



**Technical Support Document for the
Draft Fifth Contaminant Candidate List
(CCL 5) -
Contaminant Information Sheets**

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Abbreviations and Acronyms

CASRN	Chemical Abstract Services Registry Number
CCL	Contaminant Candidate List
CCL 1	EPA's First Contaminant Candidate List
CCL 2	EPA's Second Contaminant Candidate List
CCL 3	EPA's Third Contaminant Candidate List
CCL 4	EPA's Fourth Contaminant Candidate List
CCL 5	EPA's Fifth Contaminant Candidate List
CERCLA	Comprehensive Environmental Response, Compensation, and Liability Act
CIS	Contaminant Information Sheet
CSF	Cancer Slope Factor
DTXSID	DSSTox Substance Identifier
FIFRA	Federal Insecticide, Fungicide, and Rodenticide Act
EEC	Estimated environmental concentrations
EDWC	Estimated drinking water concentrations
fHQ	Final Hazard Quotient
HRL	Health Reference Level
KH	Henry's Law Constant
Kow	Octanol-Water Partition Coefficient
LOAEL	Lowest Observed Adverse Effect Level
NPDWR	National Primary Drinking Water Regulation
NHANES	National Health and Nutrition Examination Survey
NOAEL	No Observed Adverse Effect Level
OPP	Office of Pesticide Programs
OW	Office of Water
PWS	Public Water System
PCCL	Preliminary Contaminant Candidate List
QSAR	Quantitative Structure-activity Relationship
SDWA	Safe Drinking Water Act
SL	Screening Level
USEPA	United States Environmental Protection Agency

Chapter 1 Introduction

Section 1412(b)(1)(B)(i) of the Safe Drinking Water Act (SDWA), as amended in 1996, requires the United States Environmental Protection Agency (EPA) to publish every five years a list of drinking water contaminants which are not subject to any proposed or promulgated National Primary Drinking Water Regulations (NPDWRs), are known or anticipated to occur in public water systems (PWSs), and may require regulation under the SDWA. This list is known as the Contaminant Candidate List, or CCL. The SDWA directs the agency to consider health effects and occurrence information for unregulated contaminants to identify those that present the greatest public health concern related to exposure from drinking water. EPA uses this list of unregulated contaminants to help identify priority contaminants for regulatory decision making and to prioritize research and data collection efforts.

EPA followed a 3-step process to identify chemicals for inclusion on the Draft CCL 5. These steps included:

Step 1. Building a broad universe of potential drinking water contaminants (called the CCL 5 Chemical Universe). EPA evaluated 134 data sources and identified 43 that were related to potential drinking water chemical contaminants and met established CCL assessment factors. From these data sources, EPA identified and extracted occurrence and health effects data for the 21,894 chemicals that form the CCL 5 Chemical Universe.

Step 2. Screening the CCL 5 Chemical Universe to identify a list of chemicals that should be further evaluated (called the Preliminary CCL 5 (PCCL 5)). EPA established and applied a data-driven screening points system to identify and prioritize a subset of chemicals with the greatest potential for public health concern. The agency also incorporated publicly nominated chemicals to the PCCL 5.

Step 3. Classifying PCCL 5 chemicals to select the Draft CCL 5 chemicals. EPA compiled occurrence and health effects information and imported it into a standardized document format, called the Contaminant Information Sheet (CIS). The agency provided the CISs for use by two evaluation teams of EPA scientists. The evaluation teams reviewed this information for each chemical before reaching a group decision on whether to list a chemical on the Draft CCL 5.

A more detailed description of the processes used to develop the Draft CCL 5 of chemicals using these steps can be found in the Technical Support Document for the Draft Fifth Contaminant Candidate List (CCL 5) - Chemical Contaminants¹.

The purpose of this document is to present the CISs and relevant information that helps readers understand the data provided in the CISs. The remainder of this document is organized as follows: Chapter 2 presents an overview of the Draft CCL 5 CISs; Chapter 3 provides a graphic illustration, also known as the CIS Key, to assist with interpretation of the data on the CIS.

¹ USEPA. 2021. Technical Support Document for the Draft Fifth Contaminant Candidate List (CCL 5) - Chemical Contaminants. EPA 815-R-21-005. July 2021.

Appendix A provides CISs for 214 chemicals evaluated by the evaluation teams; and Appendix B provides the references for bracketed citations on the CISs. The remaining references for data sources on the CISs are included in Appendix N of the *Draft CCL 5 Chemical Technical Support Document* (USEPA, 2021).

Chapter 2 Overview of the Draft CCL 5 CISs

This chapter presents an overview of the CISs with a brief description of the data elements presented and how they were used in the CCL 5 process. The CIS for each chemical is a concise, four-page profile that was provided to the chemical evaluators to assist them in making listing recommendations for the Draft CCL 5.

The first page of each CIS includes a summary of the chemical's attribute scores, final hazard quotient, health effects and occurrence information used to calculate the final hazard quotient, chemical use information, and the chemical's status on the CCL. The second and third pages include detailed health effects and occurrence data, respectively. The derivation and use of these data are explained in detail in the *Draft CCL 5 Chemical Technical Support Document* (USEPA, 2021). The fourth page lists the references that are cited in the CISs.

Page 1 - Summary and Decision

The first page of each chemical CIS contains six sections of information including contaminant identifiers and use characteristics, the Draft CCL 5 listing decision and final hazard quotient (fHQ), attribute scores, health effects and occurrence information, and the status of the contaminant with respect to nomination for the CCL 5 and decisions from previous CCL and regulatory determination cycles. From left to right, the six sections are described as follows:

- 1) **Contaminant Identification** – presents the contaminant name, a unique DSSTox Substance Identifier (DTXSID), the contaminant's Chemical Abstract Services Registry Number (CASRN), use information, and other notes. The DTXSID field also contains a hyperlink to the chemical's profile on EPA's CompTox Chemicals Dashboard. A second table indicates if the contaminant is on any health or occurrence-related lists (e.g., FIFRA and CERCLA lists).
- 2) **Contaminant Summary and Decision** – indicates whether the contaminant was listed on the Draft CCL 5 and presents the chemical's final hazard quotient (concentration in water divided by the health concentration).
- 3) **Contaminant Status** – indicates the status of the contaminant with respect to public nomination for the CCL 5, previous listing on CCLs 1-4, and previous negative regulatory determinations and the basis for that determination, if applicable.
- 4) **Attribute Scores** – presents assigned values/categories for each of the four CCL attributes derived from the health effects and occurrence data presented on the CISs, which are defined as follows:
 - a. **Potency** quantifies the potential for a chemical to cause adverse health effects based on the dose required to elicit the most sensitive adverse effect as identified

in a single study or assessment. Potency for chemicals is reflected in several standard toxicological parameters, including reference dose (RfD) or its equivalent, cancer slope factor (CSF) or its equivalent, no observed adverse effect level (NOAEL), or lowest observed adverse effect level (LOAEL).

- b. **Severity** is a descriptive measure of the adverse health effect associated with the toxicity value that is used as the measure of potency and corresponds with the type of adverse outcome expected to occur at the LOAEL of a chemical.
 - c. **Prevalence** provides a measure of how widespread the occurrence of the chemical is in the environment in the United States. The data used to develop the prevalence score may include the percent of PWSs or monitoring sites with detections of the contaminant, the number of states where pesticides are applied or releases to the environment are reported or chemicals are produced in pounds per year (lbs/year).
 - d. **Magnitude** refers to the quantity of a chemical that is or may be in the environment. This was measured using the median value concentration of detections (if available) in drinking water or ambient water or the total pounds of a chemical released to the environment. In cases where magnitude data are not available, persistence and mobility data (i.e., chemical property/environmental fate parameters) were used as surrogates for water occurrence or release data (see USEPA, 2021 for discussion). If a median was not available, the maximum was used.
- 5) **Health Effects Information** – presents the health effects information used to calculate the fHQ. If available, a health concentration (i.e., health reference level (HRL) or CCL Screening Level (CCL SL) was calculated from information provided by the cited assessment source. Health concentrations can be calculated for non-cancer and cancer endpoints and various target populations. The critical effect and target population from the selected assessment are also presented in this section.

Health concentrations are expressed as a concentration of a chemical in drinking water (expressed in $\mu\text{g/L}$). To determine the health concentration for a chemical, the agency considered adverse health effects that may pose a greater risk to specific life stages and other sensitive groups which represent a meaningful portion of the population. Although an HRL or SL was calculated for every qualifying or non-qualifying data element presented on the health effects page, a single health concentration was chosen to calculate the fHQ that is presented on the Summary and Decision page. More details on this process is provided in Section 4.3.1 of the *Draft CCL 5 Chemical Technical Support Document* (USEPA, 2021). The assessment used as the source of the health concentration is the same assessment used as the source of the potency and severity attribute scores. This assessment is highlighted in yellow on the health effects page.

- 6) **Occurrence Information** – presents occurrence data used to calculate the fHQ - the 90th percentile concentration occurrence value, if available, or the next highest percentile value or the maximum concentration of detections (expressed in $\mu\text{g/L}$). This section also indicates the data source, the type of water source monitored (e.g., finished or ambient water), and the monitoring date range. If measured data were unavailable, modeled

concentrations were used. A description of the selection process for the water concentration used to calculate the fHQ is provided in Section 4.3.2 and Appendix H of the *Draft CCL 5 Chemical Technical Support Document* (USEPA, 2021).

Page 2 - Health Effects Data

The second page of the CISs presents the available health effects data for each chemical. The page is split into three distinct sections:

- 1. Qualifying and Non-Qualifying Health Effects Data** – presents data elements extracted from qualifying health assessments first followed by data elements extracted from non-qualifying health assessments. Differences between these two types of assessments are described in Section 4.3.1 of the *Draft CCL 5 Chemical Technical Support Document* (USEPA, 2021). The column headings indicate the data element, the numerical or qualitative value, associated units, and assessment source and year associated with the data element. Typically, the year is the date of publication of the data, although given the variability of the formatting of the data sources, it may represent a toxicological study date or the date when the data source website was last updated or accessed. If available, the critical study and effect are noted alongside the target population and exposure factor used to derive the HRL or CCL SL; a reference to the full citation is provided on page 4 of the CIS. A notes field is filled in if other pertinent information for a particular data element or a specific data source is available. The row for the data element used to develop the potency and severity attribute scores and to calculate the final hazard quotient is shaded yellow.
- 2. Literature Search Summary** – summarizes results from the rapid systematic review conducted for relevant health effects information, as further described in Section 4.2.2 of the *Draft CCL 5 Chemical Technical Support Document* (USEPA, 2021). Search start and end dates, based on the date of the most recent published health assessment for the chemical of interest, are listed. The number of unique references identified for each chemical and deemed relevant after title-abstract screening and full-text review is also provided. If available, lowest LOAEL and highest NOAEL health effects information from animal toxicity studies are presented with the corresponding study references. Additional supplementary materials and rapid systematic review results for each chemical are accessible via the CCL 5 docket (EPA-HQ-OW-2018-0594).
- 3. Other Health Data** – at the bottom of the health effects data page of the CIS are other supporting qualitative and quantitative data. These data represent measured and modeled health effects information collected from primary data sources and the CompTox Chemicals Dashboard. Examples include cancer classifications from non-EPA sources, toxicity or benchmark values for multiple exposure durations (e.g., acute) and routes (e.g., inhalation), and quantitative structure-activity relationship (QSAR) results. Data that have been modeled are provided in a separate table from the measured data.

Page 3 - Occurrence Data

The third page of the CISs provides the available occurrence data for each chemical. Data used

to develop the occurrence attribute scores, also known as “scoring data,” are presented at the top of the page, followed by “non-scoring data”. Scoring data associated with a higher attribute score (i.e., higher prevalence or higher magnitude) is presented first. The page is split into six distinct sections:

- 1. Nationally Representative Water Data** – nationally representative finished water data represent the best estimation of the potential for human exposure; therefore, they are listed first in this section, followed by ambient water data. The column headers for the water data include the data source; number of total PWSs, sampling sites, or samples; number of positive results (referred to as “detects”); an indication as to whether these values correspond to PWSs, sampling sites, or samples; percent of PWSs, sites, or samples with detects; and where available, minimum, maximum, median, 90th percentile; units; sampling year(s); and a notes field. The row with the occurrence data element used to develop the prevalence and magnitude attribute scores is shaded yellow on the CIS.
- 2. Application, Release, and Production Data** – if water data were not available, then application, release, and production data were used to develop attribute scores to estimate the potential occurrence of chemicals in water. These include pesticide application data, toxic release data, and chemical production data, all measured in lbs/year, for the most recent year for which data were available at the time of CCL 5 data collection. In addition, the pesticide application and toxic release data provide counts for how many states a chemical was applied or released in the data collection year.
- 3. Non-Nationally Representative Water Data** – non-nationally representative water data are presented in the following order: finished water data, ambient water data, and waste water effluent data. These data were not used to develop attribute scores since they are not nationally representative; therefore, they are listed as “non-scoring data.” This section includes data from both primary and supplemental data sources. Similar to the Nationally Representative Water Data section, the data in this section includes column headers for the water occurrence data, including the data source; number of total PWSs, sampling sites, samples; number of detects, number of PWSs, sampling sites, or samples; percent of detects; and where available, minimum, maximum, median, 90th percentile; units; sampling year(s); and a notes field.
- 4. Estimated Concentration in Water** – estimated occurrence concentrations for pesticides that lacked nationally representative finished and/or nationally representative ambient water data. The data sources of presented modeled occurrence concentrations are EPA’s Office of Pesticide Programs (OPP) risk assessments. This section provides modelled concentrations, known as estimated environmental concentrations (EECs) or estimated drinking water concentrations (EDWCs), accompanied by information on the assessment source, publication date, model used, and any other relevant notes. A description of the estimated occurrence concentrations used in CCL 5 is provided in Section 4.2.1.2 of the *Draft CCL 5 Chemical Technical Support Document* (USEPA, 2021).
- 5. Predicted Exposure and Biomonitoring Data** – predicted exposure data from the EPA CompTox Dashboard provide results from qualitative structure-activity relationship

(QSAR) and ExpoCast models that have been developed to predict chemical identifications such as toxicity endpoints, physical properties, exposure and environmental fate parameters. This information is presented in addition to the biomonitoring data collected by CDC's National Health and Nutrition Examination Survey (NHANES), which provides data for detections at the 90th percentile in human tissues and fluids such as serum, blood, and urine. This information is included because the data suggest there is exposure in the U.S. population; there are serious known or suspected health effects associated with different levels of exposure; and there may be limited availability and adequacy of analytical methods, and other logistical and cost considerations that resulted in limited finished or ambient water data.

6. **Modelled Environmental Fate Parameters** – includes any available data on environmental fate parameters. These modelled parameters from the EPA CompToxDashboard provide measures of a chemical's persistence and mobility in the environment. These measures include half-life ($t_{1/2}$), boiling point, vapor pressure, solubility in water, bioconcentration factor, Henry's Law constant (K_H), and octanol-water partition coefficient (K_{ow}).

Page 4 - References

The fourth page presents the references for the bracketed citations on the first three pages. References for all primary data sources are provided in Appendix N of the *Draft CCL 5 Chemical Technical Support Document* (USEPA, 2021).

Chapter 3 CIS Key

The following four pages provide an annotated graphic illustration, known as the CIS Key, to assist with interpretation of the data on the CIS.

Contaminant Identification: Presents the contaminant name, DSSTox Substance ID (DTXSID) and Chemical Abstract Services Registry Number (CASRN), use, notes, and its status on health or occurrence related lists.

Contaminant Summary and Decision: Indicates the contaminant's status on the Draft CCL 5 and presents the final hazard quotient (concentration in water divided by the Health Reference Level (HRL) or CCL Screening Level (SL)).

Contaminant Status: Indicates if the contaminant was publicly nominated for CCL 5, its status on previous CCL cycles, and past negative regulatory determinations and the basis for that determination. If the contaminant does not have a negative regulatory determination, "Not Applicable" is recorded.

1,4-Dioxane
CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION	
Name:	1,4-Dioxane
CASRN:	123-91-1
DTXSID:	DTXSID4020533
Use:	Solvent; solvent stabilizer
Chemical Notes:	
Is the contaminant on any lists?	
CERCLA	X
FIFRA	
Human Neurotoxins	
PubMed Neurotoxins	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION						
Draft CCL5 List Decision		Final Hazard Quotient (HQ)				
List		3.1				
ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION						
Potency	Severity			Prevalence	Magnitude	
5	carcinogen with linear MOA			10	5	
Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date	
HRL	0.3	hepatocellular adenomas and carcinomas in females	general population	IRIS	2010	
Conc. in water for HQ (ug/L)		90th Percentile or Maximum (if measured conc)		Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.93		90th Percentile		Finished Water	UCMR3	2013 - 2015

PUBLIC NOMINATION STATUS			
Public Nomination			
X			
PAST CCL STATUS			
CCL 1	CCL 2	CCL 3	CCL 4
		X	X
PAST NEGATIVE REGULATORY DETERMINATION STATUS			
RD 1	RD 2	RD 3	
Not Applicable	Not Applicable	Not Applicable	
Basis			
Not Applicable			

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level (SL). The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. Source Contribution of 20%.

Occurrence information: Presents occurrence data used to calculate the final hazard quotient - the 90th percentile concentration occurrence value, if available, or the next highest percentile value or the maximum concentration of detections. If measured data were unavailable, modeled concentrations were used. Also, indicates water type, data source, and monitoring date(s).

Health Effects Information: Presents data elements used to calculate the final hazard quotient, including the Health Reference Level (HRL) or CCL Screening Level (SL), the assessment from which the HRL or CCL SL was derived, and the corresponding critical effect and target population. The assessment listed here was also used as a source for the potency and severity attribute scores.

Attribute Scores: Presents assigned values/categories for each of the four CCL attributes derived from the health effects and occurrence data presented on the CISs. Attribute scores allow EPA to compare relative toxicity and occurrence of CCL 5 chemicals.

1,4-Dioxane
CCL 5 Contaminant Information Sheet
HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations**

Data Element	Value	Units	Assessment Source	Study	Population	Exposure Factor (mg/kg-day)	Notes
Reference Dose (RfD) or Equivalent	0.1	mg/kg/day	ATSDR 2012	Kociba et al. 1974	liver effects in male rats	33.8	
Reference Dose (RfD) or Equivalent	0.03	mg/kg/day	IRIS 2010	Kociba et al. 1974	liver and kidney toxicity	33.8	178 [308]
Reference Dose (RfD) or Equivalent	0.096	mg/kg/day	WHO 2005	Kociba et al. 1974	renal tubular epithelial and hepatocellular degeneration and necrosis	33.8	568 [439]
Reference Dose (RfD) or Equivalent	0.0054	mg/kg/day	HC 2018	Kociba et al. 1974; Dourson et al. 2014	hepatocellular necrosis	33.8	32.0 [95]
Cancer Slope Factor (CSF)	0.1	(mg/kg/day) ⁻¹	IRIS 2010	Kano et al. 2009	hepatocellular adenomas and carcinomas in female mice	33.8	0.296 [308]
Cancer Classification (CC)	L		IRIS 2010				[308]

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect
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Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study
Hepatic, Systemic	440	GI, 2018	Hepatic	562	GI, 2018

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	0.4	mg/L	EPA DWSHA 2018	
Acute inhalation Minimal Risk Level (MRL)	2	ppm	CDC ATSDR	
Benchmark	0.001	mg/L	CalEPA OEHHA Chemical Database	
Cancer Slope Factor (CSF)	0.027	(mg/kg/day) ⁻¹	CalEPA OEHHA Chemical Database	
Chronic Health-Based Guidance Value	0.1	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.0001	mg/L	MN DOH	
Chronic inhalation Minimal Risk Level (MRL)	0.03	ppm	CDC ATSDR	
Drinking Water Guideline Value	0.05	mg/L	WHO Drinking Water Quality Guidelines	
Inhalation Unit Risk (IUR)	0.000005	(ug/m ³) ⁻¹	EPA IRIS	
Inhalation Unit Risk (IUR)	0.0000077	ug/m ³	CalEPA OEHHA Chemical Database	
Intermediate Inhalation Minimal Risk Level (MRL)	0.2	ppm	CDC ATSDR	
Intermediate Minimal Risk Level (MRL)	0.5	mg/kg/day	CDC ATSDR	
Lifetime Health Advisory	0.2	mg/L	EPA DWSHA 2018	
Lifetime Health Advisory	0.00035	mg/L	EPA DWSHA 2018	
Reference Concentration (RfC)	0.03	mg/m ³	EPA IRIS	
Reference Concentration (RfC)	3000	ug/m ³	CalEPA OEHHA Chemical Database	
Short-Term/Subchronic Health-Based Guidance Value	0.3	mg/L	MN DOH	
Cancer Classification (CC)				
Cancer Classification (CC)				
Cancer Classification (CC)				
Cancer Classification (CC)				
Cancer Classification (CC)				

Notes: Highlighted cells indicate values were not available. Blank fields indicate values were not available. The full citation for the critical study is provided in the references section. PECO = Population, Exposure, Critical Effect, and Outcome.

Qualifying and Non-Qualifying Health Effects Data: Presents data elements from qualifying health assessments first, followed by those from non-qualifying health assessments. The column headings summarize the data element, the numerical value (or qualitative, for cancer classifications), units and assessment source and year associated with the data element. If available, the critical study and effect are noted along with the target population, exposure factor, HRL or CCL SL, and a reference to the full citation on the references page. A notes field is filled in if other pertinent information for a particular data element is available.

Yellow shading indicates the data used to populate the potency and severity attribute scores, health effects information, and final hazard quotient sections on the Summary + Decision page.

Literature Search Summary: Summarizes the rapid systematic review results for relevant health effects information. If available, the lowest LOAEL and highest NOAEL health effects information from animal toxicology studies are presented with references. Search date ranges based on the publication date of the most recent health assessment are listed. The numbers of unique references identified and deemed relevant after title-abstract screen and full-text review are also provided.

LD50	2000	mg/kg	NIH HSDB	min
LD50	5700	mg/kg	NIH HSDB	max
Percent of active toxcast in	0.85	percent	EPA Chemistry Dashboard	
TD50	40.5	mg/kg/day	NIH CPDB	min
TD50	71900	mg/kg/day	NIH CPDB	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0335738	mol/kg	TEST QSAR	
Ames mutagenicity test	0.069	no units	TEST QSAR	
Developmental toxin test	0.408	no units	TEST QSAR	

Other Health Data: Presents supporting qualitative and quantitative health effects data. These data represent measured and modeled health effects information collected from primary data sources and the CompTox Chemicals Dashboard. Modeled data is provided in a separate table from measured data.

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1,4-Dioxane
CCL 5 Contaminant Information Sheet
OCCURRENCE DATAScoring Data
Nationally Representative Water Data

Finished Water

Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019											
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015	4,915	1,077	Sites	22	0.07	0.17	0.93	34	ug/L		
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010											
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003											
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997											
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992											
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986											

Ambient Water

National Water Quality Assessment (USGS NAWQA) (All Water)						0.57	0.568	1.83	16.0			
National Water Quality Assessment (USGS NAWQA) (Surface Water)						9.8	0.568	2.06	17.0			
National Water Quality Assessment (USGS NAWQA) (Groundwater)						0.22	0.9	1.83	3.0			

Pesticide Application Data

Number

Estimated Annual Agricultural Pesticide Use (USGS)

Non-Scoring Data

Non-Nationally Representative Water Data

Finished Water

Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	42	18	Sites	43	0.5	1.5	3.2	9.1	ug/L		
Drinking Water Monitoring Data - MA (Finished)	2006 - 2020	10	8	Sites	80	0.0081	0.2	0.51	1.1	ug/L		
Community Water System Survey (CWSS) (Finished) [178]	2006	1	NA	Sites			0.8	1.4		ug/L		

Ambient Water

Drinking Water Monitoring Data - CA (Source)	2006 - 2020	274	67	Sites	24	0.27	2	5.9	36	ug/L		
Drinking Water Monitoring Data - MA (Source)	2006 - 2020	6	5	Sites	83	0.0272	0.24	1.3	3.5	ug/L		

National Water Information System (USGS NWIS) (Surface Water)

National Water Information System (USGS NWIS) (Groundwater)

National Water Information System (USGS NWIS) (All Water)

Community Water System Survey (CWSS) (Finished) [178]

Bradley et al. 2017 (Ambient) [52]

Arnold et al. 2016 (Unfiltered) [7]

Waste Water Effluent

Estimated Concentration in Water

Predicted Exposure Data
(EPA CompTox Dashboard)

Exposure

Date

Total Predicted
Exposure (mg/kg-
bw/day)

Notes

Biomonitoring Data

Detection at 90th
Percentile

Units

Notes

NHANES biomonitoring detection in serum (1999-2016)

NHANES biomonitoring detection in blood (1999-2016)

NHANES biomonitoring detection in urine (1999-2016)

Notes: Highlighted cells indicate value
Blank fields indicate there were no data
"All Water" data from NWIS and NAW
Monitoring dates for non-scoring data
State Drinking Water UCMR 4 data used in the draft CCL 5

Nationally Representative Water Data: Scoring data presented in order of the hierarchical attribute scoring protocol established for prevalence and magnitude. Finished water data from the most recent UCMR cycle are shown first, followed by the preceding UCMR cycles, then UCM and finally NIRS. Lastly, national ambient water data from NAWQA.

Yellow shading indicates the data used to calculate the prevalence and magnitude attribute scores on the Summary + Decision Page.

Non-Nationally Representative Water Data: Non-scoring data from primary and supplemental sources that are presented in order of hierarchy, separated into three categories: finished water data, ambient water data, and waste water effluent data.

Estimated Concentration in Water: Pesticide modelled concentrations used in instances when no finished or ambient water data were available. The modelled value and units are included in this section, accompanied by information on the source, publication date, model used, and relevant notes.

Application, Release, and Production Data: Additional scoring data for Prevalence and Magnitude used to estimate potential occurrence in water in the absence of measured water data. They include application rate data for pesticides, toxic release data, and chemical production data.

Modelled Environmental Fate Parameters: Available environmental fate parameters for a chemical extracted from EPA's CompTox Dashboard. For persistence, this includes the chemical's half-life. The remaining properties relate to a chemical's mobility in the environment.

Predicted Exposure and Biomonitoring Data: Predicted daily exposure (ExpoCast) data extracted from EPA's CompTox Dashboard are presented above biomonitoring data from the National Health and Nutrition Examination Survey (NHANES) Biospecimen Program. Biomonitoring values presented are the 90th percentile concentrations of compounds in serum, blood and/or urine.

Modelled Environmental Fate Parameters
(EPA CompTox Dashboard)

Biodegradation half-life	OPERA QSAR	10.227	days	
Boiling point	OPERA QSAR	101.678	degree C	
Boiling point	TEST QSAR	99.984	degree C	
Vapor pressure	OPERA QSAR	41.0426	mmHg	
	TEST QSAR	46.9894	mmHg	
	OPERA QSAR	11.2319	mol/L	
	TEST QSAR	4.7863	mol/L	
	OPERA QSAR	0.779115	no units	
	TEST QSAR	1.49968	no units	
	OPERA QSAR	0.0000147	atm-m ³ /mol	
log Kow	OPERA QSAR	-0.200282	no units	


1,4-Dioxane

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
30	ATSDR. 2012. Toxicological Profile for 1,4-Dioxane. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. Environmental science & technology, 51(9), 4792-4802.
95	HC. 2018. Guideline Technical Document for Public Consultation, 1,4-Dioxane in Drinking Water. Health Canada (HC), Ottawa, Ontario, Canada.
178	USEPA (US Environmental Protection Agency). (2009). 2006 Community Water System Survey. Overview, 57.
308	USEPA. 2010. Chemical Assessment Summary, 1,4-Dioxane. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, D.C.
439	WHO. 2005. 1,4-Dioxane in Drinking-water. WHO Guidelines for Drinking-water Quality. World Health Organization (WHO), Geneva, Switzerland.



References: This page presents the full references for the bracketed citations on the CISs.

Appendix A Contaminant Information Sheets

This appendix contains CISs for the 214 chemicals reviewed by the evaluation teams for the Draft CCL 5. These chemicals are listed in alphabetic order in a table, followed by 859 pages of CISs in a tabular format containing background, health effects, and occurrence information. Due to the technical limitations of this section, for further assistance with reasonable accommodation please contact Brynne Storsved at storsved.brynne@epa.gov or 202-564-4004.

Chemical Name	DTXSID
1,1,2,2-Tetrachloroethane	DTXSID7021318
1,2,3-Trichloropropane	DTXSID9021390
1,3-Butadiene	DTXSID3020203
1,3-Dichloropropene	DTXSID1022057
1,4-Dioxane	DTXSID4020533
17-alpha-ethynyl estradiol	DTXSID5020576
17-beta estradiol	DTXSID0020573
1-Butanol	DTXSID1021740
1H-Benzotriazole, 4(or 5)-methyl-	DTXSID0026171
2-(2-Methyl-4-chlorophenoxy)propionic acid (MCPP)	DTXSID9024194
2,4-Dichlorophenol	DTXSID1020439
2,4-Dichlorophenoxybutyric acid	DTXSID7024035
2,4-Dinitrophenol	DTXSID0020523
2,4-Dinitrotoluene	DTXSID0020529
2,6-Dinitrotoluene	DTXSID5020528
2-Aminotoluene	DTXSID1026164
2-Hydroxyatrazine	DTXSID6037807
2-Methyl-4-chlorophenoxyacetic acid (MCPA)	DTXSID4024195
2-Methylnaphthalene	DTXSID4020878
4-Androstene-3,17-dione	DTXSID8024523
4-Nonylphenol (all isomers)	DTXSID3021857
4-tert-Octylphenol	DTXSID9022360
6-Chloro-1,3,5-triazine-2,4-diamine	DTXSID1037806
Acephate	DTXSID8023846
Acetamiprid	DTXSID0034300
Acetochlor ethanesulfonic acid	DTXSID6037483
Acetochlor oxanilic acid (OA)	DTXSID1037484
Acetophenone	DTXSID6021828
Acrolein	DTXSID5020023
Acyclovir	DTXSID1022556

Chemical Name	DTXSID
Alachlor ethanesulfonic acid (ESA)	DTXSID6037485
Alachlor OA	DTXSID1037486
Aldrin	DTXSID8020040
alpha-Hexachlorocyclohexane (alpha-HCH)	DTXSID2020684
Ametryn	DTXSID1023869
Ammonia	DTXSID0023872
Anthraquinone	DTXSID3020095
Atenolol	DTXSID2022628
Azoxystrobin	DTXSID0032520
Benfluralin	DTXSID3023899
Bensulide	DTXSID9032329
Bentazon	DTXSID0023901
Benzophenone	DTXSID0021961
Bifenthrin	DTXSID9020160
Bisphenol A	DTXSID7020182
Boron	DTXSID3023922
Boscalid	DTXSID6034392
Bromacil	DTXSID4022020
Bromochloromethane	DTXSID4021503
Bromoxynil	DTXSID3022162
Bupropion	DTXSID7022706
Butyl benzyl phthalate	DTXSID3020205
Caffeine	DTXSID0020232
Calcium	DTXSID9050484
Camphor	DTXSID5030955
Carbamazepine	DTXSID4022731
Carbaryl	DTXSID9020247
Carbendazim (MBC)	DTXSID4024729
Carbon disulfide	DTXSID6023947
Chlordecone (Kepone)	DTXSID1020770
Chlorodifluoromethane (HCFC-22)	DTXSID6020301
Chloromethane	DTXSID0021541
Chlorothalonil	DTXSID0020319
Chlorpyrifos	DTXSID4020458
Clomazone	DTXSID1032355
Clopyralid	DTXSID9029221
Clothianidin	DTXSID2034465

Chemical Name	DTXSID
Cobalt	DTXSID1031040
Cotinine	DTXSID1047576
Cycloate	DTXSID6032356
Cyfluthrin	DTXSID5035957
Cyhalothrin	DTXSID6023997
Cypermethrin	DTXSID1023998
Cyprodinil	DTXSID1032359
Deethylatrazine	DTXSID5037494
Desisopropyl atrazine	DTXSID0037495
Desvenlafaxine	DTXSID40869118
Diazepam	DTXSID4020406
Diazinon	DTXSID9020407
Dicamba	DTXSID4024018
Dichlorvos	DTXSID5020449
Dicrotophos	DTXSID9023914
Dieldrin	DTXSID9020453
Diethyl phthalate	DTXSID7021780
Difenoconazole	DTXSID4032372
Dimethenamid	DTXSID4032376
Dimethenamid oxanilic acid degradate (OXA)	DTXSID4037530
Dimethoate	DTXSID7020479
Di-n-butyl phthalate	DTXSID2021781
Diuron	DTXSID0020446
Esfenvalerate	DTXSID4032667
Ethalfuralin	DTXSID8032386
Ethion	DTXSID2024086
Ethoprop	DTXSID4032611
Ethyl dipropylthiocarbamate (EPTC)	DTXSID1024091
Famoxadone	DTXSID8034588
Fenbuconazole	DTXSID8032548
Fenitrothion	DTXSID4032613
Fenpropathrin	DTXSID0024002
Fenthion	DTXSID8020620
Fexofenadine	DTXSID00861411
Fipronil	DTXSID4034609
Fluconazole	DTXSID3020627
Flufenacet	DTXSID2032552

Chemical Name	DTXSID
Fluometuron	DTXSID8020628
Fluoranthene	DTXSID3024104
Fluoxetine	DTXSID7023067
Galaxolide	DTXSID8027373
Gemfibrozil	DTXSID0020652
Heroin	DTXSID6046761
Hexazinone	DTXSID4024145
Imazalil	DTXSID8024151
Imazapyr	DTXSID8034665
Imazaquin	DTXSID3024152
Imazethapyr	DTXSID3024287
Imidacloprid	DTXSID5032442
Indoxacarb	DTXSID1032690
Iprodione	DTXSID3024154
Isophorone	DTXSID8020759
Isopropylbenzene (Cumene)	DTXSID1021827
Isoxaflutole	DTXSID5034723
Lactofen	DTXSID7024160
lambda-Cyhalothrin	DTXSID7032559
Lidocaine	DTXSID1045166
Linuron	DTXSID2024163
Lithium	DTXSID5036761
Loratadine	DTXSID2023224
Magnesium	DTXSID0049658
Malathion	DTXSID4020791
Manganese	DTXSID2024169
Meprobamate	DTXSID3023261
Metalaxyl	DTXSID6024175
Metformin	DTXSID2023270
Methocarbamol	DTXSID6023286
Methomyl	DTXSID1022267
Methyl tert-butyl ether (MTBE)	DTXSID3020833
Methylmercury	DTXSID9024198
Metolachlor ESA	DTXSID1037567
Metolachlor OA	DTXSID6037568
Metoprolol	DTXSID2023309
Metribuzin	DTXSID6024204

Chemical Name	DTXSID
Molybdenum	DTXSID1024207
Morphine	DTXSID9023336
Morphine-3-glucuronide	DTXSID80174157
Myclobutanil	DTXSID8024315
N,N-Diethyl-m-toluamide (DEET)	DTXSID2021995
Naled	DTXSID1024209
Naphthalene	DTXSID8020913
Nicotine	DTXSID1020930
Norflurazon	DTXSID8024234
Oxadiazon	DTXSID3024239
Oxyfluorfen	DTXSID7024241
p,p'-DDE	DTXSID9020374
p-Cresol	DTXSID7021869
Pendimethalin	DTXSID7024245
Permethrin	DTXSID8022292
Phenanthrene	DTXSID6024254
Phenol	DTXSID5021124
Phorate	DTXSID4032459
Phosmet	DTXSID5024261
Phosphorus	DTXSID1024382
Phostebupirim	DTXSID1032482
Piperonyl butoxide	DTXSID1021166
Potassium	DTXSID9049748
Profenofos	DTXSID3032464
Prometon	DTXSID6022341
Prometryn	DTXSID4024272
Pronamide	DTXSID2020420
Propachlor	DTXSID4024274
Propanil	DTXSID8022111
Propargite	DTXSID4024276
Propazine	DTXSID3021196
Propiconazole	DTXSID8024280
Propoxur	DTXSID7021948
Prosulfuron	DTXSID9034868
Pymetrozine	DTXSID2032637
Pyraclostrobin	DTXSID7032638
Pyrene	DTXSID3024289

Chemical Name	DTXSID
Pyridaben	DTXSID5032573
Quinoline	DTXSID1021798
Silicon	DTXSID0051441
Sitagliptin	DTXSID70197572
Sodium	DTXSID1049774
Sulfamethoxazole	DTXSID8026064
Sulfentrazone	DTXSID6032645
Sulfomethuron-methyl	DTXSID0034936
Tamoxifen	DTXSID1034187
Tebuconazole	DTXSID9032113
Tebuthiuron	DTXSID3024316
Tefluthrin	DTXSID5032577
Terbacil	DTXSID8024317
Terbufos	DTXSID2022254
Testosterone	DTXSID8022371
Tetraconazole	DTXSID8034956
Thiabendazole	DTXSID0021337
Thiamethoxam	DTXSID2034962
Thiobencarb	DTXSID6024337
Thiram	DTXSID5021332
Tin	DTXSID1049801
Tri-allate	DTXSID5024344
Tribufos	DTXSID1024174
Tributyl phosphate	DTXSID3021986
Triclopyr	DTXSID0032497
Triclosan	DTXSID5032498
Triethyl citrate	DTXSID0040701
Trifloxystrobin	DTXSID4032580
Trifluralin	DTXSID4021395
Trimethylbenzene (1,2,4-)	DTXSID6021402
Tris(1,3-dichloro-2-propyl) phosphate (TDCP)	DTXSID9026261
Tris(2-butoxyethyl) phosphate (TBEP)	DTXSID5021758
Tris(2-chloroethyl) phosphate (TCEP)	DTXSID5021411
Tungsten	DTXSID8052481
Vanadium	DTXSID2040282
Verapamil	DTXSID9041152

1,1,2,2-Tetrachloroethane

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	1,1,2,2-Tetrachloroethane
CASRN:	79-34-5
DTXSID:	DTXSID7021318
Use:	Industrial solvent; former pesticide; in manufacture of paints, varnish, rust removers; in soil sterilization and weed killer, insecticide formulations; chemical intermediate
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	27

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	carcinogen with linear MOA	5	6

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.1	hepatocellular carcinomas	general population	IRIS	2010

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
2.684	90th Percentile	Finished Water	UCM1	1988-1992

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X	X		

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	X	Not Applicable

Basis

1,1,2,2-tetrachloroethane is not expected to occur in many PWSs today. While 1,1,2,2-tetrachloroethane was detected in both the UCM Round 1 and the UCM Round 2 surveys, the percentage of detections had decreased by the time the UCM Round 2 survey was performed in the mid-1990's [a]. In addition, USGS did not detect 1,1,2,2-tetrachloroethane in two subsequent monitoring surveys of source waters that supply community water systems, using a reporting limit that is less than the 1,1,2,2-tetrachloroethane HRL of 0.4 ug/L [b,c]. EPA believes that this decrease in detections occurred because commercial production of 1,1,2,2-tetrachloroethane ceased in the mid-1980's [d].

[a] USEPA, 2008 [297]; [b] Grady, 2003 [87]; [c] Delzer & Ivahnenko, 2003 [68]; [d] ATSDR, 1996 [4]; as cited in USEPA, 2008 [296]

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

1,1,2,2-Tetrachloroethane

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0011	mg/kg/day	CALEPA 2003	Schmidt et al. 1972	transient weight gain depression and increased liver fat content	general population	33.8	6.51	[57]	
Reference Dose (RfD) or Equivalent	0.0107	mg/kg/day	OW 2008	NTP 2004	increase in relative liver weight	general population	33.8	63.3	[287]	
Reference Dose (RfD) or Equivalent	0.01071	mg/kg/day	OW 2008	NTP 2004	increase in relative liver weight	general population	33.8	63.4	[291]	
Reference Dose (RfD) or Equivalent	0.02	mg/kg/day	IRIS 2010	NTP 2004	increased relative liver weights	general population	33.8	118	[307]	
Cancer Slope Factor (CSF)	0.15	(mg/kg/day) ⁻¹	CALEPA 2003	NCI 1978	hepatocellular carcinoma	general population	33.8	0.197	[57]	
Cancer Slope Factor (CSF)	0.085	(mg/kg/day) ⁻¹	OW 2008	NCI 1978	hepatocellular carcinomas	general population	33.8	0.348	[287]	
Cancer Slope Factor (CSF)	0.085	(mg/kg/day) ⁻¹	OW 2008	NCI 1978	hepatocellular carcinomas	general population	33.8	0.348	[291]	
Cancer Slope Factor (CSF)	0.2	(mg/kg/day) ⁻¹	IRIS 2010	NCI 1978	hepatocellular carcinomas	general population	33.8	0.148	[307]	
Cancer Classification (CC)	L		OW 2008						[287]	
Cancer Classification (CC)	L		OW 2008						[291]	
Cancer Classification (CC)	L		IRIS 2010						[307]	
			ATSDR 2008						[27]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
						2009-09-01	2020-04-07	45	0	1	

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	3	mg/L	EPA DWSHA 2018	
Cancer Slope Factor (CSF)	0.2	(mg/kg/day) ⁻¹	CalEPA OEHHA Chemical Database	
Chronic Health-Based Guidance Value	0.0002	mg/L	MN DOH	
Human Health Ambient Water Quality Criteria	0.0002	mg/L	EPA Human Health Criteria for CWA	
Inhalation Unit Risk (IUR)	0.000058	ug/m ³	CalEPA OEHHA Chemical Database	
Intermediate Minimal Risk Level (MRL)	0.5	mg/kg/day	CDC ATSDR	
Lifetime Health Advisory	0.0004	mg/L	EPA DWSHA 2018	
Public Health Goal	0.0001	mg/L	CalEPA OEHHA Public Health Goals	
Cancer Classification (CC)	2B	no units	WHO IARC	
Cancer Classification (CC)	Female.Mice P	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats N	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice P	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats E	no units	HHS NTP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	250	mg/kg	NIH HSDB	
Percent of active toxcast in vitro assays tested	2.55	percent	EPA Chemistry Dashboard	
TD50	1910	mg/kg/day	NIH CPDB	max
TD50	35.4	mg/kg/day	NIH CPDB	min

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0108893	mol/kg	TEST QSAR	
Ames mutagenicity test	0.148	no units	TEST QSAR	
Developmental toxin test	0.374	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

1,1,2,2-Tetrachloroethane

CCL 5 Contaminant Information Sheet

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997	24,800	19	Sites	0.08	0.1	0.5	1.5	2	ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992	20,407	91	Sites	0.45	0.05	0.5	2.68	200	ug/L	
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	6,771	4	Sites	0.06	0.02	0.08	0.29	0.38	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	225	2	Sites	0.89	0.02	0.08	0.164	0.2	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	6,546	2	Sites	0.03	0.06	0.22	0.316	0.38	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)	9	5,936	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	466	0	Sites	0						
Drinking Water Monitoring Data - MA (Finished)	2006 - 2020	885	0	Sites	0						
Drinking Water Monitoring Data - WA (Finished)	2006 - 2011	1,098	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	4,714	4	Sites	0.08	0.8	1.2	3.36	4.28	ug/L	
Drinking Water Monitoring Data - FL (Source)	2006 - 2011	3	0	Sites	0						
Drinking Water Monitoring Data - MA (Source)	2006 - 2020	130	0	Sites	0						
Drinking Water Monitoring Data - PA (Source)	2006 - 2011	13	0	Sites	0						
Drinking Water Monitoring Data - WA (Source)	2006 - 2011	1,521	0	Sites	0						
Drinking Water Monitoring Data - WI (Source)	2012-2019	112	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	237	0	Sites	0						
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	2,806	2	Sites	0.07	2.1	4	13.8	18	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	3,039	2	Sites	0.07	2.1	4	13.8	18	ug/L	
Arnold et al. 2016 (Unfiltered) [7]	2012 - 2013	158	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Expcast exposure		0.0000368	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)	< LOD	ng/ml	
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	14.5265	days	
Boiling point	OPERA QSAR	147.582	degree C	
Boiling point	TEST QSAR	132.363	degree C	
Vapor pressure	OPERA QSAR	7.28977	mmHg	
Vapor pressure	TEST QSAR	5.3827	mmHg	
Solubility in water	OPERA QSAR	0.0176084	mol/L	
Solubility in water	TEST QSAR	0.0107647	mol/L	
Bioconcentration factor	OPERA QSAR	11.7866	no units	
Bioconcentration factor	TEST QSAR	15.5239	no units	
Henry's Law constant	OPERA QSAR	0.000500707	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.35016	no units	

1,1,2,2-Tetrachloroethane

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
4	Agency for Toxic Substances and Disease Registry (ATSDR). 1996. Toxicological Profile for 1,1,2,2-Tetrachloroethane. Atlanta, GA: Agency for Toxic Substances and Disease Registry, Public Health Service U.S. Department of Health and Human Services. Available on the Internet at: http://www.atsdr.cdc.gov/toxprofiles/tp93.html .
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
27	ATSDR. 2008. Toxicological Profile for 1,1,2,2-Tetrachloroethane. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
57	CalEPA. 2003. Public Health Goal for 1,1,2,2-Tetrachloroethane in Drinking Water. California Environmental Protection Agency (CalEPA), Office of Environmental Health Hazard Assessment, Sacramento, CA.
68	Delzer, G.C. and T. Ivahnenko. 2003. Occurrence and Temporal Variability of Methyl tertButyl Ether (MTBE) and Other Volatile Organic Compounds in Select Sources of Drinking Water: Results of the Focused Survey. U.S. Geological Survey WaterResources Investigations Report 02-4084. 65 pp. Available on the Internet at: http://sd.water.usgs.gov/nawqa/pubs/wrir/wrir02_4084.pdf .
87	Grady, S.J. 2003. A National Survey of Methyl tert-Butyl Ether and Other Volatile Organic Compounds in Drinking-Water Sources: Results of the Random Survey. U.S. Geological Survey Water-Resources Investigations Report 02-4079. 85 pp. Available on the Internet at: http://sd.water.usgs.gov/nawqa/pubs/wrir/wrir02_4079.pdf .
287	USEPA. 2008. Drinking Water Health Advisory for 1,1,2,2-Tetrachloroethane. U.S. Environmental Protection Agency, Office of Water, Office of Science and Technology, Health and Ecological Criteria Division, Washington, D.C.
291	USEPA. 2008. Health Effects Support Document for 1,1,2,2-Tetrachloroethane. U.S. Environmental Protection Agency, Office of Water, Health and Ecological Criteria Division, Washington, D.C.
296	USEPA. 2008. Regulatory Determinations Support Document for Selected Contaminants from the Second Drinking Water Contaminant Candidate List (CCL 2). EPA Report 815-R-08-012. June 2008.
297	USEPA. 2008. The Analysis of Occurrence Data from the First Unregulated Contaminant Monitoring Regulation (UCMR 1) in Support of Regulatory Determinations for the Second Drinking Water Contaminant Candidate List. EPA 815-R-08-013. June.
307	USEPA. 2010. Chemical Assessment Summary, 1,1,2,2-Tetrachloroethane. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, D.C.

1,2,3-Trichloropropane

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	1,2,3-Trichloropropane
CASRN:	96-18-4
DTXSID:	DTXSID9021390
Use:	Paint ingredient
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	140

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	carcinogen with mutagenic MOA	8	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.002	forestomach neoplasms	general population	IRIS	2009

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.28	90th Percentile	Finished Water	UCMR3	2013-2015

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
		X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis
Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

1,2,3-Trichloropropane

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.006	mg/kg/day	OW 1989	NTP 1983 a and b	effects on body and organ weights, hematological effects, changes in clinical chemistry and histopathological effects	general population	33.8	35.5	[201]	
Reference Dose (RfD) or Equivalent	0.0057	mg/kg/day	CALEPA 2009	NTP 1993	effects on erythrocytes	general population	33.8	33.7	[59]	
Reference Dose (RfD) or Equivalent	0.004	mg/kg/day	IRIS 2009	NTP 1993	increased absolute liver weight	general population	33.8	23.7	[299]	
Cancer Slope Factor (CSF)	25	(mg/kg/day)^-1	CALEPA 2009	NTP 1993	forestomach neoplasms	general population	33.8	0.00118	[59]	
Cancer Slope Factor (CSF)	30	(mg/kg/day)^-1	IRIS 2009	NTP 1993	forestomach neoplasms	general population	33.8	0.00230	[299]	
Cancer Classification (CC)	L		IRIS 2009						[299]	
			ATSDR 1992						[8]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	0.6	mg/L	EPA DWSHA 2018	
Acute Health-Based Guidance Value	0.007	mg/L	MN DOH	
Acute Health-Based Guidance Value	0.007	mg/L	MN DOH	
Acute inhalation Minimal Risk Level (MRL)	0.0003	ppm	CDC ATSDR	
Benchmark	0.000005	mg/L	CalEPA OEHHHA Chemical Database	
Chronic Health-Based Guidance Value	0.0000003	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.007	mg/L	MN DOH	
Intermediate Minimal Risk Level (MRL)	0.06	mg/kg/day	CDC ATSDR	
Public Health Goal	0.0000007	mg/L	CalEPA OEHHHA Public Health Goals	
Reference Concentration (RfC)	0.0003	mg/m^3	EPA IRIS	
Short-Term/Subchronic Health-Based Guidance Value	0.007	mg/L	MN DOH	
Cancer Classification (CC)	2A	no units	WHO IARC	
Cancer Classification (CC)	Female.Mice P	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats P	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice P	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats P	no units	HHS NTP	

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	320	mg/kg	NIH HSDB	min
LD50	505	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	1.65	percent	EPA Chemistry Dashboard	
TD50	0.806	mg/kg/day	NIH CPDB	min
TD50	454	mg/kg/day	NIH CPDB	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.00803526	mol/kg	TEST QSAR	
Ames mutagenicity test	0.673	no units	TEST QSAR	
Developmental toxin test	0.462	no units	TEST QSAR	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

1,2,3-Trichloropropane
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015	4,916	67	Sites	1.36	0.03	0.073	0.28	1.02	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997	24,088	19	Sites	0.08	0.03	0.5	16.6	3000	ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992	17,392	44	Sites	0.25	0.1	0.915	6	112	ug/L	
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	7,695	83	Sites	1.08	0.002	0.2	0.839	2.92	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	265	1	Sites	0.38	0.12	0.16	0.179	0.179	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	7,430	82	Sites	1.1	0.002	0.206	0.851	2.92	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)	2	5,040	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	502	69	Sites	14	0.001	0.014	0.6	29	ug/L	
Drinking Water Monitoring Data - MA (Finished)	2006 - 2020	885	0	Sites	0						
Drinking Water Monitoring Data - WA (Finished)	2006 - 2011	1,204	0	Sites	0						
Community Water System Survey (CWSS) (Finished) [178]	2006	1	NA	Sites			400	400		ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	4,640	373	Sites	8.04	0.0018	0.032	0.31	270	ug/L	
Drinking Water Monitoring Data - FL (Source)	2006 - 2011	3	1	Sites	33	1.9	1.9	1.9	1.9	ug/L	
Drinking Water Monitoring Data - MA (Source)	2006 - 2020	130	0	Sites	0						
Drinking Water Monitoring Data - PA (Source)	2006 - 2011	14	0	Sites	0						
Drinking Water Monitoring Data - WA (Source)	2006 - 2011	1,690	1	Sites	0.06	0.0322	0.0335	0.0345	0.0348	ug/L	
Drinking Water Monitoring Data - WI (Source)	2012-2019	112	1	Sites	0.89	0.33	0.33	0.33	0.33	ug/L	
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	222	0	Sites	0						
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3,422	51	Sites	1.49	0.002	0.0157	0.161	1.16	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	3,640	51	Sites	1.4	0.002	0.0157	0.161	1.16	ug/L	
Arnold et al. 2016 (Unfiltered) [7]	2012 - 2013	685	12	Sites	1.75	0.005	0.0215	0.132	0.526	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Exposure exposure		1.33E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)	< LOD	ng/ml	
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.59332	days	
Boiling point	OPERA QSAR	147.27	degree C	
Boiling point	TEST QSAR	145.101	degree C	
Vapor pressure	OPERA QSAR	6.2604	mmHg	
Vapor pressure	TEST QSAR	6.56145	mmHg	
Solubility in water	OPERA QSAR	0.0143205	mol/L	
Solubility in water	TEST QSAR	0.0117761	mol/L	
Bioconcentration factor	OPERA QSAR	11.92	no units	
Bioconcentration factor	TEST QSAR	16.1808	no units	
Henry's Law constant	OPERA QSAR	0.000365755	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.27667	no units	

1,2,3-Trichloropropane

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
8	ATSDR. 1992. Toxicological Profile for 1,2,3-Trichloropropane. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
59	CalEPA. 2009. Public Health Goals for Chemicals in Drinking Water, 1,2,3-Trichloropropane. California Environmental Protection Agency (CalEPA), Office of Environmental Health Hazard Assessment, Pesticide and Environmental Toxicology Branch, Sacramento, CA.
178	USEPA (US Environmental Protection Agency). (2009). 2006 Community Water System Survey. Overview, 57.
201	USEPA. 1989. 1,2,3-Trichloropropane Drinking Water Health Advisory. U.S. Environmental Protection Agency, Office of Water, Washington, D.C.
299	USEPA. 2009. Chemical Assessment Summary, 1,2,3-Trichloropropane. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, D.C.

1,2,4-Trimethylbenzene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	1,2,4-Trimethylbenzene
CASRN:	95-63-6
DTXSID:	DTXSID6021402
Use:	Chemical intermediate; vermifuge
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.17

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	non-cancer effects	6	6

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	60	decreased pain sensitivity	general population	IRIS	2016

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
10	90th Percentile	Finished Water	UCM1	1988-1992

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X	X		

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

1,2,4-Trimethylbenzene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.01	mg/kg/day	IRIS 2016	Korsak and Rydzynski 1996	decreased pain sensitivity	general population	33.8	59.2	[373]	NOTE: IRIS utilized PBPK modeling to extrapolate an oral RfD from an inhalation study
Cancer Classification (CC)	D		OW 1987						[194]	
Cancer Classification (CC)	D		PPRTV 2007						[278]	
Cancer Classification (CC)	I		IRIS 2016						[373]	NOTE: IRIS utilized PBPK modeling to extrapolate an oral RfD from an inhalation study

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
						2015-09-01	2020-04-06	17	0	0	

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Health-Based Guidance Value	0.1	mg/L	MN DOH	
Benchmark	0.33	mg/L	CalEPA OEHHA Chemical Database	
Chronic Health-Based Guidance Value	0.1	mg/L	MN DOH	
Reference Concentration (RfC)	0.06	mg/m ³	EPA IRIS	
Reference Concentration (RfC)	0.08	mg/m ³	EPA IRIS	
Reference Concentration (RfC)	0.2	mg/m ³	EPA IRIS	
Reference Concentration (RfC)	3	mg/m ³	EPA IRIS	
Reference Concentration (RfC)	4	mg/m ³	EPA IRIS	
Short-Term/Subchronic Health-Based Guidance Value	0.1	mg/L	MN DOH	
Subchronic Provisional RfD	0.04	mg/m ³	EPA IRIS	
Subchronic Provisional RfD	0.04	mg/m ³	EPA IRIS	

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	3280	mg/kg	NIH HSDB	min
LD50	6000	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	0.9	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0282488	mol/kg	TEST QSAR	
Ames mutagenicity test			TEST QSAR	
Developmental toxin test	0.482	no units	TEST QSAR	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
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EPA - Office of Water

1,2,4-Trimethylbenzene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997	22,965	174	Sites	0.76	0.1	0.8	5.42	137	ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992	12,755	106	Sites	0.83	0.02	1	10	77	ug/L	
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	7,705	695	Sites	9.02	0.004	0.03	0.199	260	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	265	76	Sites	29	0.005	0.0255	0.21	3.6	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	7,440	619	Sites	8.32	0.004	0.033	0.196	260	ug/L	
Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data			Number of States	Amount Released (lbs/year)	Chemical Production Data		
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			50	6,616,209	Chemical Data Reporting (CDR) Results (EPA) (2016)		
									Production Volume (lbs/year)		
									250M - 500M		

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	405	5	Sites	1.23	0.039	1.15	8.02	22.3	ug/L	
Drinking Water Monitoring Data - MA (Finished)	2006 - 2020	884	11	Sites	1.24	0.5	0.68	2.1	2.4	ug/L	
Drinking Water Monitoring Data - WA (Finished)	2006 - 2011	1,188	1	Sites	0.08	1.4	1.4	1.4	1.4	ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	4,250	14	Sites	0.33	0.034	0.645	2.45	3.5	ug/L	
Drinking Water Monitoring Data - MA (Source)	2006 - 2020	130	2	Sites	1.54	0.6	0.79	0.798	0.8	ug/L	
Drinking Water Monitoring Data - PA (Source)	2006 - 2011	13	0	Sites	0						
Drinking Water Monitoring Data - WA (Source)	2006 - 2011	1,665	0	Sites	0						
Drinking Water Monitoring Data - WI (Source)	2012-2019	101	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	219	13	Sites	5.94	0.011	0.033	0.0545	0.072	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3,487	204	Sites	5.85	0.01	0.0525	0.304	180	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	3,703	217	Sites	5.86	0.01	0.047	0.299	180	ug/L	
Arnold et al. 2016 (Unfiltered) [7]	2012 - 2013	685	18	Sites	2.63	0.012	0.039	0.161	0.274	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.0000518	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.62726	days	
Boiling point	OPERA QSAR	169.007	degree C	
Boiling point	TEST QSAR	178.053	degree C	
Vapor pressure	OPERA QSAR	1.87805	mmHg	
Vapor pressure	TEST QSAR	1.49279	mmHg	
Solubility in water	OPERA QSAR	0.000492809	mol/L	
Solubility in water	TEST QSAR	0.00155239	mol/L	
Bioconcentration factor	OPERA QSAR	144.739	no units	
Bioconcentration factor	TEST QSAR	218.776	no units	
Henry's Law constant	OPERA QSAR	0.00706473	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.61901	no units	

1,2,4-Trimethylbenzene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
194	USEPA. 1987. Drinking Water Health Advisory for 1,2,4-trimethylbenzene. U.S. Environmental Protection Agency, Office of Health and Environmental Assessment, Environmental Criteria and Assessment Office, Cincinnati, OH.
278	USEPA. 2007. Provisional Peer-Reviewed Toxicity Values for 1,2,4-Trimethylbenzene. U.S. Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment, Superfund Health Risk Technical Support Center, Cincinnati, OH.
373	USEPA. 2016. Toxicological Review of Trimethylbenzenes. U.S. Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, D.C.

1,3-Butadiene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	1,3-Butadiene
CASRN:	106-99-0
DTXSID:	DTXSID3020203
Use:	Rubber chemical
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	
Human Neurotoxics	
PubMed Neurotoxics	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
		1	6

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
				IRIS	2002

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.518	90th Percentile	Finished Water	UCMR3	2013-2015

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
		X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

1,3-Butadiene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Cancer Classification (CC)	B2		IRIS 2002						[249]	NOTE: according to IRIS: "Oral RfD not calculated because 1,3-butadiene is a gas, is poorly soluble in water, and causes hazard by inhalation only"
			ATSDR 2012						[29]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Cancer Slope Factor (CSF)	0.6	(mg/kg/day) ⁻¹	CALEPA 2009	Melnick et al. 1990	lung alveolar and bronchiolar neoplasms	general population	33.8	0.0493	[60]	

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
						2001-11-01	2020-02-13	1334	0	45	

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Cancer Classification (CC)	1	no units	WHO IARC	
Cancer Slope Factor (CSF)	0.6	(mg/kg/day) ⁻¹	CalEPA OEHHA Chemical Database	
Inhalation Unit Risk (IUR)	0.00017	ug/m ³	CalEPA OEHHA Chemical Database	
Inhalation Unit Risk (IUR)	0.00003	(ug/m ³) ⁻¹	EPA IRIS	
Reference Concentration (RfC)	2	ug/m ³	CalEPA OEHHA Chemical Database	
Reference Concentration (RfC)	0.002	mg/m ³	EPA IRIS	
Cancer Classification (CC)	Female.Mice P	no units	HHS NTP	
Cancer Classification (CC)	Female.Mice P	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats NT	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats NT	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice P	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice P	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats NT	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats NT	no units	HHS NTP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	5480	mg/kg	NIH HSDB	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0291072	mol/kg	TEST QSAR	
Ames mutagenicity test			TEST QSAR	
Developmental toxin test	0.572	no units	TEST QSAR	

1,3-Butadiene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015	4,916	2	Sites	0.04	0.32	0.43	0.518	0.54	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	1,411	1	Sites	0.07	0.649	0.649	0.649	0.649	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	51	1	Sites	1.96	0.649	0.649	0.649	0.649	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	1,360	0	Sites	0						

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)	33	1,241,320	Chemical Data Reporting (CDR) Results (EPA) (2016)	18 - 58

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	47	0	Sites	0						
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	824	1	Sites	0.12	0.81	0.81	0.81	0.81	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	871	1	Sites	0.11	0.81	0.81	0.81	0.81	ug/L	
Arnold et al. 2016 (Unfiltered) [7]	2012 - 2013	527	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	7.4766	days	
Boiling point	OPERA QSAR	2.82833	degree C	
Boiling point	TEST QSAR	18.339	degree C	
Vapor pressure	OPERA QSAR	1266.91	mmHg	
Vapor pressure	TEST QSAR	1213.39	mmHg	
Solubility in water	OPERA QSAR	0.0170752	mol/L	
Solubility in water	TEST QSAR	0.021727	mol/L	
Bioconcentration factor	OPERA QSAR	11.0376	no units	
Bioconcentration factor	TEST QSAR	7.31139	no units	
Henry's Law constant	OPERA QSAR	0.0679036	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.92103	no units	

1,3-Butadiene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
29	ATSDR. 2012. Toxicological Profile for 1,3-Butadiene. U.S. Department of Health and Human Services, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
60	CalEPA. 2009. Technical Support Document for Cancer Potency Factors, Appendix B. California Environmental Protection Agency (CalEPA), Office of Environmental Health Hazard Assessment, Air Toxicology and Epidemiology Branch, Sacramento, CA.
249	USEPA. 2002. Chemical Assessment Summary, 1,3-Butadiene. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, D.C.

1,3-Dichloropropene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	1,3-Dichloropropene
CASRN:	542-75-6
DTXSID:	DTXSID1022057
Use:	pesticide; in organic synthesis
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	X
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	8.2

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	carcinogen with linear MOA	1	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.2	forestomach, liver, adrenal, and thyroid tumors found in male rats	general population	OPP	2008

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
1.63	90th Percentile	Finished Water	UCM1	1988-1992

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X	X		

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	X	Not Applicable

Basis

1,3-DCP appears to occur infrequently at health levels of concern in PWSS. While 1,3-DCP was detected in the UCM Round 1 (late 1980's) and the UCM Round 2 (mid 1990's) surveys [a], it was not detected in a subsequent evaluation of 796 small systems from the UCMR 1 survey [b]. In addition, the USGS did not detect 1,3-DCP in two occurrence studies performed between 1999 and 2001 using monitoring levels that were lower than the HRL [c,d]. EPA believes the 1999 pesticide labeling requirements, which are intended to mitigate risks to drinking water, may be one reason for the lack of occurrence of 1,3-DCP at levels of concern in subsequent monitoring surveys.

[a] USEPA, 2008 [298]; [b] USEPA, 2008 [297]; [c] Grady, 2003 [87]; [d] Delzer & Ivahnenko, 2003 [68]; as cited in USEPA, 2008 [296]

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

1,3-Dichloropropene

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.025	mg/kg/day	OPP 2008	Stott et al. 1995	decreased body weight gain, increased incidence of basal cell hyperplasia of nonglandular stomach mucosa	general population	33.8	148	[285]	
Cancer Slope Factor (CSF)	0.122	(mg/kg/day) ⁻¹	OPP 2008	NTP 1985; Stott et al. 1995	forestomach, liver, adrenal, and thyroid tumors found in male rats	general population	33.8	0.243	[285]	
Cancer Classification (CC)	L		OPP 2008						[285]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References Identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	0.03	mg/L	EPA DWSHA 2018	
Cancer Slope Factor (CSF)	0.091	(mg/kg/day) ⁻¹	CalEPA OEHHA Chemical Database	
Chronic Health-Based Guidance Value	0.0002	mg/L	MN DOH	
Chronic inhalation Minimal Risk Level (MRL)	0.007	ppm	CDC ATSDR	
Drinking Water Guideline Value	0.02	mg/L	WHO Drinking Water Quality Guidelines	
Human Health Ambient Water Quality Criteria	0.00027	mg/L	EPA Human Health Criteria for CWA	
Inhalation Unit Risk (IUR)	0.000004	(ug/m ³) ⁻¹	EPA IRIS	
Intermediate Inhalation Minimal Risk Level (MRL)	0.008	ppm	CDC ATSDR	
Intermediate Minimal Risk Level (MRL)	0.04	mg/kg/day	CDC ATSDR	
Lifetime Health Advisory	0.0004	mg/L	EPA DWSHA 2018	
Public Health Goal	0.0002	mg/L	CalEPA OEHHA Public Health Goals	
Reference Concentration (RfC)	0.02	mg/m ³	EPA IRIS	
Cancer Classification (CC)	2B	no units	WHO IARC	
Cancer Classification (CC)	Female.Mice P	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats SE	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice IS	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats P	no units	HHS NTP	

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	713	mg/kg	NIH HSDB	max
LD50	94	mg/kg	NIH HSDB	min
LOAEL	12.5	mg/kg/day	EPA Toxicity Reference Database	
NOAEL	2.5	mg/kg/day	EPA Toxicity Reference Database	
Percent of active toxcast in vitro assays tested	0	percent	EPA Chemistry Dashboard	
TD50	1930	mg/kg/day	NIH CPDB	max
TD50	33.2	mg/kg/day	NIH CPDB	min

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.00398107	mol/kg	TEST QSAR	
Ames mutagenicity test	1.133	no units	TEST QSAR	
Developmental toxin test	0.342	no units	TEST QSAR	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

1,3-Dichloropropene

CCL 5 Contaminant Information Sheet

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003	796	0	Sites	0					ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997	16,787	58	Sites	0.35	0.2	0.5	0.99	39	ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992	9,164	15	Sites	0.16	0.5	1	1.63	2	ug/L	
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	24	59,344,846	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	10	7,907	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	464	2	Sites	0.43	0.5	1	1	1	ug/L	
Drinking Water Monitoring Data - MA (Finished)	2006 - 2020	879	1	Sites	0.11	1.3	1.3	1.3	1.3	ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	4,667	5	Sites	0.11	0.52	0.605		10	ug/L	
Drinking Water Monitoring Data - FL (Source)	2006 - 2011	2	0	Sites	0						
Drinking Water Monitoring Data - MA (Source)	2006 - 2020	129	0	Sites	0						
Drinking Water Monitoring Data - PA (Source)	2006 - 2011	13	0	Sites	0						
Drinking Water Monitoring Data - WI (Source)	2012-2019	112	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	94	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		3.56E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	5.3718	days	
Boiling point	OPERA QSAR	97.6161	degree C	
Boiling point	TEST QSAR	97.43	degree C	
Vapor pressure	OPERA QSAR	31.8587	mmHg	
Vapor pressure	TEST QSAR	41.9759	mmHg	
Solubility in water	OPERA QSAR	0.0196733	mol/L	
Solubility in water	TEST QSAR	0.0229087	mol/L	
Bioconcentration factor	OPERA QSAR	7.94771	no units	
Bioconcentration factor	TEST QSAR	12.3027	no units	
Henry's Law constant	OPERA QSAR	0.00202678	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.02743	no units	

1,3-Dichloropropene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
68	Delzer, G.C. and T. Ivahnenko. 2003. Occurrence and Temporal Variability of Methyl tertButyl Ether (MTBE) and Other Volatile Organic Compounds in Select Sources of Drinking Water: Results of the Focused Survey. U.S. Geological Survey WaterResources Investigations Report 02-4084. 65 pp. Available on the Internet at: http://sd.water.usgs.gov/nawqa/pubs/wrir/wrir02_4084.pdf .
87	Grady, S.J. 2003. A National Survey of Methyl tert-Butyl Ether and Other Volatile Organic Compounds in Drinking-Water Sources: Results of the Random Survey. U.S. Geological Survey Water-Resources Investigations Report 02-4079. 85 pp. Available on the Internet at: http://sd.water.usgs.gov/nawqa/pubs/wrir/wrir02_4079.pdf .
285	USEPA. 2008. 1,3-Dichloropropene: Proposed New Use for Drip Irrigation in Vineyards: Revised HED Human Health Risk Assessment. EPA-HQ-OPP-2013-0154-0006. DP No. D347789. U.S. Environmental Protection Agency, Office of Prevention, Pesticides and Toxic Substances, Washington, D.C.
296	USEPA. 2008. Regulatory Determinations Support Document for Selected Contaminants from the Second Drinking Water Contaminant Candidate List (CCL 2). EPA Report 815-R-08-012. June 2008.
297	USEPA. 2008. The Analysis of Occurrence Data from the First Unregulated Contaminant Monitoring Regulation (UCMR 1) in Support of Regulatory Determinations for the Second Drinking Water Contaminant Candidate List. EPA 815-R-08-013. June.
298	USEPA. 2008. The Analysis of Occurrence Data from the Unregulated Contaminant Monitoring (UCM) Program and National Inorganics and Radionuclides Survey (NIRS) in Support of Regulatory Determinations for the Second Drinking Water Contaminant Candidate List. EPA 815-D-08-014. June.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

1,4-Dioxane

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	1,4-Dioxane
CASRN:	123-91-1
DTXSID:	DTXSID4020533
Use:	Solvent; solvent stabilizer
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	3.1

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	carcinogen with linear MOA	10	5

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.3	hepatocellular adenomas and carcinomas in females	general population	IRIS	2010

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.93	90th Percentile	Finished Water	UCMR3	2013 - 2015

PUBLIC NOMINATION STATUS

Public Nomination
X

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
		X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

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1,4-Dioxane

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.1	mg/kg/day	ATSDR 2012	Kociba et al. 1974	liver effects in male rats	general population	33.8	592	[30]	
Reference Dose (RfD) or Equivalent	0.03	mg/kg/day	IRIS 2010	Kociba et al. 1974	liver and kidney toxicity	general population	33.8	178	[308]	
Reference Dose (RfD) or Equivalent	0.096	mg/kg/day	WHO 2005	Kociba et al. 1974	renal tubular epithelial and hepatocellular degeneration and necrosis	general population	33.8	568	[439]	
Reference Dose (RfD) or Equivalent	0.0054	mg/kg/day	HC 2018	Kociba et al. 1974; Dourson et al. 2014	hepatocellular necrosis	general population	33.8	32.0	[95]	
Cancer Slope Factor (CSF)	0.1	(mg/kg/day) ⁻¹	IRIS 2010	Kano et al. 2009	hepatocellular adenomas and carcinomas in female mice	general population	33.8	0.296	[308]	
Cancer Classification (CC)	L		IRIS 2010						[308]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Hepatic, Systemic	440	Gi, 2018	Hepatic	562	Gi, 2018						1

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	0.4	mg/L	EPA DWSHA 2018	
Acute inhalation Minimal Risk Level (MRL)	2	ppm	CDC ATSDR	
Benchmark	0.001	mg/L	CalEPA OEHH Chemical Database	
Cancer Slope Factor (CSF)	0.027	(mg/kg/day) ⁻¹	CalEPA OEHH Chemical Database	
Chronic Health-Based Guidance Value	0.1	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.0001	mg/L	MN DOH	
Chronic inhalation Minimal Risk Level (MRL)	0.03	ppm	CDC ATSDR	
Drinking Water Guideline Value	0.05	mg/L	WHO Drinking Water Quality Guidelines	
Inhalation Unit Risk (IUR)	0.000005	(ug/m ³) ⁻¹	EPA IRIS	
Inhalation Unit Risk (IUR)	0.0000077	ug/m ³	CalEPA OEHH Chemical Database	
Intermediate Inhalation Minimal Risk Level (MRL)	0.2	ppm	CDC ATSDR	
Intermediate Minimal Risk Level (MRL)	0.5	mg/kg/day	CDC ATSDR	
Lifetime Health Advisory	0.2	mg/L	EPA DWSHA 2018	
Lifetime Health Advisory	0.00035	mg/L	EPA DWSHA 2018	
Reference Concentration (RfC)	0.03	mg/m ³	EPA IRIS	
Reference Concentration (RfC)	3000	ug/m ³	CalEPA OEHH Chemical Database	
Short-Term/Subchronic Health-Based Guidance Value	0.3	mg/L	MN DOH	
Cancer Classification (CC)	2B	no units	WHO IARC	
Cancer Classification (CC)	Female.Mice P	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats P	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice P	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats P	no units	HHS NTP	

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	2000	mg/kg	NIH HSDB	min
LD50	5700	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	0.85	percent	EPA Chemistry Dashboard	
TD50	40.5	mg/kg/day	NIH CPDB	min
TD50	71900	mg/kg/day	NIH CPDB	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0335738	mol/kg	TEST QSAR	
Ames mutagenicity test	0.069	no units	TEST QSAR	
Developmental toxin test	0.408	no units	TEST QSAR	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

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1,4-Dioxane
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015	4,915	1,077	Sites	22	0.07	0.17	0.93	34	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	1,406	8	Sites	0.57	0.568	1.83	16.5	18.9	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	51	5	Sites	9.8	0.568	2.06	17.6	18.9	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	1,355	3	Sites	0.22	0.9	1.83	3.06	3.58	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)	24	617,134	Chemical Data Reporting (CDR) Results (EPA) (2016)	1M - 10M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	42	18	Sites	43	0.5	1.5	3.2	9.1	ug/L	
Drinking Water Monitoring Data - MA (Finished)	2006 - 2020	10	8	Sites	80	0.0081	0.2	0.51	1.1	ug/L	
Community Water System Survey (CWSS) (Finished) [178]	2006	1	NA	Sites			0.8	1.4		ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	274	67	Sites	24	0.27	2	5.9	36	ug/L	
Drinking Water Monitoring Data - MA (Source)	2006 - 2020	6	5	Sites	83	0.0272	0.24	1.3	3.5	ug/L	
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	114	16	Sites	14	0.124	1.32	6.94	15.9	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	955	105	Sites	11	0.083	3.3	7.6	36	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,068	121	Sites	11	0.083	3.2	7.6	36	ug/L	
Community Water System Survey (CWSS) (Ambient) [178]	2006	1	NA	Sites			0.9	1.3		ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	4	Sites	11	0.7226	0.987	2.77	3.537	ug/L	
Arnold et al. 2016 (Unfiltered) [7]	2012 - 2013	527	2	Sites	0.38	1	1.5	1.9	2	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.0000011	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)	< LOD	ng/ml	
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	10.227	days	
Boiling point	OPERA QSAR	101.678	degree C	
Boiling point	TEST QSAR	99.984	degree C	
Vapor pressure	OPERA QSAR	41.0426	mmHg	
Vapor pressure	TEST QSAR	46.9894	mmHg	
Solubility in water	OPERA QSAR	11.2319	mol/L	
Solubility in water	TEST QSAR	4.7863	mol/L	
Bioconcentration factor	OPERA QSAR	0.779115	no units	
Bioconcentration factor	TEST QSAR	1.49968	no units	
Henry's Law constant	OPERA QSAR	0.0000147	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	-0.200282	no units	

1,4-Dioxane

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
30	ATSDR. 2012. Toxicological Profile for 1,4-Dioxane. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. Environmental science & technology, 51(9), 4792-4802.
95	HC. 2018. Guideline Technical Document for Public Consultation, 1,4-Dioxane in Drinking Water. Health Canada (HC), Ottawa, Ontario, Canada.
178	USEPA (US Environmental Protection Agency). (2009). 2006 Community Water System Survey. Overview, 57.
308	USEPA. 2010. Chemical Assessment Summary, 1,4-Dioxane. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington D.C.
439	WHO. 2005. 1,4-Dioxane in Drinking-water. WHO Guidelines for Drinking-water Quality. World Health Organization (WHO), Geneva, Switzerland.

1-Butanol

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	1-Butanol
CASRN:	71-36-3
DTXSID:	DTXSID1021740
Use:	Paint solvent; chemical intermediate; food additive
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.016

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	non-cancer effects	9	8

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	600	ataxia and hypoactivity	general population	IRIS	1987

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
9.64712	90th Percentile	Finished Water	UCMR4	2018-2019

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
		X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

1-Butanol

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.1	mg/kg/day	IRIS 1987	USEPA 1986	hypoactivity and ataxia	general population	33.8	592	[193]	
Cancer Classification (CC)	D		IRIS 1987						[193]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Developmental	300	Sitarek, 1994	Reproductive	5654	Ema, 2005	1986-03-01	2020-03-16	4072	2	8	2

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Chronic Health-Based Guidance Value	0.7	mg/L	MN DOH	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	790	mg/kg	NIH HSDB	
Percent of active toxcast in vitro assays tested	1.23	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0105439	mol/kg	TEST QSAR	
Ames mutagenicity test	0.112	no units	TEST QSAR	
Developmental toxin test	0.677	no units	TEST QSAR	

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1-Butanol
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019	3,689	145	Sites	3.93	2	3.5	9.65	101.5552	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	1,406	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	51	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	1,355	0	Sites	0						

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)	46	9,818,559	Chemical Data Reporting (CDR) Results (EPA) (2016)	18 - 58

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	43	0	Sites	0						
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	1,104	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,147	0	Sites	0						
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	1	Sites	2.63	5.743	5.74	5.74	5.743	ug/L	
Arnold et al. 2016 (Unfiltered) [7]	2012 - 2013	527	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.0000587	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.44861	days	
Boiling point	OPERA QSAR	111.366	degree C	
Boiling point	TEST QSAR	118.364	degree C	
Vapor pressure	OPERA QSAR	7.55899	mmHg	
Vapor pressure	TEST QSAR	5.29663	mmHg	
Solubility in water	OPERA QSAR	1.20266	mol/L	
Solubility in water	TEST QSAR	0.626614	mol/L	
Bioconcentration factor	OPERA QSAR	4.82083	no units	
Bioconcentration factor	TEST QSAR	3.34965	no units	
Henry's Law constant	OPERA QSAR	0.00000978	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	0.850878	no units	

1-Butanol

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
193	USEPA. 1987. Chemical Assessment Summary, n-Butanol. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, D.C.

1H-Benzotriazole, 4(or 5)-methyl-
CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	1H-Benzotriazole, 4(or 5)-methyl-
CASRN:	29385-43-1
DTXSID:	DTXSID0026171
Use:	In water treatment, corrosion inhibitor for copper and its alloys
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0091

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	non-cancer effects	10	5

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	100	renal proximal tubule regeneration	general population	MDH	2019

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.9104	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

1H-Benzotriazole, 4(or 5)-methyl-
CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.017	mg/kg/day	MDH 2019	JBRC 2007	renal proximal tubule regeneration	general population	33.8	101	[148]	NOTE: the toxicity value was derived from a surrogate chemical (1H-benzotriazole)

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
							2020-03-13	86	1	2	0

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	800	mg/kg	NIH HSDB	
Percent of active toxcast in vitro assays tested	5.14	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity test			TEST QSAR	
Developmental toxin test			TEST QSAR	

1H-Benzotriazole, 4(or 5)-methyl-

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	557	62	Sites	11	0.00672	0.242	0.91	4.17	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	75	51	Sites	68	0.00672	0.256	0.912	4.17	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	482	11	Sites	2.28	0.0284	0.0506	0.366	2.98	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	1M - 10M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Bradley et al. 2018 (Finished) [53]	2016	26	3	Sites	12	0.0130716	0.0333	0.0352	0.0357109	ug/L	
Ambient Water											
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	20	Sites	53	0.0213052	0.664	2.33	4.6612843	ug/L	
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	20	Sites	95	0.1313613	1.36	9.3	27.69201	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exposure exposure		0.000000337	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

1H-Benzotriazole, 4(or 5)-methyl-

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Reference Number	Full Reference
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. <i>Environmental science & technology</i> , 52(23), 13972-13985.
148	MDH. 2019. Toxicological Summary for: Tolytriazole and 5-Methyl-1H-Benzotriazole. Health Based Guidance for Water. Minnesota Department of Health (MDH), Environmental Health Division, Health Risk Assessment Unit, St Paul, MN.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.

17-alpha-Ethynyl estradiol

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	17-alpha-Ethynyl estradiol
CASRN:	57-63-6
DTXSID:	DTXSID5020576
Use:	Pharmaceutical, hormone
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	X
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	21

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
10	reproductive and developmental effects	4	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	0.00007	lowest therapeutic dose: synthetic estrogen for birth control	bottle-fed infants	FDA; NIH	2018; 2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.001452	90th Percentile	Finished Water	UCMR3	2013-2015

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
		X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

17-alpha-Ethinyl estradiol

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	1.04167E-08	mg/kg/day	FDA 2018; NIH 2018	Allergan, Inc. 2017	lowest therapeutic dose: synthetic estrogen for birth control	bottle-fed infants	151	6.94e-05	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved
Reference Dose (RfD) or Equivalent	1.04167E-08	mg/kg/day	FDA 2018; NIH 2018	Allergan, Inc. 2017	lowest therapeutic dose: synthetic estrogen for birth control	general population	33.8	0.000245	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Health-Based Guidance Value	0.0000005	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.0000002	mg/L	MN DOH	
Maximum Recommended Daily Dose	0.0005	mg/kg/day	FDA	
Screening level for pharmaceutical - general population	0.000000245	mg/L	EPA Office of Water	
Screening level for pharmaceutical - infants	6.94E-08	mg/L	EPA Office of Water	
Short-Term/Subchronic Health-Based Guidance Value	0.0000002	mg/L	MN DOH	
Cancer Classification (CC)	Female.Rats	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats EE	no units	HHS NTP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1200	mg/kg	NIH HSDB	min
LD50	5000	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	28	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.00798	mol/kg	TEST QSAR	
Ames mutagenicity test	0	no units	TEST QSAR	
Developmental toxin test	1	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
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EPA - Office of Water

17-alpha-Ethynyl estradiol
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
				Prevalence				Magnitude			
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015	1,201	4	Sites	0.33	0.0011	0.0012	0.00145	0.00156	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
				Prevalence				Magnitude			
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	581	2	Sites	0.34	0.00066	0.000705	0.000732	0.00075	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	33	1	Sites	3.03	0.00075	0.00075	0.00075	0.00075	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	548	1	Sites	0.18	0.00066	0.00066	0.00066	0.00066	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
				Prevalence				Magnitude			
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	1	0	Sites	0						
Furlong et al 2017 (Finished) [83]	2007 - 2012	NA	NA	Sites	0					ug/L	
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
				Prevalence				Magnitude			
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	1	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	255	5	Sites	1.96	0.00056	0.00121	0.00164	0.0017	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	353	1	Sites	0.28	0.00647	0.00647	0.00647	0.00647	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	608	6	Sites	0.99	0.00056	0.00139	0.00361	0.00647	ug/L	
Furlong et al 2017 (Ambient) [83]	2007 - 2012	NA	NA	Sites	0					ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	1	Sites	2.63	0.000884	0.000884	0.000884	0.000884	ug/L	
Bexfield et al. 2019 (Groundwater) [49]	2013 - 2015	1,091	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Benotti et al. (2009) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.0014	ug/L	
Huang et al. (2001) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						7e-05	ug/L	
Kolpin et al. (2002) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.273	ug/L	
Zuo et al. (2006) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.0047	ug/L	
Waste Water Effluent											
				Prevalence				Magnitude			
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	5	Sites	24	0.00053	0.00145	0.0018	0.00182	ug/L	
Auriol et al. (2008) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						0.006	ug/L	
Chimchirian et al. (2007) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						0.0012	ug/L	
Huang et al. (2001) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						0.0024	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Expcast exposure		3.38E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	58.463	days	
Boiling point	OPERA QSAR	390.506	degree C	
Boiling point	TEST QSAR	383.097	degree C	
Vapor pressure	OPERA QSAR	7.41E-10	mmHg	
Vapor pressure	TEST QSAR	1.27E-08	mmHg	
Solubility in water	OPERA QSAR	0.0000399	mol/L	
Solubility in water	TEST QSAR	0.0000126	mol/L	
Bioconcentration factor	OPERA QSAR	120.559	no units	
Bioconcentration factor	TEST QSAR			
Henry's Law constant	OPERA QSAR	9.14E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.66688	no units	

17-alpha-Ethynyl estradiol

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
49	Bexfield, L.M., P.L. Toccalino, K. Belitz, W.T. Foreman, and E.T. Furlong. 2019. Hormones and pharmaceuticals in groundwater used as a source of drinking water across the United States. <i>Environmental Science and Technology</i> 53: 2950-2960.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
77	FDA. 2018. Drugs @ FDA: FDA Approved Drug Products. U.S. Food and Drug Administration (FDA). https://www.accessdata.fda.gov/scripts/cder/daf/ .
83	Furlong, E.T., Batt, A.L., Glassmeyer, S.T., Noriega, M.C., Kolpin, D.W., Mash, H., Schenck, K.M. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States: Pharmaceuticals. <i>Science of The Total Environment</i> . 579 (1629-1642).
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
127	Kostich, MS, et al., 2010. Predicting variability of aquatic concentrations of human pharmaceuticals. <i>Sci. Total Environ</i> . 408 (20), 4504e4510.
150	NIH. 2018. DailyMed Database. U.S. National Library of Medicine, National Institutes of Health (NIH). https://dailymed.nlm.nih.gov/dailymed/ .
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.

17-beta-Estradiol

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	17-beta-Estradiol
CASRN:	50-28-2
DTXSID:	DTXSID0020573
Use:	Pharmaceutical, hormone
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	X
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.030

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
9	non-cancer effects	3	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	0.03	lowest therapeutic dose: hormone therapy; hypoestrogenism, treatment of vasomotor symptoms associated with menopause, etc	bottle-fed infants	FDA; NIH	2018; 2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.000886	90th Percentile	Finished Water	UCMR3	2013-2015

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
		X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		
Not Applicable		

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

17-beta-Estradiol

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	4.16667E-06	mg/kg-day	FDA 2018; NIH 2018	Epic Pharma, LLC	lowest therapeutic dose: hormone therapy, treatment of symptoms associated with menopause, hypoestrogenism, etc	bottle-fed infants	151	0.03	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels
Reference Dose (RfD) or Equivalent	4.16667E-06	mg/kg-day	FDA 2018; NIH 2018	Epic Pharma, LLC	lowest therapeutic dose: hormone therapy, treatment of symptoms associated with menopause, hypoestrogenism, etc	general population	33.8	0.1	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels
Cancer Slope Factor (CSF)	39	(mg/kg/day)^-1	CALEPA 1992	Highman et al. 1980	mammary gland adenocarcinomas	general population	33.8	0.0007	[55]	

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Cancer Slope Factor (CSF)	39	(mg/kg/day)^-1	CalEPA OEHHA Chemical Database	
Inhalation Unit Risk (IUR)	0.011	ug/m^3	CalEPA OEHHA Chemical Database	
Maximum Recommended Daily Dose	0.5	mg/kg/day	FDA	
Screening level for pharmaceutical - general population	0.000098	mg/L	EPA Office of Water	
Screening level for pharmaceutical - infants	0.0000278	mg/L	EPA Office of Water	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Percent of active toxcast in vitro assays tested	22.84	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0057943	mol/kg	TEST QSAR	
Ames mutagenicity test	0.33	no units	TEST QSAR	
Developmental toxin test	0.889	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

17-beta-Estradiol
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015	1,201	2	Sites	0.17	4.00E - 04	0.00076	0.000886	0.00091	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	580	2	Sites	0.34	0.00048	0.00051	0.000528	0.00054	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	32	2	Sites	6.25	0.00048	0.00051	0.000528	0.00054	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	548	0	Sites	0						

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	1	0	Sites	0						
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	2	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	255	14	Sites	5.49	9.00E - 05	0.00094	0.00242	0.00388	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	382	4	Sites	1.05	0.00179	0.00439	0.0063	0.0065	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	637	18	Sites	2.83	9.00E - 05	0.00148	0.0043	0.0065	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	5	Sites	13	0.000325	0.000616	0.00202	0.002354	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	3	Sites	7.89	0.00071	0.00086	0.00153	0.0017	ug/L	
Bexfield et al. 2019 (Groundwater) [49]	2013 - 2015	1,091	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	5	Sites	24	0.000707	0.00119	0.0088	0.008934	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Expcast exposure		0.000000032	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	58.4157	days	
Boiling point	OPERA QSAR	372.709	degree C	
Boiling point	TEST QSAR	378.806	degree C	
Vapor pressure	OPERA QSAR	3.41E-10	mmHg	
Vapor pressure	TEST QSAR	2.03E-08	mmHg	
Solubility in water	OPERA QSAR	0.0000158	mol/L	
Solubility in water	TEST QSAR	0.000047	mol/L	
Bioconcentration factor	OPERA QSAR	33.8438	no units	
Bioconcentration factor	TEST QSAR	160.694	no units	
Henry's Law constant	OPERA QSAR	0.00000853	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.90759	no units	

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Reference Number	Full Reference
49	Bexfield, L.M., P.L. Toccalino, K. Belitz, W.T. Foreman, and E.T. Furlong. 2019. Hormones and pharmaceuticals in groundwater used as a source of drinking water across the United States. <i>Environmental Science and Technology</i> 53: 2950-2960.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
55	CalEPA. 1992. Expedited Cancer Potency Values and Proposed Regulatory Levels for Certain Proposition 65 Carcinogens. California Environmental Protection Agency (CalEPA), Office of Environmental Health Hazard Assessment, Reproductive and Cancer Hazard Assessment Section, Sacramento, CA.
77	FDA. 2018. Drugs @ FDA: FDA Approved Drug Products. U.S. Food and Drug Administration (FDA). https://www.accessdata.fda.gov/scripts/cder/daf/ .
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
150	NIH. 2018. DailyMed Database. U.S. National Library of Medicine, National Institutes of Health (NIH). https://dailymed.nlm.nih.gov/dailymed/ .
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.

2-(2-Methyl-4-chlorophenoxy)propionic acid (MCPP)

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EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	2-(2-Methyl-4-chlorophenoxy)propionic acid (MCPP)
CASRN:	93-65-2
DTXSID:	DTXSID9024194
Use:	Herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.04

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	non-cancer effects	2	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	200	increased kidney weights and chronic nephropathy	general population	OPP	2019

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
8		EDWC SW 30-Year Mean	OPP	2019

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

2-(2-Methyl-4-chlorophenoxy)propionic acid (MCPP)

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.04	mg/kg/day	OPP 2019	Mellert et al. 1996, 1999	increased kidney weights and chronic nephropathy	general population	33.8	237	[419]	
Cancer Classification (CC)	5		OPP 2019						[419]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Drinking Water Guideline Value	0.01	mg/L	WHO Drinking Water Quality Guidelines	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1210	mg/kg	NIH HSDB	max
LD50	369	mg/kg	NIH HSDB	min
LOAEL	125	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	50	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	10	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	50	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	1.16	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	9	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	3	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0039355	mol/kg	TEST QSAR	
Ames mutagenicity test	0.046	no units	TEST QSAR	
Developmental toxin test	0.691	no units	TEST QSAR	

2-(2-Methyl-4-chlorophenoxy)propionic acid (MCPPE)

CCL 5 Contaminant Information Sheet

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	2	2,823	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	6	254	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	12	6	Sites	50	0.00052	0.0012	0.00443	0.19	ug/L	
Ambient Water											
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	27	Sites	12	0.00052	0.0014	0.014	0.16	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	218	21	Sites	9.63	0.00052	0.0027	0.0708	0.139	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	6	Sites	50	0.00052	0.0013	0.012	0.16	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	107	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					
Estimated Drinking Water Concentration (EDWC) in Surface Water, 30-Year Mean	2019	OPP	8	ug/L	Pesticide in Water Calculator (PWC), v1.52	The modeled surface water 30-year mean concentration provided by the most recent available EPA OPP health assessment was selected as the occurrence concentration for MCPPE. This value coincides with the critical effect of chronic nephropathy provided within the health effects report.					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		7.16E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.5293	days	
Boiling point	OPERA QSAR	296.689	degree C	
Boiling point	TEST QSAR	312.482	degree C	
Vapor pressure	OPERA QSAR	0.00000159	mmHg	
Vapor pressure	TEST QSAR	0.0000131	mmHg	
Solubility in water	OPERA QSAR	0.00184223	mol/L	
Solubility in water	TEST QSAR	0.00348337	mol/L	
Bioconcentration factor	OPERA QSAR	3.69239	no units	
Bioconcentration factor	TEST QSAR	5.52077	no units	
Henry's Law constant	OPERA QSAR	1.62E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.05172	no units	

2-(2-Methyl-4-chlorophenoxy)propionic acid (MCP)

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Reference Number	Full Reference
419	USEPA. 2019. Mecoprop-p (MCP-p): Acute, and Chronic Aggregate Dietary (Drinking Water Only) Exposure and Risk Assessments for the Registration Review Risk Assessment. EPA-HQ-OPP-2014-0361-0021. DP No. D452571. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

2,4-DB

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	2,4-DB
CASRN:	94-82-6
DTXSID:	DTXSID7024035
Use:	Post-emergent herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.40

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	reproductive and developmental effects	10	7

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	800	increased early resorptions; decreased body weight, increased kidney weight, increased incidence of tubular degeneration in females	women of childbearing age	OPP	2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
318.68		EDWC SW (acute)	OPP	2018

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis
Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

2,4-DB

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.15	mg/kg/day	OPP 2018	Henwood 1990a and b	increased early resorptions; decreased body weight, increased kidney weight, increased incidence of tubular degeneration in females	women of childbearing age	35.4	847	[393]	
Cancer Classification (CC)	NL		OPP 2018						[393]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	20	mg/L	EPA HHBP	
Acute PAD	0.6	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.2	mg/L	EPA HHBP	
Drinking Water Guideline Value	0.09	mg/L	WHO Drinking Water Quality Guidelines	
Health-Based Screening Level	0.2	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.03	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	400	mg/kg	NIH HSDB	min
LD50	700	mg/kg	NIH HSDB	max
LOAEL	125	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	30	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	3	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	62.5	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in	2.6	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	25	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	50	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	15.8	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	4.96	mg/kg/day	EPA Toxicity Reference Database	min

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0027227	mol/kg	TEST QSAR	
Ames mutagenicity test	0.07	no units	TEST QSAR	
Developmental toxin test	0.701	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

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EPA - Office of Water

2,4-DB

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	46	1,445,891	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	60	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	12	1	Sites	8.33	0.023	0.023	0.023	0.023	ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	620	1	Sites	0.16	6.2	6.2	6.2	6.2	ug/L	
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	206	3	Sites	1.46	0.01	0.03	0.1	0.13	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	554	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	760	3	Sites	0.39	0.01	0.03	0.1	0.13	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	212	4	Sites	1.89	0.22	0.57	0.948	1.08	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	2	Sites	5.26	0.0281	0.0768	0.116	0.1255	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	106	0	Sites	0						
USGS, McKenzie River, Oregon, 2012 (Ambient) [158]	2002 - 2010	125	14	Samples	11				0.1	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					
Estimated Drinking Water Concentration (EDWC) in Surface Water (acute)	2018	OPP	318.68	ug/L	Pesticide Root Zone Model (PRZM) v3.12, Exposure Analysis Modeling System (EXAMS), v2.98.04	The critical effect of increased early resorptions is considered a less-than-chronic response seen during gestation. To be protective of pregnant women and fetuses, the modeled surface water acute concentration found in the most recent available EPA OPP health assessment was selected as the occurrence concentration for 2,4-dichlorophenoxybutyric acid.					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Expcast exposure		9.69E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.53603	days	
Boiling point	OPERA QSAR	320.542	degree C	
Boiling point	TEST QSAR	321.218	degree C	
Vapor pressure	OPERA QSAR	0.000000498	mmHg	
Vapor pressure	TEST QSAR	0.000011	mmHg	
Solubility in water	OPERA QSAR	0.000375647	mol/L	
Solubility in water	TEST QSAR	0.00034435	mol/L	
Bioconcentration factor	OPERA QSAR	3.46701	no units	
Bioconcentration factor	TEST QSAR	15.5597	no units	
Henry's Law constant	OPERA QSAR	1.43E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.38207	no units	

2,4-DB

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
158	Reconnaissance of Land-Use Sources of Pesticides in Drinking Water, McKenzie River, Oregon. U.S. Geological Survey Scientific Investigations Report 2012–5091, 46 p. plus appendixes.
393	USEPA. 2018. 2,4-DB: Draft Human Health Risk Assessment in Support of Registration Review. EPA-HQ-OPP-2013-0661-0019. DP No. D448826. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

2,4-Dichlorophenol

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	2,4-Dichlorophenol
CASRN:	120-83-2
DTXSID:	DTXSID1020439
Use:	Biocide; intermediate in production of herbicides
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.25

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	non-cancer effects	1	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	20	decreased delayed hypersensitivity response	general population	IRIS	1987

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
5	90th Percentile	All Ambient Water	NWIS	2008-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X	X		

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis
Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

2,4-Dichlorophenol

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.1	mg/kg/day	HC 1987	Kobayashi et al., 1972	changes in liver histopathology	general population	33.8	592	[98]	
Reference Dose (RfD) or Equivalent	0.003	mg/kg/day	IRIS 1987	Exon and Koller 1985	decreased delayed hypersensitivity response	general population	33.8	17.8	[189]	
Cancer Classification (CC)	NL		PPRTV 2007						[280]	
			ATSDR 1999						[14]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References Identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
						2006-07-01	2020-03-25	630	1	23	0

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	0.03	mg/L	EPA DWSHA 2018	
Chronic Health-Based Guidance Value	0.02	mg/L	MN DOH	
Human Health Ambient Water Quality Criteria	0.01	mg/L	EPA Human Health Criteria for CWA	
Intermediate Minimal Risk Level (MRL)	0.003	mg/kg/day	CDC ATSDR	
Lifetime Health Advisory	0.02	mg/L	EPA DWSHA 2018	
Maximum Allowable Concentration (MAC)	0.9	mg/L	Canadian Drinking Water Guidelines	
Subchronic Provisional RfD	0.02	mg/kg/day	EPA PPRTV	
Cancer Classification (CC)	Female.Mice NE	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats NE	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice NE	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats NE	no units	HHS NTP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	2050	mg/kg	NIH HSDB	max
LD50	500	mg/kg	NIH HSDB	min
LOAEL	543	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	768	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	194	mg/kg/day	EPA Toxicity Reference Database	
Percent of active toxcast in vitro assays tested	3.99	percent	EPA Chemistry Dashboard	
TD50	12400	mg/kg/day	NIH CPDB	min
TD50	458000	mg/kg/day	NIH CPDB	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0039355	mol/kg	TEST QSAR	
Ames mutagenicity test	0.015	no units	TEST QSAR	
Developmental toxin test	0.176	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

2,4-Dichlorophenol
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003	294	0	Sites	0					ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	22	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	13	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	9	0	Sites	0						

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)	5	34,293	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	6	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	36	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	148	25	Sites	17	0.01	0.03	5	5	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	392	8	Sites	2.04	0.01	0.02	1.88	18	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	540	33	Sites	6.11	0.01	0.03	5	18	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.00000499	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)	3	ug/l	

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.02586	days	
Boiling point	OPERA QSAR	211.815	degree C	
Boiling point	TEST QSAR	237.218	degree C	
Vapor pressure	OPERA QSAR	0.0785496	mmHg	
Vapor pressure	TEST QSAR	0.0280543	mmHg	
Solubility in water	OPERA QSAR	0.0237665	mol/L	
Solubility in water	TEST QSAR	0.00864968	mol/L	
Bioconcentration factor	OPERA QSAR	18.2343	no units	
Bioconcentration factor	TEST QSAR	57.4116	no units	
Henry's Law constant	OPERA QSAR	0.00000133	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.04309	no units	

2,4-Dichlorophenol

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
14	ATSDR. 1999. Toxicological Profile for Chlorophenols. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
98	Health Canada. 1987. Guideline Technical Document - Chlorophenols. Health Canada (HC), Water and Air Quality Bureau, Healthy Environments and Consumer Safety Branch, Ottawa, Ontario, Canada.
189	USEPA. 1987. Chemical Assessment Summary, 2,4-Dichlorophenol. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, D.C.
280	USEPA. 2007. Provisional Peer-Reviewed Toxicity Values for 2,4-Dichlorophenol. U.S. Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment, Superfund Health Risk Technical Support Center, Cincinnati, OH.

2,4-Dinitrophenol

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	2,4-Dinitrophenol
CASRN:	51-28-5
DTXSID:	DTXSID0020523
Use:	
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	X
Neurodev. Disruptors	
Androgen Receptors in vitro	X
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	2.6

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	non-cancer effects	1	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	10	lowest therapeutic dose in humans taking 2,4 dinitrophenol; cataracts were observed in patients receiving as little as 2 mg/kg/day, the lower range of the recommended therapeutic dose	general population	IRIS	2005

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
26.3	90th Percentile	All Ambient Water	NWIS	2008-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X	X		

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

2,4-Dinitrophenol

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.002	mg/kg/day	IRIS 2005	Horner, 1942	lowest therapeutic dose in humans taking 2,4 dinitrophenol; cataracts were observed in patients receiving as little as 2 mg/kg/day, the lower range of the recommended therapeutic dose	general population	33.8	11.8	[262]	NOTE: CCL screening level based on draft ATSDR (2019 assessment, based on 2008 study) is several orders of mag lower than HRL (based on 2006 assessment, 1942 study)
Cancer Classification (CC)	I		PPRTV 2007						[281]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.00007	mg/kg/day	ATSDR 2019	Caldeira da Silva et al. 2008	decreased body weight	bottle-fed infants	151	0.0900	[37]	

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
						2010-03-01	2020-04-14	326	1	3	0

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Minimal Risk Level (MRL)	0.01	mg/kg/day	CDC ATSDR	
Chronic Health-Based Guidance Value	0.01	mg/L	MN DOH	
Human Health Ambient Water Quality Criteria	0.01	mg/L	EPA Human Health Criteria for CWA	
Human Health Ambient Water Quality Criteria	0.01	mg/L	EPA Human Health Criteria for CWA	
Subchronic Provisional RfD	0.02	mg/kg/day	EPA PPRTV	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	20	mg/kg	NIH HSDB	min
LD50	72	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	11.86	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0002529	mol/kg	TEST QSAR	
Ames mutagenicity test	0.134	no units	TEST QSAR	
Developmental toxin test	0.554	no units	TEST QSAR	

2,4-Dinitrophenol

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003	294	0	Sites	0					ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	22	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	13	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	9	0	Sites	0						

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)	2	188,429	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	146	3	Sites	2.05	24	25	26.3	27	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	358	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	504	3	Sites	0.6	24	25	26.3	27	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		6.19E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.59079	days	
Boiling point	OPERA QSAR	349.689	degree C	
Boiling point	TEST QSAR	325.528	degree C	
Vapor pressure	OPERA QSAR	0.000270249	mmHg	
Vapor pressure	TEST QSAR	0.0000585	mmHg	
Solubility in water	OPERA QSAR	0.00173025	mol/L	
Solubility in water	TEST QSAR	0.0055847	mol/L	
Bioconcentration factor	OPERA QSAR	4.7119	no units	
Bioconcentration factor	TEST QSAR	2.68534	no units	
Henry's Law constant	OPERA QSAR	9.77E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.81096	no units	

2,4-Dinitrophenol

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
37	ATSDR. 2019. Toxicological Profile for Dinitrophenols DRAFT FOR PUBLIC COMMENT. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
262	USEPA. 2005. Chemical Assessment Summary 2,4-Dinitrophenol. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, DC.
281	USEPA. 2007. Provisional Peer-Reviewed Toxicity Values for 2,4-Dinitrotoluene. U.S. Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment, Superfund Health Risk Technical Support Center, Cincinnati, OH.

2,4-Dinitrotoluene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	2,4-Dinitrotoluene
CASRN:	121-14-2
DTXSID:	DTXSID0020529
Use:	Chemical intermediate; in propellants
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	8300

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	carcinogen with linear MOA	1	10

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.04	mammary gland tumors (adenomas, fibroadenomas, fibromas, adenocarcinomas/carcinomas) in female rats	general population	OW	2008

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
333	90th Percentile	Finished Water	UCMR1	2001 - 2003

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X	X		

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	X	Not Applicable

Basis

2,4-DNT appears to occur infrequently at levels of concern in PWSS. 2,4-DNT was detected only once at a minimum reporting level (MRL) of 2 µg/L in any of the PWSSs monitored under the UCMR 1 [a]. While the MRL is slightly greater than the HRL of 0.05 µg/L, this concentration is within the acceptable 10-4 to the 10-6 cancer risk range targeted by EPA [b].

[a] USEPA, 2008 [297]; [b] USEPA, 2000 [238]; as cited in USEPA, 2008 [296]

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

2,4-Dinitrotoluene

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.001	mg/kg/day	ATSDR 2016	U.S. Army. 1979; Ellis et al. 1985	"hematological effects (decreased erythrocyte count)"	general population	33.8	5.92	[34]	
Reference Dose (RfD) or Equivalent	0.002	mg/kg/day	OW 2008	Ellis et al., 1979; Ellis et al. 1985	"neurotoxicity and the presence of Heinz bodies and biliary tract hyperplasia"	general population	33.8	11.8	[288]	
Reference Dose (RfD) or Equivalent	0.002	mg/kg/day	IRIS 1992	Ellis et al. 1985	"Neurotoxicity, Heinz bodies and biliary tract hyperplasia"	general population	33.8	11.8	[214]	
Cancer Slope Factor (CSF)	0.667	(mg/kg/day)^-1	OW 2008	Ellis et al. 1979	mammary gland tumors (adenomas, fibroadenomas, fibromas, adenocarcinomas/carcinomas) in female rats	general population	33.8	0.0444	[288]	
Cancer Classification (CC)	L		OW 2008						[288]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Hepatic, Systemic	50	Maeda, 2015	Gastrointestinal	100	Maeda, 2015	2015-02-01	2019-12-17	65	1	0	1

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	1	mg/L	EPA DWSHA 2018	
Acute Minimal Risk Level (MRL)	0.05	mg/kg/day	CDC ATSDR	
Cancer Slope Factor (CSF)	0.31	(mg/kg/day)^-1	CalEPA OEHHA Chemical Database	
Human Health Ambient Water Quality Criteria	0.000049	mg/L	EPA Human Health Criteria for CWA	
Inhalation Unit Risk (IUR)	0.000089	ug/m^3	CalEPA OEHHA Chemical Database	
Intermediate Minimal Risk Level (MRL)	0.007	mg/kg/day	CDC ATSDR	
Lifetime Health Advisory	0.00005	mg/L	EPA DWSHA 2018	
Cancer Classification (CC)	2B	no units	WHO IARC	
Cancer Classification (CC)	Female.Mice N	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats P	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice N	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats P	no units	HHS NTP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1954	mg/kg	NIH HSDB	max
LD50	268	mg/kg	NIH HSDB	min
Percent of active toxcast in vitro assays tested	2.69	percent	EPA Chemistry Dashboard	
TD50	68	mg/kg/day	NIH CPDB	max
TD50	9.35	mg/kg/day	NIH CPDB	min

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0019724	mol/kg	TEST QSAR	
Ames mutagenicity test	0.808	no units	TEST QSAR	
Developmental toxin test	0.47	no units	TEST QSAR	

2,4-Dinitrotoluene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003	3,873	1	Sites	0.03	333	333	333	333	ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	22	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	13	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	9	0	Sites	0						

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)	6	10,733	Chemical Data Reporting (CDR) Results (EPA) (2016)	25K - 100K

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	54	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	265	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	160	3	Sites	1.88	4.9	5	5	5	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	410	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	567	3	Sites	0.53	4.9	5	5	5	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		3.63E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.55991	days	
Boiling point	OPERA QSAR	297.386	degree C	
Boiling point	TEST QSAR	304.767	degree C	
Vapor pressure	OPERA QSAR	0.000217133	mmHg	
Vapor pressure	TEST QSAR	0.000676083	mmHg	
Solubility in water	OPERA QSAR	0.00127277	mol/L	
Solubility in water	TEST QSAR	0.000635331	mol/L	
Bioconcentration factor	OPERA QSAR	9.38408	no units	
Bioconcentration factor	TEST QSAR	7.7983	no units	
Henry's Law constant	OPERA QSAR	7.58E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.93488	no units	

2,4-Dinitrotoluene

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
34	ATSDR. 2016. Toxicological Profile for Dinitrotoluenes. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
214	USEPA. 1992. Chemical Assessment Summary 2,4-Dinitrotoluene. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, DC.
238	USEPA. 2000. Unregulated Contaminant Monitoring Regulation Analytical Methods and Quality Control Manual. EPA 815-R-00-006.
288	USEPA. 2008. Drinking Water Health Advisory for 2,4-Dinitrotoluene and 2,6-Dinitrotoluene. EPA/822/R-08/010. U.S. Environmental Protection Agency, Office of Water, Health and Ecological Criteria Division, Washington, DC.
296	USEPA. 2008. Regulatory Determinations Support Document for Selected Contaminants from the Second Drinking Water Contaminant Candidate List (CCL 2). EPA Report 815-R-08-012. June 2008.
297	USEPA. 2008. The Analysis of Occurrence Data from the First Unregulated Contaminant Monitoring Regulation (UCMR 1) in Support of Regulatory Determinations for the Second Drinking Water Contaminant Candidate List. EPA 815-R-08-013. June.

2,6-Dinitrotoluene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	2,6-Dinitrotoluene
CASRN:	606-20-2
DTXSID:	DTXSID5020528
Use:	Chemical intermediate in the manufacture of dyes and military and commercial explosives
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	250

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	carcinogen with linear MOA	1	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.02	hepatocellular carcinomas	general population	PPRTV	2013

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
5	90th Percentile	All Ambient Water	NWIS	2008-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X	X		

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	X	Not Applicable

Basis

2,6-DNT appears to occur infrequently at levels of concern in PWSs. 2,6-DNT was not detected at a minimum reporting level (MRL) of 2 µg/L in any of the PWSs monitored under the UCMR 1 [a]. While the MRL is slightly greater than the HRL of 0.05 µg/L, this concentration is within the acceptable 10-4 to the 10-6 cancer risk range targeted by EPA [b].

[a] USEPA, 2008 [297]; [b] USEPA, 2000 [238]; as cited in USEPA, 2008 [296]

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

2,6-Dinitrotoluene

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0003	mg/kg/day	PPRTV 2013	Lee et al. 1976	Increased incidence of splenic extramedullary hematopoiesis	general population	33.8	1.78	[330]	
Reference Dose (RfD) or Equivalent	0.001	mg/kg/day	OW 2008	Lee et al. 1976	neurotoxicity, Heinz bodies, bile duct hyperplasia, liver and kidney histopathology, increased incidence of death	general population	33.8	5.92	[289]	
Cancer Slope Factor (CSF)	0.68	(mg/kg/day) ⁻¹	IRIS 1990	Ellis et al. 1979	hepatocellular carcinomas and neoplastic nodules; mammary gland adenomas, fibroadenomas, fibromas, and adenocarcinomas/carcinomas	general population	33.8	0.0435	[206]	
Cancer Slope Factor (CSF)	1.5	(mg/kg/day) ⁻¹	PPRTV 2013	Leonard et al. 1987	hepatocellular carcinomas	general population	33.8	0.0197	[330]	
Cancer Slope Factor (CSF)	0.667	(mg/kg/day) ⁻¹	OW 2008	Ellis et al. 1979; Lee et al. 1985	hepatocellular carcinomas and neoplastic nodules; mammary gland adenomas, fibroadenomas, fibromas, and adenocarcinomas/carcinomas	general population	33.8	0.0444	[289]	
Cancer Classification (CC)	B2		IRIS 1990						[206]	
Cancer Classification (CC)	S		PPRTV 2013						[330]	
Cancer Classification (CC)	L		OW 2008						[289]	
			ATSDR 2016						[34]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Hepatic, Systemic	20	Imamura, 2015				2015-02-01	2020-02-13	31	1	0	1

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	0.04	mg/L	EPA DWSHA 2018	
Acute Minimal Risk Level (MRL)	0.09	mg/kg/day	CDC ATSDR	
Intermediate Minimal Risk Level (MRL)	0.004	mg/kg/day	CDC ATSDR	
Lifetime Health Advisory	0.00005	mg/L	EPA DWSHA 2018	
Subchronic Provisional RfD	0.003	mg/kg/day	EPA PPRTV	
Cancer Classification (CC)	2B	no units	WHO IARC	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	177	mg/kg	NIH HSDB	min
LD50	621	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	1.83	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0005861	mol/kg	TEST QSAR	
Ames mutagenicity test	0.613	no units	TEST QSAR	
Developmental toxin test	0.44	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
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EPA - Office of Water

2,6-Dinitrotoluene

CCL 5 Contaminant Information Sheet

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003	3,873	0	Sites	0					ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	22	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	13	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	9	0	Sites	0						

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)	3	2,728	Chemical Data Reporting (CDR) Results (EPA) (2016)	< 25K

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	37	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	157	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	160	5	Sites	3.12	0.1	5	5	5	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	410	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	567	5	Sites	0.88	0.1	5	5	5	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.000000129	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.72441	days	
Boiling point	OPERA QSAR	297.597	degree C	
Boiling point	TEST QSAR	303.476	degree C	
Vapor pressure	OPERA QSAR	0.000411091	mmHg	
Vapor pressure	TEST QSAR	0.000429536	mmHg	
Solubility in water	OPERA QSAR	0.00117033	mol/L	
Solubility in water	TEST QSAR	0.00157761	mol/L	
Bioconcentration factor	OPERA QSAR	12.4551	no units	
Bioconcentration factor	TEST QSAR	6.20869	no units	
Henry's Law constant	OPERA QSAR	9.26E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.00324	no units	

2,6-Dinitrotoluene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
34	ATSDR. 2016. Toxicological Profile for Dinitrotoluenes. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
206	USEPA. 1990. Chemical Assessment Summary, 2,4-/2,6-Dinitrotoluene mixture. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, D.C.
238	USEPA. 2000. Unregulated Contaminant Monitoring Regulation Analytical Methods and Quality Control Manual. EPA 815-R-00-006.
289	USEPA. 2008. Drinking Water Health Advisory for 2,4-Dinitrotoluene and 2,6-Dinitrotoluene. U.S. Environmental Protection Agency, Office of Water, Office of Science and Technology, Health and Ecological Criteria Division, Washington, D.C.
296	USEPA. 2008. Regulatory Determinations Support Document for Selected Contaminants from the Second Drinking Water Contaminant Candidate List (CCL 2). EPA Report 815-R-08-012. June 2008.
297	USEPA. 2008. The Analysis of Occurrence Data from the First Unregulated Contaminant Monitoring Regulation (UCMR 1) in Support of Regulatory Determinations for the Second Drinking Water Contaminant Candidate List. EPA 815-R-08-013. June.
330	USEPA. 2013. Provisional Peer-Reviewed Toxicity Values for 2,6-Dinitrotoluene. U.S. Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment, Superfund Health Risk Technical Support Center, Cincinnati, OH.

2-Hydroxyatrazine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	2-Hydroxyatrazine
CASRN:	2163-68-0
DTXSID:	DTXSID6037807
Use:	Pesticide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.0005

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	non-cancer effects	10	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	400	histopathological changes in the kidney	general population	OPP	2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.2	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

2-Hydroxyatrazine

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0676	mg/kg/day	OPP 2018	Chow and Hart 1995	histopathological changes in the kidney	general population	33.8	400	[395]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Chronic Human Health Benchmark	0.06	mg/L	EPA HHBP	
Drinking Water Guideline Value	0.2	mg/L	WHO Drinking Water Quality Guidelines	
Health-Based Screening Level	0.06	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.01	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LOAEL	125	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	7.75	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	1.17	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	25	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic LOAEL	18.889999	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	59.599998	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	6.2	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	7.35	mg/kg/day	EPA Toxicity Reference Database	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0091833	mol/kg	TEST QSAR	
Ames mutagenicity test	0.145	no units	TEST QSAR	
Developmental toxin test	0.902	no units	TEST QSAR	

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EPA - Office of Water

2-Hydroxyatrazine
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	4,188	739	Sites	18	0.00044	0.0402	0.2	7.29	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	486	345	Sites	71	0.00044	0.042	0.2	4.6	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	3,702	394	Sites	11	0.00063	0.018	0.123	7.29	ug/L	
Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)			
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)				

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	10	9	Sites	90	0.002	0.015	0.12	0.74	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	495	303	Sites	61	0.00052	0.028	0.224	3.27	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	1,249	175	Sites	14	0.0013	0.019	0.0986	0.822	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,744	478	Sites	27	0.00052	0.0258	0.204	3.27	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	227	162	Sites	71	0.001998	0.023	0.22	1.2	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	218	153	Sites	70	0.001998	0.0238	0.0629	0.255	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	10	9	Sites	90	0.002	0.023	0.26	1.2	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	432	55	Sites	13	0.007	0.015	0.282	0.368	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	19	Sites	50	0.0055	0.0344	0.229	0.5428	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	57	Sites	8.26	8e-04	0.0103	0.0514	0.466	ug/L	
USGS, McKenzie River, Oregon, 2012 (Ambient) [158]	2002 - 2010	126	11	Samples	8.7				0.042	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.30198	days	
Boiling point	OPERA QSAR	332.794	degree C	
Boiling point	TEST QSAR	326.232	degree C	
Vapor pressure	OPERA QSAR	1.11E-10	mmHg	
Vapor pressure	TEST QSAR	8.95E-08	mmHg	
Solubility in water	OPERA QSAR	0.0000634	mol/L	
Solubility in water	TEST QSAR	0.0101859	mol/L	
Bioconcentration factor	OPERA QSAR	5.82054	no units	
Bioconcentration factor	TEST QSAR	3.22107	no units	
Henry's Law constant	OPERA QSAR	9.6E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.95934	no units	

2-Hydroxyatrazine

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
158	Reconnaissance of Land-Use Sources of Pesticides in Drinking Water, McKenzie River, Oregon. U.S. Geological Survey Scientific Investigations Report 2012–5091, 46 p. plus appendixes.
395	USEPA. 2018. Atrazine. Draft Human Health Risk Assessment for Registration Review. EPQ-HQ-OPP-2013-0266-1159. DP No. D418316. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

2-Methyl-4-chlorophenoxyacetic acid (MCPA)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	2-Methyl-4-chlorophenoxyacetic acid (MCPA)
CASRN:	94-74-6
DTXSID:	DTXSID4024195
Use:	Herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0013

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	non-cancer effects	8	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	300	nephrotoxicity	general population	OPP	2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.3986	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

2-Methyl-4-chlorophenoxyacetic acid (MCPA)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.044	mg/kg/day	OPP 2018	Kirsch, 1988	nephrotoxicity	general population	33.8	260	[402]	
Cancer Classification (CC)	NL		OPP 2018						[402]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	0.1	mg/L	EPA DWSHA 2018	
Chronic Health-Based Guidance Value	0.003	mg/L	MN DOH	
Lifetime Health Advisory	0.03	mg/L	EPA DWSHA 2018	
Maximum Allowable Concentration (MAC)	0.1	mg/L	Canadian Drinking Water Guidelines	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	439	mg/kg	NIH HSDB	min
LD50	800	mg/kg	NIH HSDB	max
LOAEL	1.02	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	120	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	0.21	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	60	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	1.59	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	177	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic LOAEL	3	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	1	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	42	mg/kg/day	EPA Toxicity Reference Database	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0032359	mol/kg	TEST QSAR	
Ames mutagenicity test	0.056	no units	TEST QSAR	
Developmental toxin test	0.691	no units	TEST QSAR	

2-Methyl-4-chlorophenoxyacetic acid (MCPA)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
402	USEPA. 2018. MCPA. Draft Human Health Risk Assessment in Support of Registration Review. EPA-HQ-OPP-2014-0180-0043. DP No. D446323. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

2-Methylnaphthalene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	2-Methylnaphthalene
CASRN:	91-57-6
DTXSID:	DTXSID4020878
Use:	Insecticide; small quantities for the production of alkylmethylnaphthalene sulfonates as textile auxiliaries, surfactants, and emulsifiers.
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0021

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	non-cancer effects	8	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	20	pulmonary alveolar proteinosis	general population	IRIS	2003

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.0416	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

2-Methylnaphthalene

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.004	mg/kg/day	IRIS 2003	Murata et al. 1997	pulmonary alveolar proteinosis	general population	33.8	23.7	[254]	
Reference Dose (RfD) or Equivalent	0.04	mg/kg/day	ATSDR 2005	Murata et al. 1997	pulmonary alveolar proteinosis	general population	33.8	237	[23]	
Cancer Classification (CC)	I		PPRTV 2007						[279]	
Cancer Classification (CC)	I		IRIS 2003						[254]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
						2006-09-01	2020-03-25	71	0	0	

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Chronic Health-Based Guidance Value	0.008	mg/L	MN DOH	
Subchronic Provisional RfD	0.004	mg/kg/day	EPA PPRTV	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1630	mg/kg	NIH HSDB	
Percent of active toxcast in vitro assays tested	0	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0094406	mol/kg	TEST QSAR	
Ames mutagenicity test			TEST QSAR	
Developmental toxin test	0.514	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

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2-Methylnaphthalene

CCL 5 Contaminant Information Sheet

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	567	12	Sites	2.12	0.003	0.013	0.0416	0.16	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	88	8	Sites	9.09	0.003	0.01	0.028	0.05	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	479	4	Sites	0.84	0.011	0.0275	0.108	0.16	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	1M - 10M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	750	120	Sites	16	0.003	0.01	0.05	6	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	782	65	Sites	8.31	0.003	0.014	0.0343	610	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,532	185	Sites	12	0.003	0.012	0.0499	610	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	2	Sites	5.26	0.0076	0.00875	0.00967	0.0099	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	0	Sites	0						
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.00000578	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	14.9141	days	
Boiling point	OPERA QSAR	246.408	degree C	
Boiling point	TEST QSAR	246.201	degree C	
Vapor pressure	OPERA QSAR	0.026447	mmHg	
Vapor pressure	TEST QSAR	0.0272898	mmHg	
Solubility in water	OPERA QSAR	0.000157227	mol/L	
Solubility in water	TEST QSAR	0.00013213	mol/L	
Bioconcentration factor	OPERA QSAR	72.8094	no units	
Bioconcentration factor	TEST QSAR	358.922	no units	
Henry's Law constant	OPERA QSAR	0.000535625	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.94282	no units	

2-Methylnaphthalene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
23	ATSDR. 2005. Toxicological Profile for Naphthalene, 1-Methylnaphthalene, and 2-Methylnaphthalene. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
254	USEPA. 2003. Chemical Assessment Summary, 2-Methylnaphthalene. U.S. Environmental Protection Agency, National Center for Environmental Protection, Integrated Risk Information System (IRIS), Washington, D.C.
279	USEPA. 2007. Provisional Peer-Reviewed Toxicity Values for 2-Methylnaphthalene. U.S. Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment, Superfund Health Risk Technical Support Center, Cincinnati, OH.

6-Chloro-1,3,5-triazine-2,4-diamine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	6-Chloro-1,3,5-triazine-2,4-diamine
CASRN:	3397-62-4
DTXSID:	DTXSID1037806
Use:	Herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.00095

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	reproductive and developmental effects	10	5

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	400	attenuation of LH surge in females ages 13-49 (estrous cycle disruption)	women of childbearing age	OPP	2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.382	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

6-Chloro-1,3,5-triazine-2,4-diamine
CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.076	mg/kg/day	OPP 2018	Cooper et al. 2010	attenuation of LH surge in females ages 13-49 (estrous cycle disruption)	women of childbearing age	35.4	429	[395]	
Cancer Classification (CC)	NL		OPP 2018						[395]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.3	mg/L	EPA HHBP	
Acute PAD	0.01	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.012	mg/L	EPA HHBP	
Health-Based Screening Level	0.012	mg/L	Health-based screening levels from USGS	
Maximum Allowable Daily Level	100	ug/day	CalEPA OEHHA Chemical Database	
Population-Adjusted Dose (PAD)	0.0018	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LOAEL	25	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	75	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	2.5	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	25	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	0	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	7.5999999	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	0.7	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0062374	mol/kg	TEST QSAR	
Ames mutagenicity test	0.176	no units	TEST QSAR	
Developmental toxin test	0.628	no units	TEST QSAR	

Scoring Data											
Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
		Prevalence				Magnitude					
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	3,405	656	Sites	19	0.0012	0.103		6.68	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	456	278	Sites	61	0.0013	0.105	0.365	2.4	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	2,949	378	Sites	13	0.0012	0.057	0.778	6.68	ug/L	

Non-Scoring Data													
Non-Nationally Representative Water Data			Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water				Prevalence				Magnitude					
USDA Pesticide Data Program (PDP) (Finished)			2001 - 2013	10	3	Sites	30	0.025	0.05	0.05	0.05	ug/L	
Ambient Water				Prevalence				Magnitude					
Drinking Water Monitoring Data - WI (Source)			2012-2019	2	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)			2008 - 2017	354	137	Sites	39	0.0032	0.0842	0.223	1.35	ug/L	
National Water Information System (USGS NWIS) (Groundwater)			2008 - 2017	731	188	Sites	26	0.0036	0.16	0.867	2.45	ug/L	
National Water Information System (USGS NWIS) (All Water)			2008 - 2017	1,085	325	Sites	30	0.0032	0.0984	0.406	2.45	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)			2001 - 2013	227	76	Sites	33	0.015	0.05	0.368	2.9	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)			2001 - 2013	218	73	Sites	33	0.015	0.0865	0.457	2.9	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)			2001 - 2013	10	3	Sites	30	0.025	0.05	0.05	0.12	ug/L	
Bradley et al. 2017 (Ambient) [52]			2012 - 2014	38	7	Sites	18	0.027	0.074	0.122	0.17	ug/L	
Arnold et al. 2016 (Filtered) [7]			2012 - 2013	584	86	Sites	15	0.0012	0.132	1.28	6.3	ug/L	
Waste Water Effluent				Prevalence				Magnitude					
Estimated Concentration in Water		Date	Source	Value	Units	Model	Notes						

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	8.42524	days	
Boiling point	OPERA QSAR	317.078	degree C	
Boiling point	TEST QSAR	277.429	degree C	
Vapor pressure	OPERA QSAR	7.01E-09	mmHg	
Vapor pressure	TEST QSAR	0.00000585	mmHg	
Solubility in water	OPERA QSAR	0.00462445	mol/L	
Solubility in water	TEST QSAR	0.0302691	mol/L	
Bioconcentration factor	OPERA QSAR	2.87554	no units	
Bioconcentration factor	TEST QSAR	1.65577	no units	
Henry's Law constant	OPERA QSAR	7.17E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	-0.196188	no units	

6-Chloro-1,3,5-triazine-2,4-diamine

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
395	USEPA. 2018. Atrazine. Draft Human Health Risk Assessment for Registration Review. EPQ-HQ-OPP-2013-0266-1159. DP No. D418316. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.

Acephate

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Acephate
CASRN:	30560-19-1
DTXSID:	DTXSID8023846
Use:	Insecticide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.44

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	reproductive and developmental effects	9	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.4	inhibition of brain acetylcholinesterase in male postnatal day 11 pups	bottle-fed infants	OPP	2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.1758	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
		X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Acephate

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0003	mg/kg/day	OPP 2018	Hoberman 2003	inhibition of brain AChE in male pups on PND 11.	bottle-fed infants	151	0.397	[394]	
Cancer Classification (CC)	C		OPP 2018						[394]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.03	mg/L	EPA HHBP	
Acute PAD	0.005	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.0077	mg/L	EPA HHBP	
Health-Based Screening Level	0.0077	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.0012	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	233	mg/kg	NIH HSDB	min
LD50	945	mg/kg	NIH HSDB	max
LOAEL	0.25	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	75	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	2.5	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	20	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	1.43	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	0.12	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0019999	mol/kg	TEST QSAR	
Ames mutagenicity test	0.202	no units	TEST QSAR	
Developmental toxin test	0.743	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Acephate
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water		Prevalence				Magnitude					
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water		Prevalence				Magnitude					
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	1,760	135	Sites	7.67	0.00051	0.0212	0.176	10.4	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	322	131	Sites	41	0.00051	0.0212	0.175	10.4	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	1,438	4	Sites	0.28	0.00267	0.00749	0.14	0.229	ug/L	
Pesticide Application Data		Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data		Number of States	Amount Released (lbs/year)	Chemical Production Data		Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)		36	4,373,575	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)		4	27,210	Chemical Data Reporting (CDR) Results (EPA) (2016)		25K - 100K

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water		Prevalence				Magnitude					
Ambient Water		Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	3	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	307	33	Sites	11	0.00082	0.0445	0.277	10.4	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	528	2	Sites	0.38	0.00788	0.113	0.176	0.218	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	835	35	Sites	4.19	0.00082	0.0445	0.275	10.4	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	118	34	Sites	29	0.132	0.454	2.7	13.5	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	0	Sites	0						
Waste Water Effluent		Prevalence				Magnitude					
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		6.17E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)	< LOD	ug/l	

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.55348	days	
Boiling point	OPERA QSAR	271.255	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.00000222	mmHg	
Vapor pressure	TEST QSAR			
Solubility in water	OPERA QSAR	3.1318	mol/L	
Solubility in water	TEST QSAR	0.408319	mol/L	
Bioconcentration factor	OPERA QSAR	1.22201	no units	
Bioconcentration factor	TEST QSAR			
Henry's Law constant	OPERA QSAR	4.76E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	-0.710368	no units	

Acephate

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
394	USEPA. 2018. Acephate. Revised Draft Human Health Risk Assessment (DRA) in Support of Registration Review. EPA-HQ-OPP-2008-0915-0025. DP No. D446177. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Acetamiprid

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Acetamiprid
CASRN:	135410-20-7
DTXSID:	DTXSID0034300
Use:	Insecticide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.000065

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	non-cancer effects	10	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	400	reduced body weight and body weight gain in females, hepatocellular vacuolation in males	general population	OPP	2017

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.02615	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Acetamiprid

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.071	mg/kg/day	OPP 2017	Hatch 1999	reduced body weight and body weight gain in females, hepatocellular vacuolation in males	general population	33.8	420	[375]	
Cancer Classification (CC)	NL		OPP 2017						[375]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.7	mg/L	EPA HHBP	
Acute PAD	0.1	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.45	mg/L	EPA HHBP	
Health-Based Screening Level	0.45	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.071	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	146	mg/kg	NIH HSDB	min
LD50	217	mg/kg	NIH HSDB	max
LOAEL	17.5	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	65.599998	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	25.2	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	8.8	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	1.74	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	250.10001	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic LOAEL	32	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	129.4	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	14	mg/kg/day	EPA Toxicity Reference Database	min

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0028314	mol/kg	TEST QSAR	
Ames mutagenicity test	0.819	no units	TEST QSAR	
Developmental toxin test	0.6	no units	TEST QSAR	

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Acetamiprid
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OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	5	2	Sites	40	0.0025	0.004	0.0262	0.0456	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	5	2	Sites	40	0.0025	0.004	0.0262	0.0456	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	36	107,391	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	10	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	130	7	Sites	5.38	0.0023	0.0144	0.137	0.227	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	12	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	142	7	Sites	4.93	0.0023	0.0144	0.137	0.227	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	227	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	218	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	10	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	178	8	Sites	4.49	0.0262	0.0606	0.165	0.199	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	1	Sites	2.63	0.0395	0.0395	0.0395	0.0395	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exposure exposure		8.48E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.87165	days	
Boiling point	OPERA QSAR	315.067	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.0000916	mmHg	
Vapor pressure	TEST QSAR			
Solubility in water	OPERA QSAR	0.044269	mol/L	
Solubility in water	TEST QSAR	0.0494311	mol/L	
Bioconcentration factor	OPERA QSAR	9.32437	no units	
Bioconcentration factor	TEST QSAR			
Henry's Law constant	OPERA QSAR	3.46E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.19577	no units	

Acetamiprid

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Reference Number	Full Reference
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
375	USEPA. 2017. Acetamiprid. Acute and Chronic Dietary Exposure and Risk Assessment for Registration Review. EPA-HQ-OPP-2012-0329-0022. DP No. D443740. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Acetochlor ethanesulfonic acid (ESA)

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Acetochlor ethanesulfonic acid (ESA)
CASRN:	187022-11-3
DTXSID:	DTXSID6037483
Use:	Pesticide degradate
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.004

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	reproductive and developmental effects	3	7

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	300	decreased body weight and weight gain, decreased food utilization; increased TSH, T4, and T3; increased relative testes weight	general population	MDH	2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
1.190526	90th Percentile	Finished Water	UCMR2	2008-2010

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X	X	X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Acetochlor ethanesulfonic acid (ESA)

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.056	mg/kg/day	MDH 2018	Lees 2000	decreased body weight and weight gain, decreased food utilization; increased TSH, T4, and T3; increased relative testes weight	general population	33.8	331	[142]	

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Health-Based Guidance Value	0.5	mg/L	MN DOH	
Acute Health-Based Guidance Value	0.6	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.3	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.3	mg/L	MN DOH	
Short-Term/Subchronic Health-Based Guidance Value	0.5	mg/L	MN DOH	
Short-Term/Subchronic Health-Based Guidance Value	0.6	mg/L	MN DOH	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Percent of active toxcast in vitro assays tested	0.71	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.011695	mol/kg	TEST QSAR	
Ames mutagenicity test	0.55	no units	TEST QSAR	
Developmental toxin test	1.155	no units	TEST QSAR	

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Acetochlor ethanesulfonic acid (ESA)
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010	1,198	2	Sites	0.17	1.10526	1.15	1.19	1.2	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	2,719	325	Sites	12	0.012	0.266	1.11	13.2	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	419	212	Sites	51	0.012	0.272	1.12	13.2	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	2,300	113	Sites	4.91	0.02	0.14	0.823	12.3	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	4	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	7	Sites	41	0.0027	0.039	0.484	1.2	ug/L	
Bradley et al. 2018 (Finished) [53]	2016	26	3	Sites	12	0.05	0.09	0.106	0.11	ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	2	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	354	73	Sites	21	0.02	0.174	0.62	1.75	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	826	52	Sites	6.3	0.02	0.15	0.478	0.88	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,180	125	Sites	11	0.02	0.17	0.581	1.75	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	155	Sites	68	0.002664	0.063	0.51	1.9	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	148	Sites	68	0.002664	0.0654	0.161	1.75	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	7	Sites	58	0.0027	0.059	0.579	1.9	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	9	Sites	24	0.02	0.06	0.566	0.67	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	23	Sites	3.94	0.038	0.178	0.481	0.695	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Expcast exposure		0.000000125	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.28498	days	
Boiling point	OPERA QSAR	314.606	degree C	
Boiling point	TEST QSAR	382.116	degree C	
Vapor pressure	OPERA QSAR	0.000000167	mmHg	
Vapor pressure	TEST QSAR			
Solubility in water	OPERA QSAR	0.0136286	mol/L	
Solubility in water	TEST QSAR	0.00744732	mol/L	
Bioconcentration factor	OPERA QSAR	9.7255	no units	
Bioconcentration factor	TEST QSAR	7.31139	no units	
Henry's Law constant	OPERA QSAR	5.13E-10	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.7785	no units	

Acetochlor ethanesulfonic acid (ESA)

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. <i>Environmental science & technology</i> , 52(23), 13972-13985.
140	MDH. 2016. Toxicological Summary for: Alachlor ESA and Alachlor OXA. Health Based Guidance for Water. Minnesota Department of Health (MDH), Environmental Health Division, Health Risk Assessment Unit, St Paul, MN.
142	MDH. 2018. Toxicological Summary for: Acetochlor ESA. Health Based Guidance for Water. Minnesota Department of Health (MDH), Environmental Health Division, Health Risk Assessment Unit, St Paul, MN.

Acetochlor oxanilic acid (OA)

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Acetochlor oxanilic acid (OA)
CASRN:	194992-44-4
DTXSID:	DTXSID1037484
Use:	Pesticide degradate
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.01

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	non-cancer effects	1	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	100	decreased body weight, body weight gain, and food utilization; decreased thyroid stimulating hormone	general population	MDH	2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
1.039	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X	X	X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Acetochlor oxanilic acid (OA)

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.019	mg/kg/day	MDH 2018	Albin and Kraus 2000; Williams 2000	decreased body weight, body weight gain, and food utilization; decreased thyroid stimulating hormone	general population	33.8	112	[143]	

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Health-Based Guidance Value	0.1	mg/L	MN DOH	
Acute Health-Based Guidance Value	0.2	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.09	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.1	mg/L	MN DOH	
Short-Term/Subchronic Health-Based Guidance Value	0.1	mg/L	MN DOH	
Short-Term/Subchronic Health-Based Guidance Value	0.2	mg/L	MN DOH	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0098628	mol/kg	TEST QSAR	
Ames mutagenicity test	0.261	no units	TEST QSAR	
Developmental toxin test	0.88	no units	TEST QSAR	

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EPA - Office of Water

Acetochlor oxanilic acid (OA)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010	1,198	0	Sites	0					ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	2,724	246	Sites	9.03	0.0053	0.217	1.04	15.4	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	422	203	Sites	48	0.0053	0.218	1.04	15.4	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	2,302	43	Sites	1.87	0.02	0.14	0.5	15	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	4	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	7	Sites	41	0.00113	0.048	0.615	1.3	ug/L	
Bradley et al. 2018 (Finished) [53]	2016	26	3	Sites	12	0.02	0.17	0.186	0.19	ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	2	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	355	87	Sites	25	0.0194	0.15	0.567	1.76	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	830	30	Sites	3.61	0.02	0.05	0.295	0.54	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,185	117	Sites	9.87	0.0194	0.133	0.532	1.76	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	129	Sites	56	0.00113	0.062	0.74	1.9	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	122	Sites	56	0.002331	0.0544	0.0986	1.03	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	7	Sites	58	0.00113	0.0705	0.82	1.9	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	6	Sites	16	0.03	0.075	0.54	0.56	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	6	Sites	1.03	0.103	0.172	0.438	0.628	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		8.59E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.35388	days	
Boiling point	OPERA QSAR	320.906	degree C	
Boiling point	TEST QSAR	367.714	degree C	
Vapor pressure	OPERA QSAR	0.000000214	mmHg	
Vapor pressure	TEST QSAR	0.000000653	mmHg	
Solubility in water	OPERA QSAR	0.00519245	mol/L	
Solubility in water	TEST QSAR	0.00289068	mol/L	
Bioconcentration factor	OPERA QSAR	2.91563	no units	
Bioconcentration factor	TEST QSAR	1.2331	no units	
Henry's Law constant	OPERA QSAR	7.1E-10	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.60609	no units	

Acetochlor oxanilic acid (OA)

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. <i>Environmental science & technology</i> , 52(23), 13972-13985.
143	MDH. 2018. Toxicological Summary for: Acetochlor OXA. Health Based Guidance for Water. Minnesota Department of Health (MDH), Environmental Health Division, Health Risk Assessment Unit, St Paul MN.

Acetophenone

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Acetophenone
CASRN:	98-86-2
DTXSID:	DTXSID6021828
Use:	Photosensitizing agents; flavoring
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0005

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	no adverse effects	8	5

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	600	no adverse effects identified at the highest dose tested	general population	IRIS	1988

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.3	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Acetophenone

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.1	mg/kg/day	IRIS 1988	Hagen et al. 1967	no adverse effects identified at the highest dose tested	general population	33.8	592	[197]	NOTE: the 2011 PPRTV assessment declines to derive a chronic RfD for acetophenone because a non-cancer assessment is available
Cancer Classification (CC)	D		IRIS 1988						[197]	NOTE: the 2011 PPRTV assessment declines to derive a chronic RfD for acetophenone because a non-cancer assessment is available
Cancer Classification (CC)	D		PPRTV 2011						[322]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
						2010-06-01	2020-04-14	232	2	0	

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Subchronic Provisional RfD	0.8	mg/kg/day	EPA PPRTV	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	3000	mg/kg	NIH HSDB	max
LD50	740	mg/kg	NIH HSDB	min
Percent of active toxcast in vitro assays tested	0.88	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0125893	mol/kg	TEST QSAR	
Ames mutagenicity test	0.094	no units	TEST QSAR	
Developmental toxin test	0.333	no units	TEST QSAR	

Acetophenone

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	563	11	Sites	1.95	0.1	0.2	0.3	0.5	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	88	11	Sites	12	0.1	0.2	0.3	0.5	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	475	0	Sites	0						

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)	13	981,013	Chemical Data Reporting (CDR) Results (EPA) (2016)	10M - 50M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	4		0.58		0.58	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	743	49	Sites	6.59	0.1	0.3	4.07	5.3	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	715	6	Sites	0.84	0.2	0.35	2.08	2.5	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,458	55	Sites	3.77	0.1	0.3	3.25	5.3	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	1	Sites	50	0.3	0.3	0.3	0.3	ug/L	
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	9	Sites	43	0.22	0.29	0.36	0.37	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.0000215	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	5.40713	days	
Boiling point	OPERA QSAR	200.433	degree C	
Boiling point	TEST QSAR	209.024	degree C	
Vapor pressure	OPERA QSAR	0.427749	mmHg	
Vapor pressure	TEST QSAR	0.542001	mmHg	
Solubility in water	OPERA QSAR	0.0393752	mol/L	
Solubility in water	TEST QSAR	0.0215278	mol/L	
Bioconcentration factor	OPERA QSAR	9.03932	no units	
Bioconcentration factor	TEST QSAR	7.63836	no units	
Henry's Law constant	OPERA QSAR	0.000011	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.70555	no units	

Acetophenone

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
197	USEPA. 1988. Chemical Assessment Summary, Acetophenone. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, DC.
322	USEPA. 2011. Provisional Peer-Reviewed Toxicity Values for Acetophenone. U.S. Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment, Superfund Health Risk Technical Support Center, Cincinnati, OH.

Acrolein

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Acrolein
CASRN:	107-02-8
DTXSID:	DTXSID5020023
Use:	Aquatic herbicide; rodenticide; industrial chemical
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.14

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	non-cancer effects	3	7

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	20	forestomach squamous epithelial hyperplasia	general population	ATSDR	2007

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
2.7	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
		X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Acrolein

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0005	mg/kg/day	IRIS 2003	Parent et al., 1992c	increased mortality	general population	33.8	2.96	[258]	
Reference Dose (RfD) or Equivalent	0.004	mg/kg/day	ATSDR 2007	NTP 2006	forestomach squamous epithelial hyperplasia	general population	33.8	23.7	[26]	NOTE: no toxicity values were provided in the 2015 OPP assessment because chronic and acute oral exposures to acrolein are not expected based on use patterns, physical-chemical properties, and plant metabolism data. Therefore, the ATSDR assessment was chosen as
Cancer Classification (CC)	I		OPP 2015						[338]	
Cancer Classification (CC)	I		IRIS 2003						[258]	
			PPRTV 2002						[252]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Inhalation Minimal Risk Level (MRL)	0.003	ppm	CDC ATSDR	
Cancer Classification (CC)	3	no units	WHO IARC	
Human Health Ambient Water Quality Criteria	0.003	mg/L	EPA Human Health Criteria for CWA	
Intermediate Inhalation Minimal Risk Level (MRL)	0.00004	ppm	CDC ATSDR	
Intermediate Minimal Risk Level (MRL)	0.004	mg/kg/day	CDC ATSDR	
Reference Concentration (RfC)	0.35	ug/m^3	CalEPA OEHHA Chemical Database	
Reference Concentration (RfC)	0.00002	mg/m^3	EPA IRIS	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	10.3	mg/kg	NIH HSDB	min
LD50	46	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	0.85	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0011588	mol/kg	TEST QSAR	
Ames mutagenicity test	0.51	no units	TEST QSAR	
Developmental toxin test	0.641	no units	TEST QSAR	

Acrolein

CCL 5 Contaminant Information Sheet

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	1,183	3	Sites	0.25	1	2	2.7	3	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	102	3	Sites	2.94	1	2	2.7	3	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	1,081	0	Sites	0						

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)	25	1,242,926	Chemical Data Reporting (CDR) Results (EPA) (2016)	250M - 500M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	2	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	19	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	69	5	Sites	7.25	0.4	1.3	4.44	7.5	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	21	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	89	5	Sites	5.62	0.4	1.3	4.44	7.5	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	2	0	Sites	0						
Arnold et al. 2016 (Unfiltered) [7]	2012 - 2013	527	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.000000128	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHanes biomonitoring detection in serum (1999-2016)			
NHanes biomonitoring detection in blood (1999-2016)			
NHanes biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.67473	days	
Boiling point	OPERA QSAR	59.2581	degree C	
Boiling point	TEST QSAR	52.443	degree C	
Vapor pressure	OPERA QSAR	199.082	mmHg	
Vapor pressure	TEST QSAR	210.378	mmHg	
Solubility in water	OPERA QSAR	4.7652	mol/L	
Solubility in water	TEST QSAR	1.77419	mol/L	
Bioconcentration factor	OPERA QSAR	3.77906	no units	
Bioconcentration factor	TEST QSAR			
Henry's Law constant	OPERA QSAR	0.0000817	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	0.0512154	no units	

Acrolein

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
26	ATSDR. 2007. Toxicological Profile for Acrolein. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
252	USEPA. 2002. Provisional Peer-Reviewed Toxicity Values for Acrolein. U.S. Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment, Superfund Health Risk Technical Support Center, Cincinnati, OH.
258	USEPA. 2003. Toxicological Review of Acrolein (CAS No. 107-02-8). U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, D.C.
338	USEPA. 2015. Acrolein: Human Health Assessment Scoping Document in Support of Registration Review. EPA-HQ-OPP-2015-0571-0005. DP No. D427578. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Acyclovir

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Acyclovir
CASRN:	59277-89-3
DTXSID:	DTXSID1022556
Use:	antiviral
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.012

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	non-cancer effects	9	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	20	lowest therapeutic dose: antiviral/reduce duration and severity of herpes and chickenpox infection	bottle-fed infants	FDA; NIH	2018; 2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.248	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Acyclovir

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	HRL (ug/L)	Assessment Full Citation	Notes
Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations										
Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0025	mg/kg/day	FDA 2018; NIH 2018	Ranbaxy Laboratories Ltd.	lowest therapeutic dose: antiviral/reduce duration and severity of herpes and chickenpox infection	bottle-fed infants	151	17.0	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels
Reference Dose (RfD) or Equivalent	0.0025	mg/kg/day	FDA 2018; NIH 2018	Ranbaxy Laboratories Ltd.	lowest therapeutic dose: antiviral/reduce duration and severity of herpes and chickenpox infection	general population	33.8	59.0	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References Identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Cancer Classification (CC)	3	no units	WHO IARC	
Maximum Recommended Daily Dose	13.3	mg/kg/day	FDA	
Screening level for pharmaceutical - general population	0.058823529	mg/L	EPA Office of Water	
Screening level for pharmaceutical - infants	0.016666667	mg/L	EPA Office of Water	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	10000	mg/kg	NIH HSDB	
Percent of active toxcast in vitro assays tested	2.13	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0013836	mol/kg	TEST QSAR	
Ames mutagenicity test	0.173	no units	TEST QSAR	
Developmental toxin test	0.62	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
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EPA - Office of Water

Acyclovir
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	557	16	Sites	2.87	0.00428	0.02	0.248	0.787	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	75	16	Sites	21	0.00428	0.02	0.248	0.787	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	482	0	Sites	0						

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	205	53	Sites	26	0.00644	0.0506	0.238	4.35	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	401	2	Sites	0.5	0.0565	5.23	8.33	10.4	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	606	55	Sites	9.08	0.00644	0.0509	0.259	10.4	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	14	Sites	37	0.0080967	0.314	0.484	0.6951437	ug/L	
Bexfield et al. 2019 (Groundwater) [49]	2013 - 2015	1,106	1	Sites	0.09	0.0056912	0.00569	0.00569	0.0056912	ug/L	
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	20	Sites	95	0.1394549	0.723	1.43	1.978684	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.000000148	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.54608	days	
Boiling point	OPERA QSAR	307.772	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	3.19E-10	mmHg	
Vapor pressure	TEST QSAR	0.000000125	mmHg	
Solubility in water	OPERA QSAR	0.00889126	mol/L	
Solubility in water	TEST QSAR	0.018239	mol/L	
Bioconcentration factor	OPERA QSAR	1.585	no units	
Bioconcentration factor	TEST QSAR	0.179061	no units	
Henry's Law constant	OPERA QSAR	7.37E-11	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	-1.51937	no units	

Acyclovir

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
49	Bexfield, L.M., P.L. Toccalino, K. Belitz, W.T. Foreman, and E.T. Furlong. 2019. Hormones and pharmaceuticals in groundwater used as a source of drinking water across the United States. Environmental Science and Technology 53: 2950-2960.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. Environmental science & technology, 51(9), 4792-4802.
77	FDA. 2018. Drugs @ FDA: FDA Approved Drug Products. U.S. Food and Drug Administration (FDA). https://www.accessdata.fda.gov/scripts/cder/daf/ .
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. Science of The Total Environment. v581-582, (909-922).
150	NIH. 2018. DailyMed Database. U.S. National Library of Medicine, National Institutes of Health (NIH). https://dailymed.nlm.nih.gov/dailymed/ .
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. Science of the Total Environment, 636, 69-79.

Alachlor ethanesulfonic acid (ESA)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Alachlor ethanesulfonic acid (ESA)
CASRN:	142363-53-9
DTXSID:	DTXSID6037485
Use:	Pesticide degradate
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.018

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	non-cancer effects	3	7

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	70	hematological effects including decreased erythrocyte count, hemolytic anemia, decreased hemoglobin, decreased hematocrit and red cells, increased MCH and MCHC, and decreased body weight and body weight gain	general population	MDH	2016

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
1.26	90th Percentile	Finished Water	UCMR2	2008-2010

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X	X	X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Alachlor ethanesulfonic acid (ESA)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.012	mg/kg/day	MDH 2016	Heydens et al. 1996; EPA 1998; WDHFS 2005	hematological effects including decreased erythrocyte count, hemolytic anemia, decreased hemoglobin, decreased hematocrit and red cells, increased MCH and MCHC, and decreased body weight and body weight gain	general population	33.8	71.0	[140]	

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Chronic Health-Based Guidance Value	0.05	mg/L	MN DOH	
Short-Term/Subchronic Health-Based Guidance Value	0.1	mg/L	MN DOH	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.011885	mol/kg	TEST QSAR	
Ames mutagenicity test	0.566	no units	TEST QSAR	
Developmental toxin test	1.193	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

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Alachlor ethanesulfonic acid (ESA)
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
			Prevalence					Magnitude			
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010	1,198	3	Sites	0.25	1	1.2	1.26	1.3	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
			Prevalence					Magnitude			
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	2,708	553	Sites	20	0.015	0.15	1.1	34	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	418	163	Sites	39	0.015	0.14	0.81	18.9	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	2,290	390	Sites	17	0.02	0.215	2.38	34	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
			Prevalence					Magnitude			
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	4	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	11	Sites	65	0.0028	0.017	0.0989	1.443	ug/L	
Community Water System Survey (CWSS) (Finished) [178]	2006	1	NA	Sites			0.35	0.35		ug/L	
Ambient Water											
			Prevalence					Magnitude			
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	2	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	351	38	Sites	11	0.02	0.06	0.586	1.68	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	822	188	Sites	23	0.02	0.435	1.88	7.07	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,173	226	Sites	19	0.02	0.238	1.55	7.07	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	159	Sites	69	0.0028	0.0208	0.14	4.31	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	152	Sites	69	0.0028	0.0562	0.609	4.31	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	8	Sites	67	0.0028	0.017	0.1	1.037	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	56	1	Sites	1.79	0.064	0.064	0.064	0.064	ug/L	
Community Water System Survey (CWSS) (Ambient) [178]	2006	1	NA	Sites			0.28	4.19		ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	8	Sites	21	0.02	0.025	0.119	0.21	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	33	Sites	5.65	0.12	0.331	1.49	3.37	ug/L	
Waste Water Effluent											
			Prevalence					Magnitude			
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Expcast exposure		9.98E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.29515	days	
Boiling point	OPERA QSAR	314.576	degree C	
Boiling point	TEST QSAR	380.403	degree C	
Vapor pressure	OPERA QSAR	0.000000182	mmHg	
Vapor pressure	TEST QSAR			
Solubility in water	OPERA QSAR	0.0112346	mol/L	
Solubility in water	TEST QSAR	0.00360579	mol/L	
Bioconcentration factor	OPERA QSAR	9.61239	no units	
Bioconcentration factor	TEST QSAR	7.53356	no units	
Henry's Law constant	OPERA QSAR	5.21E-10	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.78498	no units	

Alachlor ethanesulfonic acid (ESA)

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
140	MDH. 2016. Toxicological Summary for: Alachlor ESA and Alachlor OXA. Health Based Guidance for Water. Minnesota Department of Health (MDH), Environmental Health Division, Health Risk Assessment Unit, St Paul, MN.
178	USEPA (US Environmental Protection Agency). (2009). 2006 Community Water System Survey. Overview, 57.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Alachlor oxanilic acid (OA)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Alachlor oxanilic acid (OA)
CASRN:	171262-17-2
DTXSID:	DTXSID1037486
Use:	Pesticide degradate
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.004

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	non-cancer effects	1	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	70	hematological effects including decreased erythrocyte count, hemolytic anemia, decreased hemoglobin, decreased hematocrit and red cells, increased MCH and MCHC, and decreased body weight and body weight gain	general population	MDH	2016

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.28	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X	X	X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Alachlor oxanilic acid (OA)

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.012	mg/kg/day	MDH 2016	Heydens et al. 1996; EPA 1998; WDHFS 2005	hematological effects including decreased erythrocyte count, hemolytic anemia, decreased hemoglobin, decreased hematocrit and red cells, increased MCH and MCHC, and decreased body weight and body weight gain	general population	33.8	71.0	[140]	

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Chronic Health-Based Guidance Value	0.05	mg/L	MN DOH	
Short-Term/Subchronic Health-Based Guidance Value	0.1	mg/L	MN DOH	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0100693	mol/kg	TEST QSAR	
Ames mutagenicity test	0.532	no units	TEST QSAR	
Developmental toxin test	0.974	no units	TEST QSAR	

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Alachlor oxanilic acid (OA)

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence						Magnitude			
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010	1,198	0	Sites	0					ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
		Prevalence						Magnitude			
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	2,724	271	Sites	9.95	0.0043	0.05	0.28	36	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	422	154	Sites	36	0.0043	0.0494	0.2	13.7	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	2,302	117	Sites	5.08	0.01	0.114	1.06	36	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence						Magnitude			
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	4	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	7	Sites	41	0.00102	0.008	0.052	0.4995	ug/L	
Bradley et al. 2018 (Finished) [53]	2016	26	1	Sites	3.85	0.32	0.32	0.32	0.32	ug/L	
Community Water System Survey (CWSS) (Finished) [178]	2006	1	NA	Sites							
Ambient Water											
		Prevalence						Magnitude			
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	2	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	355	44	Sites	12	0.0074	0.03	0.105	0.27	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	830	83	Sites	10	0.0157	0.0671	1.49	3.79	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,185	127	Sites	11	0.0074	0.04	0.308	3.79	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	98	Sites	43	0.001016	0.008	0.046	5.38	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	92	Sites	42	0.001016	0.017	0.338	5.38	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	6	Sites	50	0.00102	0.008	0.041	0.102	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	56	0	Sites	0						
Community Water System Survey (CWSS) (Ambient) [178]	2006	1	NA	Sites			1.85	1.85		ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	1	Sites	2.63	0.02	0.02	0.02	0.02	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	11	Sites	1.88	0.0374	0.122	0.92	1.45	ug/L	
Waste Water Effluent											
		Prevalence						Magnitude			
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Exposure exposure		0.0000001	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.46456	days	
Boiling point	OPERA QSAR	320.913	degree C	
Boiling point	TEST QSAR	368.012	degree C	
Vapor pressure	OPERA QSAR	0.000000225	mmHg	
Vapor pressure	TEST QSAR	0.00000076	mmHg	
Solubility in water	OPERA QSAR	0.00516306	mol/L	
Solubility in water	TEST QSAR	0.0033037	mol/L	
Bioconcentration factor	OPERA QSAR	2.90221	no units	
Bioconcentration factor	TEST QSAR	1.30918	no units	
Henry's Law constant	OPERA QSAR	7E-10	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.60613	no units	

Alachlor oxanilic acid (OA)

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. <i>Environmental science & technology</i> , 52(23), 13972-13985.
140	MDH. 2016. Toxicological Summary for: Alachlor ESA and Alachlor OXA. Health Based Guidance for Water. Minnesota Department of Health (MDH), Environmental Health Division, Health Risk Assessment Unit, St Paul, MN.
178	USEPA (US Environmental Protection Agency). (2009). 2006 Community Water System Survey. Overview, 57.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Aldrin

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Aldrin
CASRN:	309-00-2
DTXSID:	DTXSID8020040
Use:	Former insecticide
Chemical Notes:	Canceled pesticide. Last end of use date: 5/15/1987.

Is the contaminant on any lists?	
CERCLA	X
FIFRA	X
Human Neurotoxics	X
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	330

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	carcinogen with linear MOA	1	6

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.002	liver carcinomas	general population	OW	2003

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.667	90th Percentile	Finished Water	UCM2	1993 - 1997

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X			

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
X	Not Applicable	Not Applicable
Basis		

Aldrin may cause adverse health effects in humans, specifically neurotoxicity to the central nervous system [a,b,c]. However, its occurrence in drinking water at frequencies or concentrations significant for public health concern is low; occurrence estimates from a cross-section of States with UCM data are very low with only 0.006% of all samples and 0.02% of PWSs showing detections where the HRL is 0.002 ug/L [d,e]. Furthermore, occurrence of aldrin in drinking water supplies is likely to decrease in the coming years, since the chemical is no longer produced or used commercially [f].

[a] Jager, 1970 [113]; [b] ACGIH, 1984 [6]; [c] ATSDR, 2000 [16]; [d] USEPA, 2001 [239]; [e] USEPA, 2001 [247]; [f] ATSDR, 1993 [1]; as cited in USEPA, 2001 [179]

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0003	mg/kg/day	IRIS 1987	Fitzhugh et al. 1964	liver toxicity (lesions)	general population	33.8	0.178	[190]	
Reference Dose (RfD) or Equivalent	0.0003	mg/kg/day	ATSDR 2002	Fitzhugh et al. 1964	histopathological lesions in the liver	general population	33.8	0.178	[18]	
Reference Dose (RfD) or Equivalent	0.0003	mg/kg/day	OW 2003	Fitzhugh et al. 1964	histopathological lesions in the liver	general population	33.8	0.178	[255]	NOTE: canceled registration, OPP does not provide a publicly-available health assessment for aldrin; no new information has been published by EPA regarding health effects of aldrin - refer to the 2003 RegDet supporting documentation
Cancer Slope Factor (CSF)	17	(mg/kg/day)^-1	IRIS 1987	Davis, 1965; NCI, 1978	liver carcinoma	general population	33.8	0.00174	[190]	
Cancer Slope Factor (CSF)	17	(mg/kg/day)^-1	OW 2003	Davis, 1965; Epstein, 1975; NCI, 1978	liver carcinoma	general population	33.8	0.00174	[255]	NOTE: canceled registration, OPP does not provide a publicly-available health assessment for aldrin; no new information has been published by EPA regarding health effects of aldrin - refer to the 2003 RegDet supporting documentation
Cancer Classification (CC)	B2		IRIS 1987						[190]	
Cancer Classification (CC)	B2		OW 2003						[255]	NOTE: canceled registration, OPP does not provide a publicly-available health assessment for aldrin; no new information has been published by EPA regarding health effects of aldrin - refer to the 2003 RegDet supporting documentation
			OPP							

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	0.0003	mg/L	EPA DWSHA 2018	
Cancer Slope Factor (CSF)	17	(mg/kg/day)^-1	CalEPA OEHHA Chemical Database	
Drinking Water Guideline Value	0.0003	mg/L	WHO Drinking Water Quality Guidelines	
Human Health Ambient Water Quality Criteria	7.7E-10	mg/L	EPA Human Health Criteria for CWA	
Inhalation Unit Risk (IUR)	0.0049	(ug/m3)^-1	EPA IRIS	
Inhalation Unit Risk (IUR)	0.0049	ug/m^3	CalEPA OEHHA Chemical Database	
Lifetime Health Advisory	0.00002	mg/L	EPA DWSHA 2018	
Subchronic Provisional RfD	0.00004	mg/kg/day	EPA PPRTV	
Cancer Classification (CC)	2A	no units	WHO IARC	
Cancer Classification (CC)	Female.Mice N	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats E	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice P	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats E	no units	HHS NTP	

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	39	mg/kg	NIH HSDB	min
LD50	45	mg/kg	NIH HSDB	max
Percent of active toxicant in vitro assays tested	30.45	percent	EPA Chemistry Dashboard	
TD50	0.741	mg/kg/day	NIH CPDB	min
TD50	466	mg/kg/day	NIH CPDB	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.00010641	mol/kg	TEST QSAR	
Ames mutagenicity test	0.166	no units	TEST QSAR	
Developmental toxin test	0.493	no units	TEST QSAR	

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
The full citation for the critical study is provided in the corresponding health assessment.
PECO = Population, Exposure, Comparator, Outcome.

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Aldrin
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OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997	12,165	2	Sites	0.02	0.46	0.575	0.667	0.69	ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	192	2	Sites	1.04	0.0012	0.0256	0.0402	0.05	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	84	2	Sites	2.38	0.0012	0.0256	0.0402	0.05	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	108	0	Sites	0						

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)	7	15,373	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	169	0	Sites	0						
Drinking Water Monitoring Data - MA (Finished)	2006 - 2020	822	1	Sites	0.12	0.011	0.011	0.011	0.011	ug/L	
Drinking Water Monitoring Data - WA (Finished)	2006 - 2011	660	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	10	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	1,551	1	Sites	0.06	0.084	0.084	0.084	0.084	ug/L	
Drinking Water Monitoring Data - FL (Source)	2006 - 2011	1	0	Sites	0						
Drinking Water Monitoring Data - MA (Source)	2006 - 2020	78	0	Sites	0						
Drinking Water Monitoring Data - PA (Source)	2006 - 2011	3	1	Sites	33	0.044	0.044	0.044	0.044	ug/L	
Drinking Water Monitoring Data - WA (Source)	2006 - 2011	738	0	Sites	0						
Drinking Water Monitoring Data - WI (Source)	2012-2019	92	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	126	6	Sites	4.76	0.0016	0.011	0.08	0.207	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	297	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	423	6	Sites	1.42	0.0016	0.011	0.08	0.207	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	123	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	113	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	10	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	94	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exposure exposure		0.00000127	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)	< LOD	ng/g	
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	363.235	days	
Boiling point	OPERA QSAR	323.744	degree C	
Boiling point	TEST QSAR	355.96	degree C	
Vapor pressure	OPERA QSAR	0.0000876	mmHg	
Vapor pressure	TEST QSAR	0.0000577	mmHg	
Solubility in water	OPERA QSAR	7.58E-08	mol/L	
Solubility in water	TEST QSAR	0.00000117	mol/L	
Bioconcentration factor	OPERA QSAR	6522.68	no units	
Bioconcentration factor	TEST QSAR	4017.91	no units	
Henry's Law constant	OPERA QSAR	0.0000518	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	6.31366	no units	

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Reference Number	Full Reference
1	Agency for Toxic Substances and Disease Registry (ATSDR). 1993. Toxicological Profile for Aldrin/Dieldrin (update). Atlanta: Agency for Toxic Substances and Disease Registry. 184 pp
6	American Conference of Governmental Industrial Hygienists (ACGIH). 1984. Documentation of the Threshold Limit Values for Substances in Workroom Air. Third Edition. Cincinnati, OH: ACGIH. 139 pp.
16	ATSDR. 2000. Toxicological Profile for Aldrin/Dieldrin (Update). Atlanta, GA: Agency for Toxic Substances and Disease Registry. 280 pp.
18	ATSDR. 2002. Toxicological Profile for Aldrin/Dieldrin. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
113	Jager, K.W. 1970. Aldrin, Dieldrin, Endrin and Telodrin: An Epidemiological and Toxicological Study of Long-Term Occupational Exposure. New York: Elsevier Publishing Company. 234 pp.
179	USEPA, 2001. Regulatory Determination Support Document for Aldrin and Dieldrin. EPA 815 R-01-011.
190	USEPA. 1987. Chemical Assessment Summary, Aldrin. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, DC.
239	USEPA. 2001. Analysis of National Occurrence of the 1998 Contaminant Candidate List Regulatory Determination Priority Contaminants in Public Water Systems. Office of Water. EPA report 815-D-01-002. 77 pp.
247	USEPA. 2001. Occurrence of Unregulated Contaminants in Public Water Systems: An Initial Assessment. Office of Water. EPA report 815-P-00-001. Office of Water. 50 pp.
255	USEPA. 2003. Contaminant Candidate List Regulatory Determination Support Document for Aldrin and Dieldrin. U.S Environmental Protection Agency, Office of Water, Standards and Risk Management Division, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

alpha-Hexachlorocyclohexane

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	alpha-Hexachlorocyclohexane
CASRN:	319-84-6
DTXSID:	DTXSID2020684
Use:	Component of benzene hexachloride (BHC) former insecticide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	4.6

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	carcinogen with linear MOA	5	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.005	hepatic nodules and hepatocellular carcinomas	general population	IRIS	1987

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.0229	90th Percentile	Finished Water	UCMR4	2018-2019

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
		X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

alpha-Hexachlorocyclohexane
CCL 5 Contaminant Information Sheet
HEALTH EFFECTS DATA

EPA-OGWDW and OST

July 2021

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.008	mg/kg/day	ATSDR 2005	Fitzhugh et al. 1950	Hepatic effects: hepatic histopathological changes	general population	33.8	47.3	[22]	
Cancer Slope Factor (CSF)	6.3	(mg/kg/day) ⁻¹	IRIS 1987	Ito et al., 1973a	hepatic nodules and hepatocellular carcinomas	general population	33.8	0.00470	[187]	NOTE: this compound is a byproduct of production of gamma HCH (Lindane), which is no longer registered for use as a pesticide in the US
Cancer Classification (CC)	B2		IRIS 1987						[187]	NOTE: this compound is a byproduct of production of gamma HCH (Lindane), which is no longer registered for use as a pesticide in the US

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Cancer Slope Factor (CSF)	2.7	(mg/kg/day) ⁻¹	CalEPA OEHHA Chemical Database	
Human Health Ambient Water Quality Criteria	0.00000036	mg/L	EPA Human Health Criteria for CWA	
Inhalation Unit Risk (IUR)	0.0018	(ug/m ³) ⁻¹	EPA IRIS	
Inhalation Unit Risk (IUR)	0.00077	ug/m ³	CalEPA OEHHA Chemical Database	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	177	mg/kg	NIH HSDB	
Percent of active toxcast in vitro assays tested	14.47	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0012794	mol/kg	TEST QSAR	
Ames mutagenicity test	0.233	no units	TEST QSAR	
Developmental toxin test	0.229	no units	TEST QSAR	

alpha-Hexachlorocyclohexane
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019	3,649	20	Sites	0.55	0.01	0.0135	0.0229	0.067	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	8,230	23	Sites	0.28	4.00E - 04	0.0118	0.0646	0.21	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	1,820	20	Sites	1.1	4.00E - 04	0.0115	0.067	0.21	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	6,410	3	Sites	0.05	0.0012	0.0327	0.0511	0.059	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	34	1	Sites	2.94	0.012	0.012	0.012	0.012	ug/L	
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	6	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	253	1	Sites	0.4	0.01	0.01	0.01	0.01	ug/L	
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	242	4	Sites	1.65	0.01	0.01	0.02	0.06	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	725	2	Sites	0.28	0.0012	0.0014	0.00185	0.0021	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	967	6	Sites	0.62	0.0012	0.01	0.01	0.06	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	6	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	6	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.000000102	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	18.5267	days	
Boiling point	OPERA QSAR	236.373	degree C	
Boiling point	TEST QSAR	276.233	degree C	
Vapor pressure	OPERA QSAR	0.00355971	mmHg	
Vapor pressure	TEST QSAR	0.0106905	mmHg	
Solubility in water	OPERA QSAR	0.00000849	mol/L	
Solubility in water	TEST QSAR	0.0000484	mol/L	
Bioconcentration factor	OPERA QSAR	1506.74	no units	
Bioconcentration factor	TEST QSAR	157.761	no units	
Henry's Law constant	OPERA QSAR	0.00000734	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.66038	no units	

alpha-Hexachlorocyclohexane

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
22	ATSDR. 2005. Toxicological Profile for Alpha-, Beta-, Gamma-, and Delta-Hexachlorocyclohexane. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
187	USEPA. 1987. Chemical Assessment Summary alpha-Hexachlorocyclohexane (alpha-HCH); CASRN 319-84-6. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, DC.

Ametryn

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Ametryn
CASRN:	834-12-8
DTXSID:	DTXSID1023869
Use:	Herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.000025

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	non-cancer effects	9	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	400	degenerative and inflammatory liver effects	general population	OPP	2017

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.0101	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Ametryn

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.072	mg/kg/day	OPP 2017	O'Connor 1987	degenerative and inflammatory liver effects	general population	33.8	426	[376]	
Cancer Classification (CC)	S		OPP 2017						[376]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	9	mg/L	EPA DWSHA 2018	
Lifetime Health Advisory	0.06	mg/L	EPA DWSHA 2018	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	3170	mg/kg	NIH HSDB	max
LD50	508	mg/kg	NIH HSDB	min
LOAEL	131	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	20.9	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	14	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	2.5	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	7.08	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	36.099998	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	7.6	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0045604	mol/kg	TEST QSAR	
Ames mutagenicity test	0.207	no units	TEST QSAR	
Developmental toxin test	0.608	no units	TEST QSAR	

July 2021

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.35089	days	
Boiling point	OPERA QSAR	343.891	degree C	
Boiling point	TEST QSAR	360.753	degree C	
Vapor pressure	OPERA QSAR	0.00000211	mmHg	
Vapor pressure	TEST QSAR	0.000000871	mmHg	
Solubility in water	OPERA QSAR	0.000630959	mol/L	
Solubility in water	TEST QSAR	0.00110662	mol/L	
Bioconcentration factor	OPERA QSAR	6.50043	no units	
Bioconcentration factor	TEST QSAR	5.28445	no units	
Henry's Law constant	OPERA QSAR	2.36E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.94353	no units	

Ametryn

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
376	USEPA. 2017. Ametryn - Preliminary Human Health Risk Assessment for Registration Review. EPA-HQ-OPP-2013-0249-0022. DP No. D440785. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Ammonia

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Ammonia
CASRN:	7664-41-7
DTXSID:	DTXSID0023872
Use:	Chemical intermediate; defoliant; antifungal agent for produce
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
		1	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
1748	90th Percentile	Finished Water	DW Monitoring	2006 - 2011

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Ammonia

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Cancer Classification (CC)	D		OW 1992						[219]	
			PPRTV 2005						[263]	
			WHO 2003						[437]	
			HC 2013						[100]	NOTE: All qualifying assessments decline to quantify oral toxicity
			ATSDR 2004						[19]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Reproductive	10	Zhang, 2018	Renal, Immune, Systemic	50	Zhang, 2018	2015-09-01	2020-03-25	4315	5	20	1

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute inhalation Minimal Risk Level (MRL)	1.7	ppm	CDC ATSDR	
Chronic inhalation Minimal Risk Level (MRL)	0.1	ppm	CDC ATSDR	
Lifetime Health Advisory	30	mg/L	EPA DWSHA 2018	
Reference Concentration (RfC)	0.5	mg/m ³	EPA IRIS	
Reference Concentration (RfC)	200	ug/m ³	CalEPA OEHHA Chemical Database	
Subchronic RfC	0.1	mg/m ³	EPA PPRTV	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	350	mg/kg	NIH HSDB	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity test			TEST QSAR	
Developmental toxin test			TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Ammonia
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	10	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	10	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)	50	158,252,384	Chemical Data Reporting (CDR) Results (EPA) (2016)	308 - 408

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - WA (Finished)	2006 - 2011	18	7	Sites	39	104	1230	1748	2020	ug/L	
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	48		390		790	ug/L	
Ambient Water											
Drinking Water Monitoring Data - WA (Source)	2006 - 2011	13	6	Sites	46	19	160	1001	1460	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	64		50		240	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exposure			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Ammonia

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
19	ATSDR. 2004. Toxicological Profile for Ammonia. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. Science of The Total Environment. v581-582, (909-922).
100	Health Canada. 2013 Guideline Technical Document Ammonia. Health Canada (HC), Ottawa, Ontario, Canada.
219	USEPA. 1992. Drinking Water Health Advisories: Ammonia. U.S. Environmental Protection Agency, Office of Water, Health and Ecological Criteria Division, Washington, DC.
263	USEPA. 2005. Provisional Peer-Reviewed Toxicity Values for Ammonia. U.S. Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment, Superfund Health Risk Technical Support Center, Cincinnati, OH.
437	WHO. 2003. Ammonia in Drinking-water. Background document for development of WHO Guidelines for Drinking-water Quality. World Health Organization (WHO), Geneva, Switzerland.

ANDROSTENEDIONE

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	ANDROSTENEDIONE
CASRN:	63-05-8
DTXSID:	DTXSID8024523
Use:	
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	X
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.000012

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	reproductive and developmental effects	9	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	100	hormone-related effects on male fertility (decreased number of sperm per mg cauda epididymis)	general population	ECHA	2011

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.00116	90th Percentile	Finished Water	UCMR3	2013-2015

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

ANDROSTENEDIONE

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.025	mg/kg/day	ECHA 2011	NTP 2010; Blystone et al., 2011	hormone-related effects on male fertility (decreased number of sperm per mg cauda epididymis)	general population	33.8	148	[70]	NOTE: An ECHA Derived No Effect Level (DNEL) is used in place of the RfD

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Developmental, Reproductive	1	Sprando, 2004	Systemic, Hepatic,	60	Wiesenfeld, 2006,		2020-04-14	2928	10	18	6

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Cancer Classification (CC)	Female.Mice P	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats EE	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice P	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats EE	no units	HHS NTP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1000	mg/kg	NIH HSDB	max
LD50	500	mg/kg	NIH HSDB	min
Percent of active toxcast in vitro assays tested	14.15	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0168267	mol/kg	TEST QSAR	
Ames mutagenicity test	-0.062	no units	TEST QSAR	
Developmental toxin test	0.958	no units	TEST QSAR	

ANDROSTENEDIONE

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015	1,201	77	Sites	6.41	3.00E - 04	0.00047	0.00116	0.0041	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	529	7	Sites	1.32	0.00041	0.00088	0.00217	0.00456	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	29	6	Sites	21	0.00041	0.00072	0.00111	0.00114	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	500	1	Sites	0.2	0.00456	0.00456	0.00456	0.00456	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	252	30	Sites	12	0.00032	0.00124	0.003	0.00828	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	354	3	Sites	0.85	0.00225	0.00238	0.00321	0.00356	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	606	33	Sites	5.45	0.00032	0.00138	0.0032	0.00828	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	6	Sites	16	0.001218	0.00283	0.00458	0.006126	ug/L	
Bexfield et al. 2019 (Groundwater) [49]	2013 - 2015	1,094	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	2	Sites	100	0.00046	0.00059	0.000694	0.00072	ug/L	
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	19	Sites	90	0.000789	0.00209	0.00553	0.007467	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.00000022	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	58.1212	days	
Boiling point	OPERA QSAR	346.557	degree C	
Boiling point	TEST QSAR	358.124	degree C	
Vapor pressure	OPERA QSAR	0.000000234	mmHg	
Vapor pressure	TEST QSAR	0.000000441	mmHg	
Solubility in water	OPERA QSAR	0.000161292	mol/L	
Solubility in water	TEST QSAR	0.000065	mol/L	
Bioconcentration factor	OPERA QSAR	37.295	no units	
Bioconcentration factor	TEST QSAR	84.3335	no units	
Henry's Law constant	OPERA QSAR	0.000000295	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.87316	no units	

ANDROSTENEDIONE

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
49	Bexfield, L.M., P.L. Toccalino, K. Belitz, W.T. Foreman, and E.T. Furlong. 2019. Hormones and pharmaceuticals in groundwater used as a source of drinking water across the United States. Environmental Science and Technology 53: 2950-2960.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. Environmental science & technology, 51(9), 4792-4802.
70	ECHA. 2011. Registration Dossier for Androst-4-ene-3,17-dione. European Chemicals Agency (ECHA), Helsinki, Finland. https://echa.europa.eu/registration-dossier/-/registered-dossier/13632/1 Accessed 5/14/2020.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. Science of the Total Environment, 636, 69-79.

Anthraquinone

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Anthraquinone
CASRN:	84-65-1
DTXSID:	DTXSID3020095
Use:	Basis for the production of a large number of acid and base dyes, vat dyes, disperse dyes, and reactive dyes.
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.36

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	carcinogen with linear MOA	9	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.8	increase in hepatocellular adenoma, carcinoma, or hepatoblastoma in male mice	general population	PPRTV	2011

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.284	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Anthraquinone

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.002	mg/kg/day	PPRTV 2011	NTP (2005b)	pathology in several organs, including the liver, kidney, and spleen, in male and female F344 rats.	general population	33.8	11.8	[323]	
Cancer Slope Factor (CSF)	0.039	(mg/kg/day) ⁻¹	PPRTV 2011	NTP (2005b)	The increase in hepatocellular adenoma, carcinoma, or hepatoblastoma in male mice	general population	33.8	0.759	[323]	
Cancer Classification (CC)	L		PPRTV 2011						[323]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Immune, Renal	3.2	Dodd, 2013	Whole Body, Hepatic	3.2	Dodd, 2013	2010-02-01	2020-01-15	847	1	1	1

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Subchronic Provisional RfD	0.01	mg/kg/day	EPA PPRTV	
Cancer Classification (CC)	2B	no units	WHO IARC	
Cancer Classification (CC)	Female.Mice P	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats P	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice P	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats SE	no units	HHS NTP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	5000	mg/kg	NIH HSDB	
Percent of active toxcast in vitro assays tested	1.28	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0150314	mol/kg	TEST QSAR	
Ames mutagenicity test	0.714	no units	TEST QSAR	
Developmental toxin test	0.517	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Anthraquinone

CCL 5 Contaminant Information Sheet

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	567	28	Sites	4.94	0.01	0.05	0.284	0.78	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	88	28	Sites	32	0.01	0.05	0.284	0.78	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	479	0	Sites	0						

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	10M - 50M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	716	197	Sites	28	0.01	0.05	0.34	2.98	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	690	12	Sites	1.74	0.02	0.05	0.081	0.11	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,406	209	Sites	15	0.01	0.05	0.34	2.98	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	16	Sites	42	0.0128	0.0346	0.0522	0.0782	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	11	Sites	52	0.08	0.081	0.0818	0.082	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exposure exposure		0.00000341	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	18.7227	days	
Boiling point	OPERA QSAR	371.769	degree C	
Boiling point	TEST QSAR	357.578	degree C	
Vapor pressure	OPERA QSAR	0.000000108	mmHg	
Vapor pressure	TEST QSAR	0.000000198	mmHg	
Solubility in water	OPERA QSAR	0.0000094	mol/L	
Solubility in water	TEST QSAR	0.00000416	mol/L	
Bioconcentration factor	OPERA QSAR	28.7099	no units	
Bioconcentration factor	TEST QSAR	101.158	no units	
Henry's Law constant	OPERA QSAR	6.82E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.23488	no units	

Anthraquinone

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
323	USEPA. 2011. Provisional Peer Reviewed Toxicity Values for 9,10-Anthraquinone(CASRN 84-65-1). EPA/690/R-11/007F. U.S. Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment, Superfund Health Risk Technical Support Center, Cincinnati, OH.

Atenolol

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Atenolol
CASRN:	29122-68-7
DTXSID:	DTXSID2022628
Use:	antihypertensive; antianginal; antiarrhythmic
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.088

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	non-cancer effects	8	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	1	lowest therapeutic dose: beta blocker/blood pressure reduction	bottle-fed infants	FDA; NIH	2018; 2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.08778	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis
Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Atenolol

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.000208333	mg/kg/day	FDA 2018; NIH 2018	Caraco Pharmaceutical Laboratories, LTD.	lowest therapeutic dose:beta blocker/blood pressure reduction	bottle-fed infants	151	1.40	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels
Reference Dose (RfD) or Equivalent	0.000208333	mg/kg/day	FDA 2018; NIH 2018	Caraco Pharmaceutical Laboratories, LTD.	lowest therapeutic dose:beta blocker/blood pressure reduction	general population	33.8	4.90	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Maximum Recommended Daily Dose	3.33	mg/kg/day	FDA	
Screening level for pharmaceutical - general population	0.004901961	mg/L	EPA Office of Water	
Screening level for pharmaceutical - infants	0.001388889	mg/L	EPA Office of Water	

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	2000	mg/kg	NIH HSDB	min
LD50	3000	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	0.7	percent	EPA Chemistry Dashboard	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0089537	mol/kg	TEST QSAR	
Ames mutagenicity test	0.008	no units	TEST QSAR	
Developmental toxin test	0.512	no units	TEST QSAR	

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OCCURRENCE DATA

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	557	12	Sites	2.15	0.00166	0.0225	0.0878	0.249	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	75	12	Sites	16	0.00166	0.0225	0.0878	0.249	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	482	0	Sites	0						

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Padhye et al. 2013 (Finished) [155]	2009 - 2010	8	1	Samples	12	0	0		3.41e-05 +/- 0	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	205	41	Sites	20	0.00096	0.0194	0.149	0.515	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	401	3	Sites	0.75	0.0081	0.00869	0.00872	0.00874	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	606	44	Sites	7.26	0.00096	0.0179	0.148	0.515	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	4		0.0298		0.0298	ug/L	
Batt et al. 2016 (Ambient) [46]	2008 - 2009	182	88	Sites	48	0.0019	0.0115	0.0653	0.1864	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	15	Sites	39	0.0079363	0.171	0.422	0.5510741	ug/L	
Bexfield et al. 2019 (Groundwater) [49]	2013 - 2015	1,106	1	Sites	0.09	0.0087356	0.00874	0.00874	0.0087356	ug/L	
Padhye et al. 2013 (Ambient) [155]	2009 - 2010	8	0	Samples	0	0	0		0	ug/L	
Batt et al. (2008) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.035	ug/L	
Benotti et al. (2009) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.036	ug/L	
Conkle et al. (2008) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.02	ug/L	
Vanderford et al. (2006) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.859	ug/L	
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	21	Sites	100	0.0417468	0.579	1.47	3.233452	ug/L	
Kostich et al. 2014 (Wastewater) [126]	not reported	50	48	Sites	96	0.0085	0.596	1.73	3.0733	ug/L	
Batt et al. (2008) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						0.96	ug/L	
Conkle et al. (2008) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						1.442	ug/L	
Palmer et al. (2008) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						14.2	ug/L	
Vanderford et al. (2006) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						3.06	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Exposcast exposure		0.000000188	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.34423	days	
Boiling point	OPERA QSAR	296.692	degree C	
Boiling point	TEST QSAR	384.93	degree C	
Vapor pressure	OPERA QSAR	1.11E-09	mmHg	
Vapor pressure	TEST QSAR	2.78E-08	mmHg	
Solubility in water	OPERA QSAR	0.0489742	mol/L	
Solubility in water	TEST QSAR	0.0201372	mol/L	
Bioconcentration factor	OPERA QSAR	1.41866	no units	
Bioconcentration factor	TEST QSAR	2.208	no units	
Henry's Law constant	OPERA QSAR	4.35E-10	atm-m^3/mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	0.0522496	no units	

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Reference Number	Full Reference
46	Batt, A. L., Kincaid, T. M., Kostich, M. S., Lazorchak, J. M., & Olsen, A. R. (2016). Evaluating the extent of pharmaceuticals in surface waters of the United States using a National-scale Rivers and Streams Assessment survey. <i>Environmental toxicology and chemistry</i> , 35(4), 874-881.
49	Bexfield, L.M., P.L. Toccalino, K. Belitz, W.T. Foreman, and E.T. Furlong. 2019. Hormones and pharmaceuticals in groundwater used as a source of drinking water across the United States. <i>Environmental Science and Technology</i> 53: 2950-2960.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
77	FDA. 2018. Drugs @ FDA: FDA Approved Drug Products. U.S. Food and Drug Administration (FDA). https://www.accessdata.fda.gov/scripts/cder/daf/ .
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
126	Kostich MS, et al. 2014 Concentrations of prioritized pharmaceuticals in effluents from 50 large wastewater treatment plants in the US and implications for risk estimation. <i>Environ Pollut</i> . 2014 Jan;184:354-9. doi: 10.1016/j.envpol.2013.09.013. Epub 2013 Oct 3. PMID: 24095705.
127	Kostich, MS, et al., 2010. Predicting variability of aquatic concentrations of human pharmaceuticals. <i>Sci. Total Environ</i> . 408 (20), 4504e4510.
150	NIH. 2018. DailyMed Database. U.S. National Library of Medicine, National Institutes of Health (NIH). https://dailymed.nlm.nih.gov/dailymed/ .
155	Padhye, L.P., Yao, H., Kung'u, F.T., and Huang, C.H. Year-long evaluation on the occurrence and fate of pharmaceuticals, personal care products, and endocrine disrupting chemicals in an urban drinking water treatment plant. 2014. <i>Water Research</i> 51 (2014) 266-276.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.

Azoxystrobin

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Azoxystrobin
CASRN:	131860-33-8
DTXSID:	DTXSID0032520
Use:	Agricultural fungicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.000027

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	non-cancer effects	10	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	1000	reduced body weights in both sexes and bile duct lesions in males	general population	OPP	2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.0265	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Azoxystrobin

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.18	mg/kg/day	OPP 2018	Milburn 1995	reduced body weights in both sexes and bile duct lesions in males	general population	33.8	1070	[396]	
Cancer Classification (CC)	NL		OPP 2018						[396]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	4.5	mg/L	EPA HHBP	
Acute PAD	0.67	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	1.2	mg/L	EPA HHBP	
Health-Based Screening Level	1.2	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.18	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	5000	mg/kg	NIH HSDB	
LOAEL	25	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	500	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	150	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	22.3	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	21.17	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	211	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	250	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	22.4	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	50	mg/kg/day	EPA Toxicity Reference Database	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.001052	mol/kg	TEST QSAR	
Ames mutagenicity test	0.199	no units	TEST QSAR	
Developmental toxin test	0.961	no units	TEST QSAR	

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	1,763	263	Sites	15	0.00012	0.00323	0.0265	2.91	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	324	253	Sites	78	0.00012	0.00323	0.0265	2.91	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	1,439	10	Sites	0.69	0.00036	0.00121	0.0144	0.26	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	48	2,436,869	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	10	8	Sites	80	0.0013	0.0032	0.0375	0.39	ug/L	
Bradley et al. 2018 (Finished) [53]	2016	26	1	Sites	3.85	0.0218	0.0218	0.0218	0.0218	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	434	186	Sites	43	0.00013	0.0066	0.141	128	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	531	6	Sites	1.13	0.00061	0.00169	0.00654	0.0101	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	965	192	Sites	20	0.00013	0.00651	0.141	128	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	227	12	Sites	5.29	0.0013	0.0013	0.0196	0.662	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	218	3	Sites	1.38	0.0044	0.0084	0.467	0.662	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	10	9	Sites	90	0.0013	0.0013	0.0184	0.24	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	676	311	Sites	46	0.0033	0.0332	0.412	2.67	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	9	Sites	24	0.005	0.0281	0.252	0.2795	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	4	Sites	0.68	4e-04	0.0013	0.00194	0.002	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		2.46E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.28513	days	
Boiling point	OPERA QSAR	359.001	degree C	
Boiling point	TEST QSAR	474.033	degree C	
Vapor pressure	OPERA QSAR	1.89E-12	mmHg	
Vapor pressure	TEST QSAR	9.42E-11	mmHg	
Solubility in water	OPERA QSAR	0.0000121	mol/L	
Solubility in water	TEST QSAR	0.00000154	mol/L	
Bioconcentration factor	OPERA QSAR	12.6717	no units	
Bioconcentration factor	TEST QSAR			
Henry's Law constant	OPERA QSAR	3.48E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.71667	no units	

Azoxystrobin

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. <i>Environmental science & technology</i> , 52(23), 13972-13985.
396	USEPA. 2018. Azoxystrobin: Revised Human Health Draft Risk Assessment for Registration Review. EPA-HQ-OPP-2009-0835-0043. DP No. D444164. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Benfluralin

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Benfluralin
CASRN:	1861-40-1
DTXSID:	DTXSID3023899
Use:	Pre-emergent dinitroaniline herbicide used to control grasses and other weed species
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.00037

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	non-cancer effects	8	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	30	increased histopathologic lesions of the kidneys	general population	OPP	2017

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.011	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Benfluralin

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.005	mg/kg/day	OPP 2017	Moore 1996, 1998	increased histopathologic lesions of the kidneys	general population	33.8	29.6	[377]	
Cancer Classification (CC)	S		OPP 2017						[377]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Chronic Human Health Benchmark	0.03	mg/L	EPA HHBP	
Health-Based Screening Level	0.03	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.005	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	10000	mg/kg	NIH HSDB	max
LD50	5000	mg/kg	NIH HSDB	min
LOAEL	1000	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	25	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	475	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	5	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	9.87	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	25	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	5	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0156315	mol/kg	TEST QSAR	
Ames mutagenicity test	0.608	no units	TEST QSAR	
Developmental toxin test	1.142	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
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EPA - Office of Water

Benfluralin
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
			Prevalence					Magnitude			
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
			Prevalence					Magnitude			
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	10,167	152	Sites	1.5	0.001	0.004	0.011	0.205	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	2,044	133	Sites	6.51	0.001	0.0045	0.012	0.205	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	8,123	19	Sites	0.23	0.001	0.004	0.008	0.011	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	7	53,174	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	2	1,250	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
			Prevalence					Magnitude			
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	1	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
			Prevalence					Magnitude			
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	33	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	706	22	Sites	3.12	0.001	0.007	0.019	0.088	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	2,606	18	Sites	0.69	0.001	0.003	0.0068	0.014	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	3,311	40	Sites	1.21	0.001	0.005	0.018	0.088	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	149	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	139	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	1,268	16	Sites	1.26	0.007	0.0125	0.203	2.71	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	2	Sites	5.26	2.04e-05	5.69e-05	8.61e-05	9.34e-05	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	106	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Waste Water Effluent											
			Prevalence					Magnitude			
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Expocast exposure		0.000000121	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.54014	days	
Boiling point	OPERA QSAR	366.246	degree C	
Boiling point	TEST QSAR	361.409	degree C	
Vapor pressure	OPERA QSAR	0.0000568	mmHg	
Vapor pressure	TEST QSAR	0.00000446	mmHg	
Solubility in water	OPERA QSAR	0.000000357	mol/L	
Solubility in water	TEST QSAR	0.00000164	mol/L	
Bioconcentration factor	OPERA QSAR	941.493	no units	
Bioconcentration factor	TEST QSAR	234.963	no units	
Henry's Law constant	OPERA QSAR	0.0000487	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	5.26734	no units	

Benfluralin

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
377	USEPA. 2017. Benfluralin: Human Health Draft Risk Assessment for Registration Review. EPA-HQ-OPP-2011-0931-0039. DP No. D431028. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Bensulide

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Bensulide
CASRN:	741-58-2
DTXSID:	DTXSID9032329
Use:	Herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	X
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	120

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	reproductive and developmental effects	7	6

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	8	inhibition of red blood cell cholinesterase in pups	bottle-fed infants	OPP	2016

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
979		EDWC SW peak	OPP	2016

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
		X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Bensulide

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.006	mg/kg/day	OPP 2016	Barnett 2014	inhibition of red blood cell cholinesterase in pups	bottle-fed infants	151	7.95	[361]	
Cancer Classification (CC)	E		OPP 2016						[361]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	1	mg/L	EPA HHBP	
Acute PAD	0.15	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.03	mg/L	EPA HHBP	
Population-Adjusted Dose (PAD)	0.005	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1540	mg/kg	NIH HSDB	max
LD50	270	mg/kg	NIH HSDB	min
LOAEL	4	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	95	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	0.5	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	23	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	24.56	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	1	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	15	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	5	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0004446	mol/kg	TEST QSAR	
Ames mutagenicity test	0.636	no units	TEST QSAR	
Developmental toxin test	0.742	no units	TEST QSAR	

Bensulide

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	9	710,457	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Ambient Water											
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	544	320	Sites	59	0.02	0.69	6.38	142	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					
Estimated Drinking Water Concentration (EDWC) in Surface Water, Peak	2016	OPP	979	ug/L	Tier II Surface Water Concentration Calculator (SWCC) v1.106	The critical effect of cholinesterase inhibition in postnatal day 11 pups is considered a less-than-chronic response in a sensitive population. To be protective of this population, the modeled surface water peak concentration was selected as the occurrence concentration for bensulide.					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.000000142	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	104.45	days	
Boiling point	OPERA QSAR	394.639	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.000000972	mmHg	
Vapor pressure	TEST QSAR	0.00000121	mmHg	
Solubility in water	OPERA QSAR	0.0000651	mol/L	
Solubility in water	TEST QSAR	0.0000385	mol/L	
Bioconcentration factor	OPERA QSAR	4.85073	no units	
Bioconcentration factor	TEST QSAR	13.4276	no units	
Henry's Law constant	OPERA QSAR	0.00000159	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	4.0814	no units	

Bensulide

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Reference Number	Full Reference
361	USEPA. 2016. Bensulide: Human Health Risk Assessment to Support Registration Review. EPA-HQ-OPP-2008-0022-0019. DP No. D428598. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Bentazon

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Bentazon
CASRN:	25057-89-0
DTXSID:	DTXSID0023901
Use:	Former herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision

Not List

Final Hazard Quotient (HQ)

0.0007

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	reproductive and developmental effects	9	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	200	decreased pup body weight during lactation	bottle-fed infants	OPP	2014

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.14	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		
Not Applicable		

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Bentazon

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.15	mg/kg/day	OPP 2014	Suter et al. 1989	decreased pup body weight during lactation	bottle-fed infants	151	199	[335]	
Cancer Classification (CC)	E		OPP 2014						[335]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	0.3	mg/L	EPA DWSHA 2018	
Acute Health-Based Guidance Value	0.06	mg/L	MN DOH	
Acute Health-Based Guidance Value	0.4	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.03	mg/L	MN DOH	
Lifetime Health Advisory	0.2	mg/L	EPA DWSHA 2018	
Public Health Goal	0.2	mg/L	CalEPA OEHHA Public Health Goals	
Short-Term/Subchronic Health-Based Guidance Value	0.05	mg/L	MN DOH	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1139	mg/kg	NIH HSDB	max
LD50	383.2	mg/kg	NIH HSDB	min
LOAEL	13.1	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	249	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	3.2	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	62	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	3.41	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	243.3	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	86.1	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity test			TEST QSAR	
Developmental toxin test	1.022	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

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OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	7,741	470	Sites	6.07	0.00051	0.0129	0.14	19	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	1,195	273	Sites	23	0.00051	0.0121	0.12	19	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	6,546	197	Sites	3.01	0.00193	0.06	0.926	11.5	ug/L	
Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data			Number of States	Amount Released (lbs/year)	Chemical Production Data		Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	41	2,631,678	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)					Chemical Data Reporting (CDR) Results (EPA) (2016)		

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	211	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	8	Sites	47	3e-04	0.0013	0.00757	0.1	ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	2,231	3	Sites	0.13	4.6	5.3	8.42	9.2	ug/L	
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	476	96	Sites	20	0.00117	0.0104	0.0772	13.2	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	1,059	39	Sites	3.68	0.00601	0.0354	0.115	4.49	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,535	135	Sites	8.79	0.00117	0.0121	0.0874	13.2	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	79	Sites	34	3e-04	0.0013	0.0098	1.31	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	72	Sites	33	3e-04	0.00111	0.0186	1.31	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	7	Sites	58	3e-04	0.0014	0.0097	0.194	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	5	Sites	13	0.0116	0.0187	0.0624	0.088	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	13	Sites	1.88	0.0019	0.0216	0.124	0.398	ug/L	
USGS, McKenzie River, Oregon, 2012 (Ambient) [158]	2002 - 2010	126	4	Samples	3.2				0.03	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Expcast exposure		0.000000017	
Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.9037	days	
Boiling point	OPERA QSAR	303.93	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.000000943	mmHg	
Vapor pressure	TEST QSAR			
Solubility in water	OPERA QSAR	0.00219058	mol/L	
Solubility in water	TEST QSAR	0.0000541	mol/L	
Bioconcentration factor	OPERA QSAR	1.4173	no units	
Bioconcentration factor	TEST QSAR			
Henry's Law constant	OPERA QSAR	2.59E-10	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.10469	no units	

Bentazon

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
158	Reconnaissance of Land-Use Sources of Pesticides in Drinking Water, McKenzie River, Oregon. U.S. Geological Survey Scientific Investigations Report 2012–5091, 46 p. plus appendixes.
335	USEPA. 2014. Sodium Bentazon - Preliminary Human Health Risk Assessment for Registration Review. EPA-HQ-OPP-2010-0117. DP No. D417312. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.

Benzophenone

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Benzophenone
CASRN:	119-61-9
DTXSID:	DTXSID0021961
Use:	Chemical intermediate used pesticide, fragrance, varnish, antihistamines
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.00037

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	non-cancer effects	10	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	300	increased renal tubule hyperplasia	general population	MDH	2019

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.112	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Benzophenone

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.03	mg/kg/day	ECHA 2018	NTP 2006	"non-neoplastic kidney effects"	general population	33.8	178	[67]	
Reference Dose (RfD) or Equivalent	0.053	mg/kg/day	MDH 2019	National Toxicology Program, 2006	"Increased renal tubule hyperplasia"	general population	33.8	314	[146]	

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Hepatic	6.445	Hoshino, 2005	Female Reproductive, Nervous System, Gastrointestinal, Musculoskeletal, Endocrine	4199	Chhabra, 2000		2020-01-28	1221	7	15	5

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Cancer Classification (CC)	2B	no units	WHO IARC	
Cancer Classification (CC)	Female.Mice SE	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice SE	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats SE	no units	HHS NTP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	10000	mg/kg	NIH HSDB	max
LD50	1900	mg/kg	NIH HSDB	min
LOAEL	130	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	8.776	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	40.52	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	5	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	3.43	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0262422	mol/kg	TEST QSAR	
Ames mutagenicity test	0.378	no units	TEST QSAR	
Developmental toxin test	0.553	no units	TEST QSAR	

Benzophenone

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	556	74	Sites	13	0.01	0.04	0.112	0.4	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	86	29	Sites	34	0.01	0.04	0.117	0.33	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	470	45	Sites	9.57	0.01	0.06	0.105	0.4	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	1M - 10M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	713	243	Sites	34	0.01	0.05	0.13	6.83	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	688	89	Sites	13	0.01	0.025	0.076	0.34	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,401	332	Sites	24	0.01	0.04	0.12	6.83	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	12	Sites	32	0.0714	0.184	0.214	0.221	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	2	Sites	100						
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	20	Sites	95	0.051	0.17	0.34	0.36	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.0000335	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.31313	days	
Boiling point	OPERA QSAR	306.491	degree C	
Boiling point	TEST QSAR	303.142	degree C	
Vapor pressure	OPERA QSAR	0.00114394	mmHg	
Vapor pressure	TEST QSAR	0.000349945	mmHg	
Solubility in water	OPERA QSAR	0.00063623	mol/L	
Solubility in water	TEST QSAR	0.00027227	mol/L	
Bioconcentration factor	OPERA QSAR	25.7151	no units	
Bioconcentration factor	TEST QSAR	87.9023	no units	
Henry's Law constant	OPERA QSAR	0.0000011	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.27814	no units	

Benzophenone

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Reference Number	Full Reference
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
67	Danish Environmental Protection Agency. 2018. Substance Evaluation Conclusion as required by REACH Article 48 and Evaluation Report for Benzophenone EC No 204-337-6 CAS No 119-61-9. Copenhagen, Denmark. EC No 204-337-6
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
146	MDH. 2019 Toxicological Summary for Benzophenone. Minnesota Department of Health (MDH), Environmental Health Division, Health Risk Assessment Unit, St Paul, MN.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.

Bifenthrin

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Bifenthrin
CASRN:	82657-04-3
DTXSID:	DTXSID9020160
Use:	Insecticide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0012

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	reproductive and developmental effects	7	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	10	reduced locomotor activity	bottle-fed infants	OPP	2012

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.0122	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Bifenthrin

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.01	mg/kg/day	OPP 2012	Wolansky et al. 2006	reduced locomotor activity	bottle-fed infants	151	13.2	[324]	
Cancer Classification (CC)	C		OPP 2012						[324]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.07	mg/L	EPA HHBP	
Acute PAD	0.01	mg/kg/day	EPA HHBP	
Health-Based Screening Level	0.07	mg/L	Health-based screening levels from USGS	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	4450	mg/kg	NIH HSDB	max
LD50	54.5	mg/kg	NIH HSDB	min
LOAEL	16.299999	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	2	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	1	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	7.4	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	10.19	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	5	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	7.5	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	2.5	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	4.3	mg/kg/day	EPA Toxicity Reference Database	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0001361	mol/kg	TEST QSAR	
Ames mutagenicity test	0.392	no units	TEST QSAR	
Developmental toxin test	0.781	no units	TEST QSAR	

Scoring Data

Nationally Representative Water Data		Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water												
Unregulated Contaminant Monitoring Rule (UCMR) 4		2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3		2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2		2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1		2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2		1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1		1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)		1984 - 1986										
Ambient Water												
National Water Quality Assessment (USGS NAWQA) (All Water)		1991 - 2017	1,994	21	Sites	1.05	5.00E - 05	0.00232	0.0122	0.129	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)		1991 - 2017	339	18	Sites	5.31	5.00E - 05	0.00239	0.0109	0.0446	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)		1991 - 2017	1,655	3	Sites	0.18	8.00E - 05	0.00061	0.0905	0.129	ug/L	
Pesticide Application Data		Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data		Number of States	Amount Released (lbs/year)	Chemical Production Data		Production Volume (lbs/year)	
Estimated Annual Agricultural Pesticide Use (USGS)		48	1,403,807	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)		10	16,519	Chemical Data Reporting (CDR) Results (EPA) (2016)			

Non-Scoring Data

Non-Storing Data												
Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes	
Finished Water			Prevalence					Magnitude				
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	2	Sites	12	0.0053	0.0207	0.0329	0.036	ug/L		
Ambient Water			Prevalence					Magnitude				
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	436	21	Sites	4.82	0.00148	0.0116	0.0581	0.35	ug/L		
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	530	0	Sites	0							
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	966	21	Sites	2.17	0.00148	0.0116	0.0581	0.35	ug/L		
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	201	1	Sites	0.5	0.008	0.008	0.008	0.008	ug/L		
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	190	0	Sites	0							
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	1	Sites	8.33	0.008	0.008	0.008	0.008	ug/L		
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	4,917	970	Sites	20	0.00062	0.0123	0.0799	5.633527	ug/L		
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	1	Sites	2.63	0.0218	0.0218	0.0218	0.0218	ug/L		
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	1	Sites	0.17	1e-04	1e-04	1e-04	1e-04	ug/L		
Waste Water Effluent			Prevalence					Magnitude				
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes						

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exposurecast exposure		2.33E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.54094	days	
Boiling point	OPERA QSAR	370.963	degree C	
Boiling point	TEST QSAR	411.331	degree C	
Vapor pressure	OPERA QSAR	0.000000153	mmHg	
Vapor pressure	TEST QSAR	0.000000121	mmHg	
Solubility in water	OPERA QSAR	0.000000189	mol/L	
Solubility in water	TEST QSAR	4.98E-08	mol/L	
Bioconcentration factor	OPERA QSAR	4985.6	no units	
Bioconcentration factor	TEST QSAR	381.944	no units	
Henry's Law constant	OPERA QSAR	4.88E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	6.79073	no units	

Bifenthrin

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
324	USEPA. 2012. Bifenthrin: Human Health Risk Assessment to Support Section 3 New Uses for a Bed Bug Treatment, Grass Grown for Seed, Tolerances for Imported Tea, and a Section 18 Emergency Exemption Use on Apple, Nectarine, and Peach. EPA-HQ-OPP-2016-0236-0007. DP No. D372550. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Bisphenol A (4,4'-Isopropylidenediphenol)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Bisphenol A (4,4'-Isopropylidenediphenol)
CASRN:	80-05-7
DTXSID:	DTXSID7020182
Use:	Production of polycarbonate and epoxy resins. Formerly used as fungicide.
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxics	
PubMed Neurotoxics	X
Neurodev. Disruptors	
Androgen Receptors in vitro	X
Compounds with neurodev effects, Mundy et al 2015	X

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.067

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	non-cancer effects	8	5

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	20	hepatocyte hypertrophy and increased liver weight (absolute and relative)	general population	ECHA	2015

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
1.6016	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Bisphenol A (4,4'-Isopropylidenediphenol)

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.05	mg/kg/day	IRIS 1988	NTP 1982	"reduced mean bodyweight"	general population	33.8	296	[196]	
Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations										
Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.004	mg/kg/day	ECHA 2015	Tyl et al. 2008	hepatocyte hypertrophy and increased liver weight (absolute and relative)	general population	33.8	0.0237	[72]	NOTE: Due to the large amount of literature published after the 1988 IRIS assessment (an estimated 800 studies were expected to be relevant and require full text review), no additional searches are going to be taken at this time. If BPA is listed on the CCL, efforts to update EPA assessment may
Reference Dose (RfD) or Equivalent	0.016	mg/kg/day	NSF 2008	Tyl et al. (2007)	reduced body weight gain in rats and minimal to mild hepatocyte hypertrophy in adult F0 and F1 males and F1 female mice	general population	33.8	94.7	[444]	
Reference Dose (RfD) or Equivalent	0.0065	mg/kg/day	MDH 2015	Tyl et al. 2008	"Centrilobular hepatocyte hypertrophy, increased kidney weight"	general population	33.8	38.5	[138]	

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
						1987-09-01	2019-12-17	9149	230	20	Screening stopped in the middle of title/abstract screening due to extremely high number of includes, which was deemed outside the scope of this rapid systematic review. No further work on this chemical.

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Health-Based Guidance Value	0.1	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.02	mg/L	MN DOH	
Short-Term/Subchronic Health-Based Guidance Value	0.02	mg/L	MN DOH	
Cancer Classification (CC)	Female.Mice	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats E	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice E	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats E	no units	HHS NTP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	2230	mg/kg	NIH HSDB	min
LD50	5280	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	21.33	percent	EPA Chemistry Dashboard	
TD50	1320000	mg/kg/day	NIH CPDB	max
TD50	445	mg/kg/day	NIH CPDB	min

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0179887	mol/kg	TEST QSAR	
Ames mutagenicity test	0.086	no units	TEST QSAR	
Developmental toxin test	0.711	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Bisphenol A (4,4'-isopropylidenediphenol)
CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	732	12	Sites	1.64	0.03	0.251	1.6	2.64	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	86	4	Sites	4.65	0.03	0.105	0.273	0.278	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	646	8	Sites	1.24	0.107	0.298	2.13	2.64	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)	29	3,104,838	Chemical Data Reporting (CDR) Results (EPA) (2016)	1B - 5B

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	1	0	Sites	0						
Bradley et al. 2018 (Finished) [53]	2016	26	1	Sites	3.85	9.157284	9.16	9.16	9.157284	ug/L	
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Padhye et al. 2013 (Finished) [155]	2009 - 2010	8	4	Samples	50	0	2.7e-06		4.43e-05 +/- 1.01e-05	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	2	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,200	205	Sites	17	0.01	0.08	0.49	4.97	ug/L	
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	532	157	Sites	30	0.01	0.08	0.464	2.97	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	619	47	Sites	7.59	0.02	0.09	1.05	4.97	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,151	204	Sites	18	0.01	0.08	0.49	4.97	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	4		0.029		0.029	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	15	Sites	39	0.0253	0.0649	0.134	0.163	ug/L	
Bexfield et al. 2019 (Groundwater) [49]	2013 - 2015	1,077	7	Sites	0.65	0.171062	0.193	0.34	0.430036	ug/L	
Padhye et al. 2013 (Ambient) [155]	2009 - 2010	8	6	Samples	75	0	1.27e-05		2.19e-05 +/- 1.6e-06	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	2	Sites	100						
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	20	2	Sites	10	0.152752	0.242	0.401	0.441148	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.0000211	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)	4.9	ug/l	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	15.1318	days	
Boiling point	OPERA QSAR	343.216	degree C	
Boiling point	TEST QSAR	359.933	degree C	
Vapor pressure	OPERA QSAR	6.83E-08	mmHg	
Vapor pressure	TEST QSAR	0.00000259	mmHg	
Solubility in water	OPERA QSAR	0.000535206	mol/L	
Solubility in water	TEST QSAR	0.00124451	mol/L	
Bioconcentration factor	OPERA QSAR	43.6947	no units	
Bioconcentration factor	TEST QSAR	117.22	no units	
Henry's Law constant	OPERA QSAR	0.000000126	atm-m^3/mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.35076	no units	

Bisphenol A (4,4'-Isopropylidenediphenol)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
49	Bexfield, L.M., P.L. Toccalino, K. Belitz, W.T. Foreman, and E.T. Furlong. 2019. Hormones and pharmaceuticals in groundwater used as a source of drinking water across the United States. <i>Environmental Science and Technology</i> 53: 2950-2960.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. <i>Environmental science & technology</i> , 52(23), 13972-13985.
72	ECHA. 2015. Committee for Risk Assessment (RAC) Opinion on an Annex XV dossier proposing restrictions on bisphenol A. European Chemicals Agency (ECHA), Helsinki, Finland. ECHA/RAC/RES-O-0000001412-86-56/F.
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
138	MDH. 2015. Toxicological Summary for: Bisphenol A. Minnesota Department of Health (MDH), Environmental Health Division, Health Risk Assessment Unit, St Paul, MN.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
155	Padhye, L.P., Yao, H., Kung'u, F.T., and Huang, C.H. Year-long evaluation on the occurrence and fate of pharmaceuticals, personal care products, and endocrine disrupting chemicals in an urban drinking water treatment plant. 2014. <i>Water Research</i> 51 (2014) 266-276.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
196	USEPA. 1988. Chemical Assessment Summary Bisphenol A. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, DC.
444	Willhite, C., Ball, G., and McLellan, C. 2008. <i>Journal of Toxicology and Environmental Health, Part B</i> . 11:69-146.

Boron

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Boron
CASRN:	7440-42-8
DTXSID:	DTXSID3023922
Use:	Former pesticide; oxygen scavenger; catalyst; in composite structural materials
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.48

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	reproductive and developmental effects	10	10

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	1000	decreased fetal body weights	women of childbearing age	OW	2008

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
475	90th Percentile	Finished Water	NIRS	1984-1986

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X	X		

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	X	Not Applicable
Basis		

Boron was found at levels greater than the HRL (and ½ the HRL) in several of the ground water systems surveyed by NIRS, it was not found at levels greater than the HRL (or ½ the HRL) in the surface waters sources evaluated in the AwwaRF study [a, b, d]. EPA believes that the overall national occurrence and exposure from both surface and ground water systems together is likely to be lower than the values observed for the NIRS ground water data [c,d].

[a] Frey, et al, 2004 [82]; [b] Seidel, 2006 [162]; [c] USEPA, 2004 [261]; [d] USEPA, 2008 [298]; as cited in USEPA, 2008 [296]

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Boron
CCL 5 Contaminant Information Sheet
HEALTH EFFECTS DATA
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Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.035	mg/kg/day	HC 1990	Weir and Fisher 1972	testicular atrophy and spermatogenesis arrest	general population	33.8	207	[90]	
Reference Dose (RfD) or Equivalent	0.17	mg/kg/day	OW 2008	Allen et al. 1996; Heindel et al. 1992; Price et al. 1994 and	decreased fetal body weights	women of childbearing age	35.4	960	[292]	
Reference Dose (RfD) or Equivalent	0.2	mg/kg/day	ATSDR 2010	Weir and Fisher 1972	testicular atrophy and systemic effects	general population	33.8	1180	[28]	
Reference Dose (RfD) or Equivalent	0.17	mg/kg/day	WHO 2009	Allen et al. 1996; Heindel et al. 1992; Price et al. 1994 and	decreased fetal body weights	women of childbearing age	35.4	960	[441]	
Reference Dose (RfD) or Equivalent	0.2	mg/kg/day	IRIS 2004	Price et al., 1996a; Heindel et al.,	decreased fetal weight	women of childbearing age	35.4	1130	[259]	
Cancer Classification (CC)	I		IRIS 2004						[259]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Reproductive	1	Marat, 2018	Developmental, Systemic	125	El-Dakdoky, 2013	2009-11-01	2020-02-13	2877	9	30	4

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	3	mg/L	EPA DWSHA 2018	
Acute Health-Based Guidance Value	0.5	mg/L	MN DOH	
Acute inhalation Minimal Risk Level (MRL)	0.3	mg/m ³	CDC ATSDR	
Chronic Health-Based Guidance Value	0.5	mg/L	MN DOH	
Drinking Water Guideline Value	2.4	mg/L	WHO Drinking Water Quality Guidelines	
Lifetime Health Advisory	6	mg/L	EPA DWSHA 2018	
Maximum Allowable Concentration (MAC)	5	mg/L	Canadian Drinking Water Guidelines	
Short-Term/Subchronic Health-Based Guidance Value	0.5	mg/L	MN DOH	

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity test			TEST QSAR	
Developmental toxin test			TEST QSAR	

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
The full citation for the critical study is provided in the corresponding health assessment.
PECO = Population, Exposure, Comparator, Outcome.

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Boron
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986	989	810	Sites	82	5	47	475	3950	ug/L	
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	6,327	6,014	Sites	95	0	38	210	8470	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	414	388	Sites	94	0	40	193	4200	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	5,913	5,626	Sites	95	1	33	247	8470	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	25K - 100K

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	273	192	Sites	70	0.076	180	500	9000	ug/L	
Community Water System Survey (CWSS) (Finished) [178]	2006	5	NA	Sites			140	200		ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	1,929	1,184	Sites	61	0.0151	240	1000	235000	ug/L	
Drinking Water Monitoring Data - WI (Source)	2012-2019	1	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	2,101	1,959	Sites	93	1.79	55	301	56700	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	8,067	7,586	Sites	94	1	65	728	564000	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	10,148	9,526	Sites	94	1	60	467	564000	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	757	738	Sites	97	3	34	446	4080	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Boron

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
28	ATSDR. 2010. Toxicological Profile for Boron. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
82	Frey, M.M., C. Seidel, M. Edwards, J. Parks, and L. McNeill. 2004. Occurrence Survey for Boron and Hexavalent Chromium. AwwaRF Report 91044F.
90	HC. 1990. Guideline Technical Document - Boron. Health Canada (HC), Water and Air Quality Bureau, Healthy Environments and Consumer Safety Branch, Ottawa, Ontario, Canada.
162	Seidel, C. 2006. Email Communication to Brent Ranalli at The Cadmus Group, Inc. [concerning boron data from an AwwaRF-sponsored study, with data in an attached spreadsheet]. Denver, CO: McGuire Malcolm Pirnie. May 19.
178	USEPA (US Environmental Protection Agency). (2009). 2006 Community Water System Survey. Overview, 57.
259	USEPA. 2004. Chemical Assessment Summary, Boron. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, D.C.
261	USEPA. 2004. Integrated Risk Information System (IRIS), Boron and Compounds. August. Available on the Internet at: http://www.epa.gov/iris/subst/0410.htm . Accessed February 2, 2005.
292	USEPA. 2008. Health Effects Support Document for Boron. U.S. Environmental Protection Agency, Office of Water, Health and Ecological Criteria Division, Washington, D.C.
296	USEPA. 2008. Regulatory Determinations Support Document for Selected Contaminants from the Second Drinking Water Contaminant Candidate List (CCL 2). EPA Report 815-R-08-012. June 2008.
298	USEPA. 2008. The Analysis of Occurrence Data from the Unregulated Contaminant Monitoring (UCM) Program and National Inorganics and Radionuclides Survey (NIRS) in Support of Regulatory Determinations for the Second Drinking Water Contaminant Candidate List. EPA 815-D-08-014. June.
441	WHO. 2009. Boron in Drinking-water. Background document for development of WHO Guidelines for Drinking-water Quality. World Health Organization (WHO), Geneva, Switzerland.

Boscalid

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Boscalid
CASRN:	188425-85-6
DTXSID:	DTXSID6034392
Use:	Fungicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.000026

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	non-cancer effects	10	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	1000	thyroid lesions	general population	OPP	2019

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.0258	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Boscalid

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.22	mg/kg/day	OPP 2019	Mellert et al. 2001a and b; MRID 45723501	thyroid lesions	general population	33.8	1300	[414]	
Cancer Classification (CC)	S		OPP 2019						[414]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Chronic Human Health Benchmark	1.4	mg/L	EPA HHBP	
Health-Based Screening Level	1.4	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.218	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	5000	mg/kg	NIH HSDB	
LOAEL	1034.5	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	57.400002	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	12.5	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	300	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	6.37	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	78.099998	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	788	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	277	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	8.1	mg/kg/day	EPA Toxicity Reference Database	min

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0093325	mol/kg	TEST QSAR	
Ames mutagenicity test	0.516	no units	TEST QSAR	
Developmental toxin test	0.762	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
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EPA - Office of Water

Boscalid
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	14	3	Sites	21	0.0057	0.0102	0.0258	0.0288	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	14	3	Sites	21	0.0057	0.0102	0.0258	0.0288	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	42	782,294	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	5	0	Sites	0						
Bradley et al. 2018 (Finished) [53]	2016	26	3	Sites	12	0.0029	0.0034	0.00556	0.0061	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	136	70	Sites	51	0.0014	0.0208	0.215	11.2	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	139	70	Sites	50	0.0014	0.0208	0.215	11.2	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	221	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	216	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	5	0	Sites	0						
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	11	Sites	29	0.0052	0.009	0.215	0.6781	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		1.82E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.73188	days	
Boiling point	OPERA QSAR	396.769	degree C	
Boiling point	TEST QSAR	446.25	degree C	
Vapor pressure	OPERA QSAR	5.4E-09	mmHg	
Vapor pressure	TEST QSAR	1.04E-08	mmHg	
Solubility in water	OPERA QSAR	0.000026	mol/L	
Solubility in water	TEST QSAR	0.0000553	mol/L	
Bioconcentration factor	OPERA QSAR	776.451	no units	
Bioconcentration factor	TEST QSAR	107.152	no units	
Henry's Law constant	OPERA QSAR	2.84E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.15332	no units	

Boscalid

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. <i>Environmental science & technology</i> , 52(23), 13972-13985.
414	USEPA. 2019. Boscalid. Human Health Risk Assessment for Registration Review. EPA-HQ-OPP-2014-0199-0020. DP No. D451675. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.

Bromacil

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Bromacil
CASRN:	314-40-9
DTXSID:	DTXSID4022020
Use:	Herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0012

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	non-cancer effects	9	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	100	decreases in mean absolute body weight and decreased food efficiency	general population	OPP	2016

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.12	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Bromacil

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0196	mg/kg/day	OPP 2016	Bogdanffy 1989	decreases in mean absolute body weight and decreased food efficiency	general population	33.8	116	[362]	
Cancer Classification (CC)	C		OPP 2016						[362]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	5	mg/L	EPA DWSHA 2018	
Lifetime Health Advisory	0.07	mg/L	EPA DWSHA 2018	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	5200	mg/kg	NIH HSDB	max
LD50	641	mg/kg	NIH HSDB	min
LOAEL	300	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	9.8199997	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	100	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	2.64	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	2.9	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0047643	mol/kg	TEST QSAR	
Ames mutagenicity test	0.514	no units	TEST QSAR	
Developmental toxin test	0.87	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
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Bromacil
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	7,914	482	Sites	6.09	0.00043	0.0124	0.12	21.7	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	1,235	268	Sites	22	0.00055	0.0117	0.095	5.42	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	6,680	214	Sites	3.2	0.00043	0.05	0.956	21.7	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	3	253,973	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	174	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	15	4	Sites	27	0.0086	0.045	0.0654	0.069	ug/L	
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	2,117	1	Sites	0.05	1.5	1.5	1.5	1.5	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	227	53	Sites	23	0.002	0.016	0.179	21.8	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	46	Sites	21	0.002	0.0445	1.8	21.8	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	10	7	Sites	70	0.002	0.014	0.0573	0.41	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	2,953	100	Sites	3.39	0.027	0.122	2.22	68	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	5	Sites	13	0.02	0.028	0.0948	0.1	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	32	Sites	4.64	4e-04	0.0164	1.07	7.76	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	0	Sites	0						
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		8.46E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.35662	days	
Boiling point	OPERA QSAR	290.845	degree C	
Boiling point	TEST QSAR	315.49	degree C	
Vapor pressure	OPERA QSAR	0.00178266	mmHg	
Vapor pressure	TEST QSAR	0.000000402	mmHg	
Solubility in water	OPERA QSAR	0.324213	mol/L	
Solubility in water	TEST QSAR	0.00179473	mol/L	
Bioconcentration factor	OPERA QSAR	2.42732	no units	
Bioconcentration factor	TEST QSAR	3.5156	no units	
Henry's Law constant	OPERA QSAR	0.00000138	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.07377	no units	

Bromacil

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
362	USEPA. 2016. Bromacil and its Lithium Salt - Draft Human Health Risk Assessment for Registration Review. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Bromoxynil

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Bromoxynil
CASRN:	1689-84-5
DTXSID:	DTXSID3022162
Use:	Herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.73

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	carcinogen with linear MOA	6	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.3	hepatocellular tumors	general population	OPP	2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.22	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Bromoxynil
CCL 5 Contaminant Information Sheet
HEALTH EFFECTS DATA

EPA-OGWDW and OST

July 2021

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.015	mg/kg/day	OPP 2018	Harling et al. 1988 and 1989	increased incidence of panting and decreased absolute body weight	general population	33.8	88.8	[397]	
Cancer Slope Factor (CSF)	0.103	(mg/kg/day) ⁻¹	OPP 2018	Budd and Rinde 1997	hepatocellular tumors	general population	33.8	0.287	[397]	
Cancer Classification (CC)	C		OPP 2018						[397]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.5	mg/L	EPA HHBP	
Acute PAD	0.08	mg/kg/day	EPA HHBP	
Cancer Slope Factor (CSF)	0.103	(mg/kg/day) ⁻¹	EPA HHBP	
Chronic Human Health Benchmark	0.000311	mg/L	EPA HHBP	
Chronic Human Health Benchmark	0.096	mg/L	EPA HHBP	
Health-Based Screening Level	0.000311	mg/L	Health-based screening levels from USGS	
Health-Based Screening Level	0.096	mg/L	Health-based screening levels from USGS	
Maximum Allowable Concentration (MAC)	0.005	mg/L	Canadian Drinking Water Guidelines	
Population-Adjusted Dose (PAD)	0.015	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	365	mg/kg	NIH HSDB	max
LD50	63	mg/kg	NIH HSDB	min
LOAEL	1.5	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	12	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	0.3	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	3.7	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	14.48	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0011535	mol/kg	TEST QSAR	
Ames mutagenicity test	0.367	no units	TEST QSAR	
Developmental toxin test			TEST QSAR	

Technical Support Document for the
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EPA - Office of Water

Bromoxynil
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	7,736	60	Sites	0.78	6.00E - 04	0.0228	0.22	6.1	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	1,196	53	Sites	4.43	6.00E - 04	0.0235	0.219	6.1	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	6,540	7	Sites	0.11	0.01	0.02	0.121	0.311	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	36	2,957,908	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	2	31	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	13	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	476	9	Sites	1.89	0.0056	0.01	0.19	0.269	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	1,059	1	Sites	0.09	0.01	0.01	0.01	0.01	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,535	10	Sites	0.65	0.0056	0.01	0.182	0.269	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	8	1	Sites	12	0.065	0.065	0.065	0.065	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	2	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	6	1	Sites	17	0.065	0.065	0.065	0.065	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	4	Sites	11	0.0128	0.0194	0.0902	0.1185	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.000000092	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.8868	days	
Boiling point	OPERA QSAR	306.681	degree C	
Boiling point	TEST QSAR	295.87	degree C	
Vapor pressure	OPERA QSAR	0.000000232	mmHg	
Vapor pressure	TEST QSAR	0.000264241	mmHg	
Solubility in water	OPERA QSAR	0.000863573	mol/L	
Solubility in water	TEST QSAR	0.000237684	mol/L	
Bioconcentration factor	OPERA QSAR	5.7625	no units	
Bioconcentration factor	TEST QSAR	12.331	no units	
Henry's Law constant	OPERA QSAR	0.000000153	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.62395	no units	

Bromoxynil

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
397	USEPA. 2018. Bromoxynil and Bromoxynil Esters: Human Health Draft Risk Assessment for Registration Review. EPA-HQ-OPP-2012-0896-0021. DP No. D444387. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.

Bupropion

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Bupropion
CASRN:	34911-55-2
DTXSID:	DTXSID7022706
Use:	antidepressant
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.013

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	non-cancer effects	8	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	8	lowest therapeutic dose: aminoketone antidepressant/ maintaining antidepressant response, treat depressive episode	bottle-fed infants	FDA; NIH	2018; 2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.10344	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Bupropion

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.00125	mg/kg/day	FDA 2018; NIH 2018	Solco Healthcare US LLC	lowest therapeutic dose: aminoketone antidepressant/ maintaining antidepressant response, treat depressive episode	bottle-fed infants	151	8.30	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels
Reference Dose (RfD) or Equivalent	0.00125	mg/kg/day	FDA 2018; NIH 2018	Solco Healthcare US LLC	lowest therapeutic dose: aminoketone antidepressant/ maintaining antidepressant response, treat depressive episode	general population	33.8	29.0	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Maximum Recommended Daily Dose	7.5	mg/kg/day	FDA	
Screening level for pharmaceutical - general population	0.029411765	mg/L	EPA Office of Water	
Screening level for pharmaceutical - infants	0.008333333	mg/L	EPA Office of Water	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	575	mg/kg	NIH HSDB	min
LD50	600	mg/kg	NIH HSDB	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0045709	mol/kg	TEST QSAR	
Ames mutagenicity test	0.071	no units	TEST QSAR	
Developmental toxin test	0.358	no units	TEST QSAR	

Technical Support Document for the
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Bupropion
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	557	11	Sites	1.97	0.00107	0.0139	0.103	0.148	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	75	11	Sites	15	0.00107	0.0139	0.103	0.148	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	482	0	Sites	0						
									</		

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	12		0.0103		0.01091	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	205	47	Sites	23	6.00E - 04	0.00403	0.2	0.339	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	401	4	Sites	1	0.00282	0.0162	0.0284	0.034	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	606	51	Sites	8.42	6.00E - 04	0.00467	0.198	0.339	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	20		0.00636		0.00941	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	12	Sites	32	0.0007854	0.048	0.0796	0.1595924	ug/L	
Bexfield et al. 2019 (Groundwater) [49]	2013 - 2015	1,106	3	Sites	0.27	0.0044212	0.0093	0.02	0.0226803	ug/L	
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	18	Sites	86	0.0179911	0.0935	0.988	89.4629985	ug/L	
Shultz et al. (2008) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						0.6	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.38965	days	
Boiling point	OPERA QSAR	307.696	degree C	
Boiling point	TEST QSAR	295.443	degree C	
Vapor pressure	OPERA QSAR	0.00000469	mmHg	
Vapor pressure	TEST QSAR	0.0000116	mmHg	
Solubility in water	OPERA QSAR	0.000646695	mol/L	
Solubility in water	TEST QSAR	0.000368978	mol/L	
Bioconcentration factor	OPERA QSAR	69.189	no units	
Bioconcentration factor	TEST QSAR	50.3501	no units	
Henry's Law constant	OPERA QSAR	3.04E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.91432	no units	

Bupropion

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
49	Bexfield, L.M., P.L. Toccalino, K. Belitz, W.T. Foreman, and E.T. Furlong. 2019. Hormones and pharmaceuticals in groundwater used as a source of drinking water across the United States. <i>Environmental Science and Technology</i> 53: 2950-2960.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
77	FDA. 2018. Drugs @ FDA: FDA Approved Drug Products. U.S. Food and Drug Administration (FDA). https://www.accessdata.fda.gov/scripts/cder/daf/ .
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
127	Kostich, MS, et al., 2010. Predicting variability of aquatic concentrations of human pharmaceuticals. <i>Sci. Total Environ.</i> 408 (20), 4504e4510.
150	NIH. 2018. DailyMed Database. U.S. National Library of Medicine, National Institutes of Health (NIH). https://dailymed.nlm.nih.gov/dailymed/ .
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.

Butyl benzyl phthalate

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Butyl benzyl phthalate
CASRN:	85-68-7
DTXSID:	DTXSID3020205
Use:	Chemical intermediate; plasticizer
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	X
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.065

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
3	carcinogen with linear MOA	9	7

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	20	increased incidence of pancreatic cancer in male F334 rats	general population	PPRTV	2002

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
1.3	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Butyl benzyl phthalate

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.2	mg/kg/day	IRIS 1989	NTP 1985	"Significantly increased liver- to-body weight and liver-to-brain weight ratios"	general population	33.8	1180	[203]	
Reference Dose (RfD) or Equivalent	0.2	mg/kg/day	OW 1991	NTP 1985	increased liver weight in rats	general population	33.8	1180	[211]	
Cancer Slope Factor (CSF)	0.0019	(mg/kg/day) ⁻¹	PPRTV 2002	NTP 1997a	increased incidence of pancreatic cancer in male F334 rats	general population	33.8	15.6	[253]	
Cancer Classification (CC)	C		OW 1991						[211]	
Cancer Classification (CC)	C		PPRTV 2002						[253]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Neurological, Systemic	2	Betz, 2013	Hematologic	1500	Uriu-Adams, 2001	2001-10-01	2019-12-17	656	12	34	11

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Health-Based Guidance Value	0.1	mg/L	MN DOH	
Acute Health-Based Guidance Value	0.1	mg/L	MN DOH	
Cancer Classification (CC)	3	no units	WHO IARC	
Chronic Health-Based Guidance Value	0.1	mg/L	MN DOH	
Human Health Ambient Water Quality Criteria	0.0001	mg/L	EPA Human Health Criteria for CWA	
Maximum Allowable Daily Level	1200	ug/day	CalEPA OEHHA Chemical Database	
Short-Term/Subchronic Health-Based Guidance Value	0.1	mg/L	MN DOH	
Cancer Classification (CC)	Female.Mice N	no units	HHS NTP	
Cancer Classification (CC)	Female.Mice NT	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats EE	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats P	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice N	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice NT	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats IS	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats SE	no units	HHS NTP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	13750	mg/kg	NIH HSDB	max
LD50	2000	mg/kg	NIH HSDB	min
LOAEL	100	mg/kg/day	EPA Toxicity Reference Database	
Percent of active toxcast in vitro assays tested	9.87	percent	EPA Chemistry Dashboard	
TD50	347	mg/kg/day	NIH CPDB	min
TD50	47000	mg/kg/day	NIH CPDB	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0591562	mol/kg	TEST QSAR	
Ames mutagenicity test	0.035	no units	TEST QSAR	
Developmental toxin test	0.749	no units	TEST QSAR	

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EPA - Office of Water

Butyl benzyl phthalate

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	22	2	Sites	9.09	1.3	1.3	1.3	1.3	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	13	2	Sites	15	1.3	1.3	1.3	1.3	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	9	0	Sites	0						

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	10M - 50M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	21	1	Sites	4.76	0.005	0.029	0.0674	0.077	ug/L	
Drinking Water Monitoring Data - WA (Finished)	2006 - 2011	484	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	221	2	Sites	0.9	0.003	0.042	5.41	8.5	ug/L	
Drinking Water Monitoring Data - WA (Source)	2006 - 2011	638	1	Sites	0.16	4.7	5.2	5.6	5.7	ug/L	
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	143	15	Sites	10	0.2	0.8	5	5	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	344	17	Sites	4.94	0.5	0.8	1.11	2.1	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	487	32	Sites	6.57	0.2	0.8	5	5	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.000115	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.35267	days	
Boiling point	OPERA QSAR	365.191	degree C	
Boiling point	TEST QSAR	392.394	degree C	
Vapor pressure	OPERA QSAR	0.00000447	mmHg	
Vapor pressure	TEST QSAR	0.00000433	mmHg	
Solubility in water	OPERA QSAR	0.00000908	mol/L	
Solubility in water	TEST QSAR	0.0000185	mol/L	
Bioconcentration factor	OPERA QSAR	19.3088	no units	
Bioconcentration factor	TEST QSAR	16.6725	no units	
Henry's Law constant	OPERA QSAR	2.82E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	4.46009	no units	

Butyl benzyl phthalate

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Reference Number	Full Reference
203	USEPA. 1989. Chemical Assessment Summary Butyl benzyl phthalate. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, DC.
211	USEPA. 1991. Drinking Water Criteria Document for Phthalic Acid Esters (PAES). U.S. Environmental Protection Agency, Office of Water, Health and Ecological Criteria Division, Washington, DC.
253	USEPA. 2002. Provisional Peer Reviewed Toxicity Values for Butyl benzyl phthalate (CASRN 85-68-7) Derivation of a Carcinogenicity Assessment. U.S. Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment, Superfund Health Risk Technical Support Center, Cincinnati, OH.

Caffeine

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Caffeine
CASRN:	58-08-2
DTXSID:	DTXSID0020232
Use:	CNS stimulant
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	X

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
		10	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.2782	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Caffeine
CCL 5 Contaminant Information Sheet
HEALTH EFFECTS DATA

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Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
										NOTE: Though there are over the-counter labels for caffeine, there are no FDA approved formulations for adults. For this reason, a health concentration was not developed.

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References Identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Cancer Classification (CC)	3	no units	WHO IARC	
Maximum Recommended Daily Dose	10	mg/kg/day	FDA	
Screening level for pharmaceutical - general population	0.058823529	mg/L	EPA Office of Water	
Screening level for pharmaceutical - infants	0.016666667	mg/L	EPA Office of Water	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	127	mg/kg	NIH HSDB	min
LD50	230	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	7.84	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0011429	mol/kg	TEST QSAR	
Ames mutagenicity test	0.192	no units	TEST QSAR	
Developmental toxin test	0.799	no units	TEST QSAR	

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EPA - Office of Water

Caffeine
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
		Prevalence				Magnitude					
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	3,465	417	Sites	12	0.0025	0.046	0.278	15	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	341	222	Sites	65	0.004	0.0554	0.325	15	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	3,124	195	Sites	6.24	0.0025	0.01	0.0384	2.82	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	100K - 500K

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	58	9	Sites	16	0.051	0.064	0.17	0.37	ug/L	
Bradley et al. 2018 (Finished) [53]	2016	26	1	Sites	3.85	0.0589107	0.0589	0.0589	0.0589107	ug/L	
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Community Water System Survey (CWSS) (Finished) [178]	2006	1	NA	Sites			0.017	0.017		ug/L	
Padhye et al. 2013 (Finished) [155]	2009 - 2010	8	3	Samples	38	0	0		1.16e-05 +/- 7e-07	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
		Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	266	34	Sites	13	0.05	0.19	0.427	1.5	ug/L	
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	1,019	526	Sites	52	0.00583	0.06	0.322	18	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	1,697	69	Sites	4.07	0.005	0.0323	0.108	0.267	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	2,715	595	Sites	22	0.005	0.06	0.314	18	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	12		0.0703		0.09089	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	28	Sites	74	0.0068603	0.0874	0.227	1.275935	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	106	0	Sites	0						
Bexfield et al. 2019 (Groundwater) [49]	2013 - 2015	1,106	11	Sites	0.99	0.1254262	0.246	0.974	1.359395	ug/L	
Padhye et al. 2013 (Ambient) [155]	2009 - 2010	8	4	Samples	50	0	2.7e-06		1.59e-05 +/- 6e-07	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	2	Sites	100	0.002	0.0145	0.0247	0.025	ug/L	
USGS, McKenzie River, Oregon, 2012 (Ambient) [158]	2002 - 2010	126	40	Samples	32				11.4	ug/L	
Waste Water Effluent											
		Prevalence				Magnitude					
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	21	Sites	100	0.0189615	0.14	1.8	3.1	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Expcast exposure		0.0000242	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.52242	days	
Boiling point	OPERA QSAR	286.771	degree C	
Boiling point	TEST QSAR	337.485	degree C	
Vapor pressure	OPERA QSAR	0.00000208	mmHg	
Vapor pressure	TEST QSAR	0.00000241	mmHg	
Solubility in water	OPERA QSAR	0.101085	mol/L	
Solubility in water	TEST QSAR	0.054325	mol/L	
Bioconcentration factor	OPERA QSAR	1.86426	no units	
Bioconcentration factor	TEST QSAR	1.31522	no units	
Henry's Law constant	OPERA QSAR	0.00000159	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	-0.119469	no units	

Caffeine

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
49	Bexfield, L.M., P.L. Toccalino, K. Belitz, W.T. Foreman, and E.T. Furlong. 2019. Hormones and pharmaceuticals in groundwater used as a source of drinking water across the United States. Environmental Science and Technology 53: 2950-2960.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. Environmental science & technology, 51(9), 4792-4802.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. Environmental science & technology, 52(23), 13972-13985.
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. Science of The Total Environment. v581-582, (909-922).
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
155	Padhye, L.P., Yao, H., Kung'u, F.T., and Huang, C.H. Year-long evaluation on the occurrence and fate of pharmaceuticals, personal care products, and endocrine disrupting chemicals in an urban drinking water treatment plant. 2014. Water Research 51 (2014) 266-276.
158	Reconnaissance of Land-Use Sources of Pesticides in Drinking Water, McKenzie River, Oregon. U.S. Geological Survey Scientific Investigations Report 2012–5091, 46 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. Science of the Total Environment, 636, 69-79.
178	USEPA (US Environmental Protection Agency). (2009). 2006 Community Water System Survey. Overview, 57.

Calcium

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Calcium
CASRN:	7440-70-2
DTXSID:	DTXSID9050484
Use:	Element, used in alloys and deoxidizer for copper, beryllium, steel
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
		10	10

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
96865	90th Percentile	Finished Water	NIRS	1984-1986

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Calcium

CCL 5 Contaminant Information Sheet

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July 2021

HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
			HC 2019						[97]	NOTE: There is no evidence of adverse health effects from calcium in drinking water

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	2500	mg/day	IOM 2010		no adverse effects	general population	2413	207000	[111]	

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity test			TEST QSAR	
Developmental toxin test			TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
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EPA 815-R-21-006
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EPA - Office of Water

Calcium
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986	989	986	Sites	100	25	37453	96865	1116000	ug/L	
Ambient Water											
		Prevalence				Magnitude					
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	12,127	12,124	Sites	100	20	37000	94540	5200000	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	2,626	2,626	Sites	100	22	33700	82000	5200000	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	9,502	9,499	Sites	100	20	51800	120000	1940000	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	1M - 10M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	660	653	Sites	99	100	49000	96000	1.2e+08	ug/L	
Drinking Water Monitoring Data - MA (Finished)	2006 - 2020	549	532	Sites	97	30	17600	49200	481000	ug/L	
Drinking Water Monitoring Data - WA (Finished)	2006 - 2011	221	215	Sites	97	780	22000	56950	121000	ug/L	
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	100		39300		78400	ug/L	
Community Water System Survey (CWSS) (Finished) [178]	2006	11	NA	Sites			30000	95000		ug/L	
Ambient Water											
		Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	5,442	5,427	Sites	100	100	43000	121000	1.3e+08	ug/L	
Drinking Water Monitoring Data - MA (Source)	2006 - 2020	88	88	Sites	100	202	27700	52790	539000	ug/L	
Drinking Water Monitoring Data - ME (Source)	2009	1	1	Sites	100	25000	25000	25000	25000	ug/L	
Drinking Water Monitoring Data - PA (Source)	2006 - 2011	13	13	Sites	100	2100	45700	103360	197000	ug/L	
Drinking Water Monitoring Data - WA (Source)	2006 - 2011	344	341	Sites	99	810	24900	66730	140000	ug/L	
Drinking Water Monitoring Data - WI (Source)	2012-2019	147	146	Sites	99	550	53000	94480	3e+05	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	100		38900		129000	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	758	757	Sites	100	42	32600	100400	476000	ug/L	
Waste Water Effluent											
		Prevalence				Magnitude					
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Calcium

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. Science of The Total Environment. v581-582, (909-922).
97	HC. 2019. Guidelines for Canadian Drinking Water Quality Summary Table. Health Canada (HC), Water and Air Quality Bureau, Health Environments and Consumer Safety Branch, Ottawa, Ontario, Canada.
111	IOM. 2010. Dietary Reference Intakes for Calcium and Vitamin D. Institute of Medicine (IOM), National Academies of Science, Washington, D.C.
178	USEPA (US Environmental Protection Agency). (2009). 2006 Community Water System Survey. Overview, 57.

Camphor

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Camphor
CASRN:	76-22-2
DTXSID:	DTXSID5030955
Use:	Starting reagent for organic synthesis. Used as an odorant and flavorant. Plasticizer in cosmetics and as a preservative.
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
		9	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.0592	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Camphor

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
										NOTE: No health assessments found

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
							2020-04-07	1181	2	8	0

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1310	mg/kg	NIH HSDB	
Percent of active toxcast in vitro assays tested	0.43	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0098855	mol/kg	TEST QSAR	
Ames mutagenicity test	-0.018	no units	TEST QSAR	
Developmental toxin test	0.94	no units	TEST QSAR	

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EPA - Office of Water

Camphor
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	571	28	Sites	4.9	0.004	0.0125	0.0592	7.6	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	88	25	Sites	28	0.004	0.013	0.0598	7.6	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	483	3	Sites	0.62	0.004	0.006	0.0368	0.05	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	100K - 500K

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	721	340	Sites	47	0.005	0.03	0.11	3.9	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	692	27	Sites	3.9	0.004	0.028	0.34	1.08	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,413	367	Sites	26	0.004	0.03	0.11	3.9	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	15	1	Sites	6.67	0.105	0.105	0.105	0.105	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	14	Sites	37	0.0108	0.0214	0.0415	0.0486	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	8	Sites	38	0.025	0.045	0.075	0.13	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.0000102	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	5.16263	days	
Boiling point	OPERA QSAR	204.644	degree C	
Boiling point	TEST QSAR	203.784	degree C	
Vapor pressure	OPERA QSAR	0.340707	mmHg	
Vapor pressure	TEST QSAR	0.214289	mmHg	
Solubility in water	OPERA QSAR	0.00489575	mol/L	
Solubility in water	TEST QSAR	0.0111944	mol/L	
Bioconcentration factor	OPERA QSAR	14.6711	no units	
Bioconcentration factor	TEST QSAR	55.7186	no units	
Henry's Law constant	OPERA QSAR	0.0000794	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.64083	no units	

Camphor

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Reference Number	Full Reference
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Carbamazepine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Carbamazepine
CASRN:	298-46-4
DTXSID:	DTXSID4022731
Use:	analgesic; anticonvulsant
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	X

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.013

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	non-cancer effects	9	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	6	lowest therapeutic dose: anticonvulsant/seizure therapy	bottle-fed infants	FDA; NIH	2018; 2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.07999	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Carbamazepine

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations										
Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.000833333	mg/kg/day	FDA 2018; NIH 2018	Caraco Pharmaceutical Laboratories,	lowest therapeutic dose: anticonvulsant/ seizure therapy	bottle-fed infants	151	5.60	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved
Reference Dose (RfD) or Equivalent	0.000833333	mg/kg/day	FDA 2018; NIH 2018	Caraco Pharmaceutical Laboratories,	lowest therapeutic dose: anticonvulsant/ seizure therapy	general population	33.8	20.0	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
							2020-01-28	10463			

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Health-Based Guidance Value	0.04	mg/L	MN DOH	
Acute Health-Based Guidance Value	0.04	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.04	mg/L	MN DOH	
Maximum Recommended Daily Dose	26.7	mg/kg/day	FDA	
Screening level for pharmaceutical - general population	0.019607843	mg/L	EPA Office of Water	
Screening level for pharmaceutical - infants	0.005555556	mg/L	EPA Office of Water	
Short-Term/Subchronic Health-Based Guidance Value	0.04	mg/L	MN DOH	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Percent of active toxcast in vitro assays tested	2.19	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0068707	mol/kg	TEST QSAR	
Ames mutagenicity test	0.428	no units	TEST QSAR	
Developmental toxin test	0.792	no units	TEST QSAR	

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OCCURRENCE DATA

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Scoring Data											
Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	626	62	Sites	9.9	0.00021	0.00478	0.08	0.468	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	75	41	Sites	55	0.00021	0.00475	0.0821	0.334	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	551	21	Sites	3.81	0.00033	0.00495	0.0571	0.468	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data											
Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	1	0	Sites	0						
Bradley et al. 2018 (Finished) [53]	2016	26	2	Sites	7.69	0.0005503	0.000656	0.00074	0.0007611	ug/L	
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	8		0.0177		0.0265	ug/L	
Padhye et al. 2013 (Finished) [155]	2009 - 2010	8	1	Samples	12	0	0		2.5e-05 +/- 8.8e-06	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Kleywegt et al. (2011) via Uslu et al. (2013) (Finished) [433]	2011	NA	NA						0.601	ug/L	
Tabe et al. (2009) via Uslu et al. (2013) (Finished) [433]	2009	NA	NA						4e-04	ug/L	
Kormos et al. (2007) via Uslu et al. (2013) (Finished) [433]	2007	NA	NA						0.721	ug/L	
IL EPA (2008) via Uslu et al. (2013) (Finished) [433]	2008	NA	NA						0.007	ug/L	
Snyder et al. (2007) via Kumar et al. (2010) (Finished) [128]	2007	20	NA	Samples		0.0011	0.0028		0.0057	ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	1	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	502	246	Sites	49	0.00018	0.012	0.114	0.521	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	940	58	Sites	6.17	0.00046	0.0157	0.301	1	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,441	304	Sites	21	0.00018	0.012	0.13	1	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	28		0.0159		0.0357	ug/L	
Batt et al. 2016 (Ambient) [46]	2008 - 2009	182	74	Sites	41	0.0015	0.0116	0.0514	0.2493	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	22	Sites	58	0.0008717	0.0707	0.204	0.3827473	ug/L	
Bexfield et al. 2019 (Groundwater) [49]	2013 - 2015	1,106	18	Sites	1.63	0.0029133	0.00852	0.102	0.1620862	ug/L	
Padhye et al. 2013 (Ambient) [155]	2009 - 2010	8	8	Samples	100	5e-07 +/- 1e-07	9e-07		4.1e-06 +/- 1.2e-06	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	2	Sites	100	0.001	0.0055	0.0122	0.014	ug/L	
Kleywegt et al. (2011) via Uslu et al. (2013) (Ambient) [433]	2011	NA	NA						0.749	ug/L	
Tabe et al. (2009) via Uslu et al. (2013) (Ambient) [433]	2009	NA	NA						0.002	ug/L	
Kormos et al. (2007) via Uslu et al. (2013) (Ambient) [433]	2007	NA	NA						1.015	ug/L	
Rahman et al. (2010) via Uslu et al. (2013) (Ambient) [433]	2010	NA	NA						0.0779	ug/L	
IL EPA (2008) via Uslu et al. (2013) (Ambient) [433]	2008	NA	NA						0.009	ug/L	
Snyder et al. (2007) via Kumar et al. (2010) (Ambient) [128]	2007	20	NA	Samples		0.0012	0.0031		0.039	ug/L	
Batt et al. (2008) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.02	ug/L	

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	5.03451	days	
Boiling point	OPERA QSAR	320.593	degree C	
Boiling point	TEST QSAR	384.336	degree C	
Vapor pressure	OPERA QSAR	6.85E-10	mmHg	
Vapor pressure	TEST QSAR	3.22E-08	mmHg	
Solubility in water	OPERA QSAR	0.000382424	mol/L	
Solubility in water	TEST QSAR	0.0000255	mol/L	
Bioconcentration factor	OPERA QSAR	16.3863	no units	
Bioconcentration factor	TEST QSAR	26.6073	no units	
Henry's Law constant	OPERA QSAR	1.02E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.46475	no units	

Carbamazepine

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46	Batt, A. L., Kincaid, T. M., Kostich, M. S., Lazorchak, J. M., & Olsen, A. R. (2016). Evaluating the extent of pharmaceuticals in surface waters of the United States using a National-scale Rivers and Streams Assessment survey. <i>Environmental toxicology and chemistry</i> , 35(4), 874-881.
49	Bexfield, L.M., P.L. Toccalino, K. Belitz, W.T. Foreman, and E.T. Furlong. 2019. Hormones and pharmaceuticals in groundwater used as a source of drinking water across the United States. <i>Environmental Science and Technology</i> 53: 2950-2960.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. <i>Environmental science & technology</i> , 52(23), 13972-13985.
77	FDA. 2018. Drugs @ FDA: FDA Approved Drug Products. U.S. Food and Drug Administration (FDA). https://www.accessdata.fda.gov/scripts/cder/daf/ .
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
126	Kostich MS, et al. 2014 Concentrations of prioritized pharmaceuticals in effluents from 50 large wastewater treatment plants in the US and implications for risk estimation. <i>Environ Pollut</i> . 2014 Jan;184:354-9. doi: 10.1016/j.envpol.2013.09.013. Epub 2013 Oct 3. PMID: 24095705.
127	Kostich, MS, et al., 2010. Predicting variability of aquatic concentrations of human pharmaceuticals. <i>Sci. Total Environ</i> . 408 (20), 4504e4510.
128	Kumar, A. and Xagorarakis, I., 2010. Human health risk assessment of pharmaceuticals in water: An uncertainty analysis for meprobamate, carbamazepine, and phenytoin. <i>Regulatory Toxicology and Pharmacology</i> , 57(2-3), pp.146-156.
150	NIH. 2018. DailyMed Database. U.S. National Library of Medicine, National Institutes of Health (NIH). https://dailymed.nlm.nih.gov/dailymed/ .
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
155	Padhye, L.P., Yao, H., Kung'u, F.T., and Huang, C.H. Year-long evaluation on the occurrence and fate of pharmaceuticals, personal care products, and endocrine disrupting chemicals in an urban drinking water treatment plant. 2014. <i>Water Research</i> 51 (2014) 266-276.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
433	Uslu, M., Jasim, S., Arvai, A., Bewtra, J. and Biswas, N., 2013. A Survey of Occurrence and Risk Assessment of Pharmaceutical Substances in the Great Lakes Basin. <i>Ozone: Science & Engineering</i> , 35(4), pp.249-262.

Carbaryl

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Carbaryl
CASRN:	63-25-2
DTXSID:	DTXSID9020247
Use:	Insecticide; veterinary medication
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	X
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	X
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.24

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	reproductive and developmental effects	1	6

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	10	brain acetylcholinesterase inhibition in pups	bottle-fed infants	OPP	2017

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
2.4	90th Percentile	Finished Water	UCM2	1993 - 1997

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Carbaryl

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.01	mg/kg/day	OPP 2017	Moser 2006	brain acetylcholinesterase inhibition in pups	bottle-fed infants	151	13.2	[378]	
Cancer Slope Factor (CSF)	0.000875	(mg/kg/day)^-1	OPP 2017	Hamada 1993	hemangiosarcoma	general population	33.8	33.8	[378]	
Cancer Classification (CC)	L		OPP 2017						[378]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	1	mg/L	EPA DWSHA 2018	
Cancer Classification (CC)	3	no units	WHO IARC	
Lifetime Health Advisory	0.04	mg/L	EPA DWSHA 2018	
Maximum Allowable Concentration (MAC)	0.09	mg/L	Canadian Drinking Water Guidelines	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	128	mg/kg	NIH HSDB	min
LD50	500	mg/kg	NIH HSDB	max
LOAEL	1248.9301	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	3.0999999	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	180.86	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	4	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	11.51	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0014689	mol/kg	TEST QSAR	
Ames mutagenicity test	0.655	no units	TEST QSAR	
Developmental toxin test	0.784	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
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EPA - Office of Water

Carbaryl

CCL 5 Contaminant Information Sheet

OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997	12,623	4	Sites	0.03	0.68	1	2.4	3	ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	11,274	820	Sites	7.27	0.00038	0.011	0.074	23.5	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	2,227	750	Sites	34	0.00038	0.011	0.074	23.5	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	9,048	70	Sites	0.77	0.00048	0.0075	0.0364	0.781	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	43	1,981,350	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	9	872	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	171	0	Sites	0						
Drinking Water Monitoring Data - MA (Finished)	2006 - 2020	820	0	Sites	0						
Drinking Water Monitoring Data - WA (Finished)	2006 - 2011	255	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	5	Sites	29	0.002	0.005	0.069	0.3	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	1,747	0	Sites	0						
Drinking Water Monitoring Data - MA (Source)	2006 - 2020	77	1	Sites	1.3	0.75	0.75	0.75	0.75	ug/L	
Drinking Water Monitoring Data - PA (Source)	2006 - 2011	1	0	Sites	0						
Drinking Water Monitoring Data - WA (Source)	2006 - 2011	422	0	Sites	0						
Drinking Water Monitoring Data - WI (Source)	2012-2019	92	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	1,564	363	Sites	23	0.00089	0.016	0.135	3.13	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3,658	24	Sites	0.66	0.00037	0.007	0.039	0.0886	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	5,221	387	Sites	7.41	0.00037	0.015	0.13	3.13	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	7	Sites	3.06	0.002	0.018	0.0643	0.33	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	2	Sites	0.91	0.0125	0.02	0.0511	0.0612	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	5	Sites	42	0.002	0.018	0.065	0.33	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	9,207	332	Sites	3.61	0.003	0.11	0.533	13	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	11	Sites	29	0.0032	0.0135	0.0899	0.257	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	796	6	Sites	0.75	5e-04	6e-04	0.0027	0.0033	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
USGS, McKenzie River, Oregon, 2012 (Ambient) [158]	2002 - 2010	133	35	Samples	26				1.3	ug/L	
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	3	Sites	14	0.093	0.093	0.093	0.093	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Expcast exposure		5.61E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.55485	days	
Boiling point	OPERA QSAR	312.24	degree C	
Boiling point	TEST QSAR	311.019	degree C	
Vapor pressure	OPERA QSAR	0.00000118	mmHg	
Vapor pressure	TEST QSAR	0.00000562	mmHg	
Solubility in water	OPERA QSAR	0.000534089	mol/L	
Solubility in water	TEST QSAR	0.000414954	mol/L	
Bioconcentration factor	OPERA QSAR	10.3318	no units	
Bioconcentration factor	TEST QSAR	4.69894	no units	
Henry's Law constant	OPERA QSAR	1.55E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.38412	no units	

Carbaryl

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
158	Reconnaissance of Land-Use Sources of Pesticides in Drinking Water, McKenzie River, Oregon. U.S. Geological Survey Scientific Investigations Report 2012–5091, 46 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
378	USEPA. 2017. Carbaryl: Draft Human Health Risk Assessment in Support of Registration Review. EPA-HQ-OPP-2010-0230-0034. DP No. D433668. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Carbendazim

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Carbendazim
CASRN:	10605-21-7
DTXSID:	DTXSID4024729
Use:	Fungicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.0076

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
3	carcinogen with linear MOA	10	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	10	hepatocellular adenoma and/or carcinoma	general population	OPP	2014

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.07612	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Carbendazim

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.025	mg/kg/day	OPP 2014	Sherman et al. 1972	decreased body weight and food consumption	general population	33.8	148	[337]	
Cancer Slope Factor (CSF)	0.00239	(mg/kg/day) ⁻¹	OPP 2014	Wood 1982; Schneider et al. 1982	hepatocellular adenoma and/or carcinoma	general population	33.8	12.4	[337]	
Cancer Classification (CC)	C		OPP 2014						[337]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.11	mg/L	EPA HHBP	
Acute PAD	0.017	mg/kg/day	EPA HHBP	
Cancer Slope Factor (CSF)	0.00239	(mg/kg/day) ⁻¹	EPA HHBP	
Chronic Human Health Benchmark	0.16	mg/L	EPA HHBP	
Chronic Human Health Benchmark	0.0134	mg/L	EPA HHBP	
Health-Based Screening Level	0.16	mg/L	Health-based screening levels from USGS	
Health-Based Screening Level	0.0134	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.025	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	15000	mg/kg	NIH HSDB	max
LD50	5000	mg/kg	NIH HSDB	min
LOAEL	16.540001	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	90	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	20	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	7.19	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	10.79	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0082794	mol/kg	TEST QSAR	
Ames mutagenicity test	0.605	no units	TEST QSAR	
Developmental toxin test	0.884	no units	TEST QSAR	

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Carbendazim

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	1,757	212	Sites	12	0.00014	0.014	0.0761	1.79	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	322	198	Sites	61	0.00014	0.014	0.0759	1.79	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	1,435	14	Sites	0.98	0.00105	0.0127	0.13	0.251	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	7	1	Sites	14	0.003	0.003	0.003	0.003	ug/L	
Ambient Water											
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	115	4	Sites	3.48	0.003	0.003	0.033	0.121	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	109	1	Sites	0.92	0.005	0.005	0.0153	0.0179	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	7	3	Sites	43	0.003	0.003	0.033	0.121	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	122	33	Sites	27	0.0043	0.0197	0.0605	0.1559	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	5	Sites	0.86	0.0013	0.0054	0.101	0.157	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.00000001	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.54241	days	
Boiling point	OPERA QSAR	275.322	degree C	
Boiling point	TEST QSAR	374.376	degree C	
Vapor pressure	OPERA QSAR	2.04E-09	mmHg	
Vapor pressure	TEST QSAR	1.17E-08	mmHg	
Solubility in water	OPERA QSAR	0.0024081	mol/L	
Solubility in water	TEST QSAR	0.000907821	mol/L	
Bioconcentration factor	OPERA QSAR	2.44925	no units	
Bioconcentration factor	TEST QSAR	1.6293	no units	
Henry's Law constant	OPERA QSAR	1.38E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.43961	no units	

Carbendazim

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
337	USEPA. 2014. Thiophanate-Methyl and Carbendazim (MBC). Human Health Assessment Scoping Document in Support of Registration Review. EPA-HQ-OPP-2014-0004-0010. DP No. D413079. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Carbon disulfide

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Carbon disulfide
CASRN:	75-15-0
DTXSID:	DTXSID6023947
Use:	Former insecticide/fumigant; rubber additive; industrial solvent; chemical intermediate
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	X
Human Neurotoxics	X
PubMed Neurotoxics	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.00067

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	reproductive and developmental effects	10	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	600	fetal toxicity and fetal malformations	women of childbearing age	IRIS	1987

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.4	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Carbon disulfide

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.1	mg/kg/day	IRIS 1987	Hardin et al. 1981	fetal toxicity and fetal malformations	women of childbearing age	35.4	565	[191]	NOTE: high volatility and very low odor threshold: from 0.0243 mg/m3 to 23.1 mg/m3 (0.0078 to 7.4 ppm)
			ATSDR 1996						[11]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Systemic, Neurological	200	Gao, 2014				1995-08-01	2020-02-13	528	10	71	2

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Minimal Risk Level (MRL)	0.01	mg/kg/day	CDC ATSDR	
Benchmark	0.16	mg/L	CalEPA OEHHA Chemical Database	
Chronic Health-Based Guidance Value	0.7	mg/L	MN DOH	
Chronic inhalation Minimal Risk Level (MRL)	0.3	ppm	CDC ATSDR	
Reference Concentration (RfC)	0.7	mg/m^3	EPA IRIS	
Reference Concentration (RfC)	800	ug/m^3	CalEPA OEHHA Chemical Database	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	2125	mg/kg	NIH HSDB	min
LD50	3188	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	0.43	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity test	0.705	no units	TEST QSAR	
Developmental toxin test			TEST QSAR	

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OCCURRENCE DATA

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	6,049	723	Sites	12	0.01	0.1	0.4	34	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	243	54	Sites	22	0.01	0.02	0.1	34	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	5,806	669	Sites	12	0.01	0.1	0.6	7.3	ug/L	
Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data		Number of States	Amount Released (lbs/year)	Chemical Production Data		Production Volume (lbs/year)	
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)		29	8,774,313	Chemical Data Reporting (CDR) Results (EPA) (2016)		250M - 500M	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	127	8	Sites	6.3	0.5	0.73	1.6	8.72	ug/L	
Bradley et al. 2018 (Finished) [53]	2016	26	9	Sites	35	0.01649	0.0211	0.151	0.2946	ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	799	20	Sites	2.5	0.51	0.74	3.4	240	ug/L	
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	187	15	Sites	8.02	0.1	0.1	0.2	0.3	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3,202	168	Sites	5.25	0.1	0.3	3	12.4	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	3,385	183	Sites	5.41	0.1	0.2	2.87	12.4	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	14	Sites	37	0.01248	0.0357	0.137	0.2378	ug/L	
Arnold et al. 2016 (Unfiltered) [7]	2012 - 2013	685	120	Sites	18	0.0102	0.0749	0.61	4.2	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.0000243	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	18.0411	days	
Boiling point	OPERA QSAR	47.2959	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	365.359	mmHg	
Vapor pressure	TEST QSAR			
Solubility in water	OPERA QSAR	0.0213938	mol/L	
Solubility in water	TEST QSAR			
Bioconcentration factor	OPERA QSAR	18.2423	no units	
Bioconcentration factor	TEST QSAR			
Henry's Law constant	OPERA QSAR	0.00944903	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.95653	no units	

Carbon disulfide

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
11	ATSDR. 1996. Toxicological Profile for Carbon Disulfide. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. Environmental science & technology, 51(9), 4792-4802.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. Environmental science & technology, 52(23), 13972-13985.
191	USEPA. 1987. Chemical Assessment Summary, Carbon Disulfide. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, D.C.

Chlordecone

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Chlordecone
CASRN:	143-50-0
DTXSID:	DTXSID1020770
Use:	Formerly as insecticide, fungicide, miticide
Chemical Notes:	Canceled pesticide. Last end of use date: 4/4/1977.

Is the contaminant on any lists?	
CERCLA	X
FIFRA	X
Human Neurotoxics	X
PubMed Neurotoxics	X
Neurodev. Disruptors	
Androgen Receptors in vitro	X
Compounds with neurodev effects, Mundy et al 2015	X

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	67

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	carcinogen with linear MOA		

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.003	liver hepatocellular carcinoma	general population	IRIS	2009

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.2	90th Percentile	All Ambient Water	NWIS	2008-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Chlordecone

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0003	mg/kg/day	IRIS 2009	Larson et al. 1979	renal lesions (glomerulosclerosis) in female rats	general population	33.8	1.78	[300]	NOTE: canceled registration, OPP does not provide a publicly-available health assessment for chlordecone; the chlordecone entry in the IRIS database was preserved at the request of EPA program offices and regions and serves as
Cancer Slope Factor (CSF)	10	(mg/kg/day) ⁻¹	IRIS 2009	NCI 1976	liver hepatocellular carcinoma	general population	33.8	0.00296	[300]	NOTE: canceled registration, OPP does not provide a publicly-available health assessment for chlordecone; the chlordecone entry in the IRIS database was preserved at the request of EPA program offices and regions and serves as
Cancer Classification (CC)	L		IRIS 2009						[300]	NOTE: canceled registration, OPP does not provide a publicly-available health assessment for chlordecone; the chlordecone entry in the IRIS database was preserved at the request of EPA program offices and regions and serves as
			OPP							

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Minimal Risk Level (MRL)	0.01	mg/kg/day	CDC ATSDR	
Cancer Slope Factor (CSF)	16	(mg/kg/day) ⁻¹	CalEPA OEHHA Chemical Database	
Inhalation Unit Risk (IUR)	0.0046	ug/m ³	CalEPA OEHHA Chemical Database	
Intermediate Minimal Risk Level (MRL)	0.0005	mg/kg/day	CDC ATSDR	
Cancer Classification (CC)	2B	no units	WHO IARC	
Cancer Classification (CC)	Female.Mice P	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats P	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice P	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats P	no units	HHS NTP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	2550	mg/kg	NIH HSDB	max
LD50	65	mg/kg	NIH HSDB	min
Percent of active toxicant in vitro assays tested	44.29	percent	EPA Chemistry Dashboard	
TD50	0.705	mg/kg/day	NIH CPDB	min
TD50	29.3	mg/kg/day	NIH CPDB	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0003882	mol/kg	TEST QSAR	
Ames mutagenicity test	0.529	no units	TEST QSAR	
Developmental toxin test			TEST QSAR	

Chlordecone

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	1	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	2	2	Sites	100	0.2	0.2	0.2	0.2	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	2	2	Sites	100	0.2	0.2	0.2	0.2	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.000000194	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	913.927	days	
Boiling point	OPERA QSAR	373.013	degree C	
Boiling point	TEST QSAR	354.456	degree C	
Vapor pressure	OPERA QSAR	0.000000162	mmHg	
Vapor pressure	TEST QSAR	0.000000465	mmHg	
Solubility in water	OPERA QSAR	0.00000296	mol/L	
Solubility in water	TEST QSAR	0.00000232	mol/L	
Bioconcentration factor	OPERA QSAR	1458.84	no units	
Bioconcentration factor	TEST QSAR			
Henry's Law constant	OPERA QSAR	0.0000926	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	5.49303	no units	

Chlordecone

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
300	USEPA. 2009. Chemical Assessment Summary, Chlordecone (Kepone). U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, D.C.

Chloromethane (Methyl chloride)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Chloromethane (Methyl chloride)
CASRN:	74-87-3
DTXSID:	DTXSID0021541
Use:	Foaming agent; in organic synthesis; naturally-occurring gas
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	X
Human Neurotoxics	X
PubMed Neurotoxics	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
		9	6

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
1.7	90th Percentile	Finished Water	UCMR3	2013-2015

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
		X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Chloromethane (Methyl chloride)
CCL 5 Contaminant Information Sheet
HEALTH EFFECTS DATA

EPA-OGWDW and OST

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Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0036	mg/kg/day	OW 1989	Repko et al., 1976	mild neurological effects	general population	33.8	21.3	[205]	
Cancer Classification (CC)	I		PPRTV 2012						[326]	NOTE: no oral toxicity values have been derived for chloromethane because it primarily exists as a gas
Cancer Classification (CC)	D		IRIS 2001						[243]	
Cancer Classification (CC)	C		OW 1989						[205]	
			ATSDR 1998						[13]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	0.4	mg/L	EPA DWSHA 2018	
Acute inhalation Minimal Risk Level (MRL)	0.5	ppm	CDC ATSDR	
Cancer Classification (CC)	3	no units	WHO IARC	
Chronic inhalation Minimal Risk Level (MRL)	0.05	ppm	CDC ATSDR	
Intermediate Inhalation Minimal Risk Level (MRL)	0.2	ppm	CDC ATSDR	
Reference Concentration (RfC)	0.09	mg/m ³	EPA IRIS	
Subchronic RfC	3	mg/m ³	EPA PPRTV	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1800	mg/kg	NIH HSDB	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0057016	mol/kg	TEST QSAR	
Ames mutagenicity test	0.487	no units	TEST QSAR	
Developmental toxin test			TEST QSAR	

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July 2021

EPA - Office of Water

Chloromethane (Methyl chloride)
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data											
Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019			Prevalence				Magnitude			
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015	4,916	138	Sites	2.81	0.2	0.4	1.7	11.3	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997	23,478	528	Sites	2.25	0.00073	1.4	5	312	ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992	20,246	248	Sites	1.22	0.01	1.9	12.2	550	ug/L	
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	7,366	189	Sites	2.57	0.02	0.1	0.2	320	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	269	53	Sites	20	0.02	0.1	0.1	320	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	7,097	136	Sites	1.92	0.1	0.1	0.2	21	ug/L	
Pesticide Application Data				Toxic Release Data				Chemical Production Data			
Number of States	Amount Applied (lbs/year)	Date		Number of States	Amount Released (lbs/year)						Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)	24	1,088,720		Chemical Data Reporting (CDR) Results (EPA) (2016)			1B - 5B

Non-Scoring Data											
Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	398	40	Sites	10	0.19	0.745	1.6	35	ug/L	
Drinking Water Monitoring Data - MA (Finished)	2006 - 2020	899	83	Sites	9.23	0.5	1.1	3.85	44.6	ug/L	
Drinking Water Monitoring Data - WA (Finished)	2006 - 2011	1,188	28	Sites	2.36	0.07	1.42	4.73	320	ug/L	
Bradley et al. 2018 (Finished) [53]	2016	26	6	Sites	23	0.1607	0.186	0.233	0.2694	ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	4,242	218	Sites	5.14	0.076	0.75	2	21.2	ug/L	
Drinking Water Monitoring Data - FL (Source)	2006 - 2011	3	2	Sites	67	0.49	36.2	64.8	72	ug/L	
Drinking Water Monitoring Data - MA (Source)	2006 - 2020	133	17	Sites	13	0.5	0.7	3.66	4.9	ug/L	
Drinking Water Monitoring Data - PA (Source)	2006 - 2011	14	0	Sites	0						
Drinking Water Monitoring Data - WA (Source)	2006 - 2011	1,666	8	Sites	0.48	0.65	0.83	5.04	6.3	ug/L	
Drinking Water Monitoring Data - WI (Source)	2012-2019	135	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	240	3	Sites	1.25	0.2	0.4	0.82	1	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3,492	38	Sites	1.09	0.1	0.4	1.1	4	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	3,728	41	Sites	1.1	0.1	0.4	1.08	4	ug/L	
Arnold et al. 2016 (Unfiltered) [7]	2012 - 2013	685	2	Sites	0.29	0.3	1.45	2.37	2.6	ug/L	
Waste Water Effluent											
				Prevalence				Magnitude			
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Expcast exposure			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	16.4952	days	
Boiling point	OPERA QSAR	-26.1513	degree C	
Boiling point	TEST QSAR	-0.434	degree C	
Vapor pressure	OPERA QSAR	2473.43	mmHg	
Vapor pressure	TEST QSAR	1866.38	mmHg	
Solubility in water	OPERA QSAR	0.0623759	mol/L	
Solubility in water	TEST QSAR	0.418794	mol/L	
Bioconcentration factor	OPERA QSAR	9.6851	no units	
Bioconcentration factor	TEST QSAR	3.8815	no units	
Henry's Law constant	OPERA QSAR	0.00943159	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	0.947026	no units	

Chloromethane (Methyl chloride)

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
13	ATSDR. 1998. Toxicological Profile for Chloromethane. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. Environmental science & technology, 52(23), 13972-13985.
205	USEPA. 1989. Chloromethane Health Advisory. U.S. Environmental Protection Agency, Office of Water, Washington, D.C.
243	USEPA. 2001. Chemical Assessment Summary, Chloromethane. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, D.C.
326	USEPA. 2012. Provisional Peer-Reviewed Toxicity Values for Chloromethane. U.S. Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment, Superfund Health Risk Technical Support Center, Cincinnati, OH.

Chlorothalonil

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Chlorothalonil
CASRN:	1897-45-6
DTXSID:	DTXSID0020319
Use:	Fungicide; bactericide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0051

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	non-cancer effects	4	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	100	renal epithelial hyperplasia in the proximal convoluted tubules of females	general population	OPP	2010

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.51	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Chlorothalonil

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.02	mg/kg/day	OPP 2010	Spencer-Briggs 1996	renal epithelial hyperplasia in the proximal convoluted tubules of females	general population	33.8	118	[309]	
Cancer Classification (CC)	L		OPP 2010						[309]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	0.2	mg/L	EPA DWSHA 2018	
Cancer Slope Factor (CSF)	0.017	(mg/kg/day)^-1	CalEPA OEHHA Chemical Database	
Chronic Health-Based Guidance Value	0.003	mg/L	MN DOH	
Lifetime Health Advisory	0.0015	mg/L	EPA DWSHA 2018	
Cancer Classification (CC)	2B	no units	WHO IARC	
Cancer Classification (CC)	Female.Mice N	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats P	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice N	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats P	no units	HHS NTP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	10000	mg/kg	NIH HSDB	max
LD50	242	mg/kg	NIH HSDB	min
LOAEL	0.9	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	500	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	1.8	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	250	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	37.28	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	2.3	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	750	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	1.5	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	250	mg/kg/day	EPA Toxicity Reference Database	max
TD50	1180	mg/kg/day	NIH CPDB	min
TD50	20100	mg/kg/day	NIH CPDB	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0048978	mol/kg	TEST QSAR	
Ames mutagenicity test	0.05	no units	TEST QSAR	
Developmental toxin test	0.29	no units	TEST QSAR	

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EPA - Office of Water

Chlorothalonil

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	5,787	21	Sites	0.36	0.01	0.09	0.51	3.33	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	951	16	Sites	1.68	0.01	0.07	0.626	3.33	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	4,836	5	Sites	0.1	0.09	0.25	0.385	0.41	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	48	11,506,189	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	7	1,036,501	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	69	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	12	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	739	3	Sites	0.41	0.018	0.033	0.0354	0.036	ug/L	
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	137	22	Sites	16	1.00E - 04	0.0046	0.0282	0.158	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	70	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	207	22	Sites	11	1.00E - 04	0.0046	0.0282	0.158	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	1	Sites	0.44	3.2	3.2	3.2	3.2	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	218	1	Sites	0.46	3.2	3.2	3.2	3.2	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	565	5	Sites	0.88	0.0067	0.105	0.159	0.187	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	5	Sites	13	0.0033	0.0061	0.00638	0.0065	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.000000218	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	5.52071	days	
Boiling point	OPERA QSAR	344.049	degree C	
Boiling point	TEST QSAR	341.73	degree C	
Vapor pressure	OPERA QSAR	0.000000897	mmHg	
Vapor pressure	TEST QSAR	0.000218776	mmHg	
Solubility in water	OPERA QSAR	0.00000281	mol/L	
Solubility in water	TEST QSAR	0.0000229	mol/L	
Bioconcentration factor	OPERA QSAR	75.4862	no units	
Bioconcentration factor	TEST QSAR	44.2	no units	
Henry's Law constant	OPERA QSAR	0.00000281	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.09917	no units	

Chlorothalonil

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
309	USEPA. 2010. Chlorothalonil. Registration Request for Use on Low-Growing Berry Subgroup 13-07G; Bushberry Subgroup 13-07B; Onion, Bulb Subgroup 3-07A; and Onion, Green Subgroup 3-07B. Human Health Risk Assessment. EPA-HQ-OPP-2018-0517-0003. DP No. D370486. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Chlorpyrifos

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Chlorpyrifos
CASRN:	2921-88-2
DTXSID:	DTXSID4020458
Use:	Insecticide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	X
Human Neurotoxicants	X
PubMed Neurotoxicants	X
Neurodev. Disruptors	X
Androgen Receptors in vitro	X
Compounds with neurodev effects, Mundy et al 2015	X

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.015

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	reproductive and developmental effects	1	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	2	decreased brain cholinesterase activity	women of childbearing age	OPP	2011

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.0305	90th Percentile	Finished Water	UCMR4	2018-2019

PUBLIC NOMINATION STATUS

Public Nomination
X

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis
Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Chlorpyrifos

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0003	mg/kg/day	OPP 2011	Hoberman 1998; Mandralla & Brzak 1998	decreased brain cholinesterase activity in pregnant dams	women of childbearing age	35.4	1.69	[318]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	0.03	mg/L	EPA DWSHA 2018	
Acute Health-Based Guidance Value	0.002	mg/L	MN DOH	
Acute Health-Based Guidance Value	0.0006	mg/L	MN DOH	
Acute Minimal Risk Level (MRL)	0.003	mg/kg/day	CDC ATSDR	
Chronic Health-Based Guidance Value	0.0006	mg/L	MN DOH	
Drinking Water Guideline Value	0.03	mg/L	WHO Drinking Water Quality Guidelines	
Intermediate Minimal Risk Level (MRL)	0.003	mg/kg/day	CDC ATSDR	
Lifetime Health Advisory	0.002	mg/L	EPA DWSHA 2018	
Maximum Allowable Concentration (MAC)	0.09	mg/L	Canadian Drinking Water Guidelines	
Short-Term/Subchronic Health-Based Guidance Value	0.0006	mg/L	MN DOH	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1000	mg/kg	NIH HSDB	max
LD50	26.9	mg/kg	NIH HSDB	min
LOAEL	15	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	0.03	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	0.01	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	3	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	18.73	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	0.75	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	0.15	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0003048	mol/kg	TEST QSAR	
Ames mutagenicity test	-0.097	no units	TEST QSAR	
Developmental toxin test	0.595	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Chlorpyrifos
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data											
Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019	3,649	1	Sites	0.03	0.0305	0.0305	0.0305	0.0305	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	11,249	620	Sites	5.51	0.00022	0.007	0.029	0.57	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	2,233	573	Sites	26	0.00022	0.007	0.029	0.57	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	9,017	47	Sites	0.52	0.00057	0.005	0.0149	0.215	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	48	7,971,347	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data											
Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	6	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	92	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	1,553	94	Sites	6.05	0.00051	0.0067	0.0618	11.3	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3,630	6	Sites	0.17	0.0028	0.00485	0.0205	0.0398	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	5,182	100	Sites	1.93	0.00051	0.0067	0.0606	11.3	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	20,007	3,554	Sites	18	7e-07	0.0188	0.162	9.4	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	30	Sites	79	2.42e-05	0.000322	0.00396	0.0904	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	1	Sites	0.14	6e-04	6e-04	6e-04	6e-04	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	1	Sites	50	0.009	0.0095	0.0099	0.01	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
USGS, McKenzie River, Oregon, 2012 (Ambient) [158]	2002 - 2010	133	1	Samples	0.8				0.01	ug/L	
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	0	Sites	0						
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exposure exposure		0.000000023	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.75106	days	
Boiling point	OPERA QSAR	371.599	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.0000259	mmHg	
Vapor pressure	TEST QSAR	0.0000308	mmHg	
Solubility in water	OPERA QSAR	0.00000316	mol/L	
Solubility in water	TEST QSAR	0.00000236	mol/L	
Bioconcentration factor	OPERA QSAR	1687.74	no units	
Bioconcentration factor	TEST QSAR	380.189	no units	
Henry's Law constant	OPERA QSAR	0.00000209	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	4.85185	no units	

Chlorpyrifos

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
158	Reconnaissance of Land-Use Sources of Pesticides in Drinking Water, McKenzie River, Oregon. U.S. Geological Survey Scientific Investigations Report 2012–5091, 46 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
318	USEPA. 2011. Chlorpyrifos: Preliminary Human Health Risk Assessment for Registration Review. EPA-HQ-OPP-2008-0850-0025. DP No. D388070. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Clomazone

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Clomazone
CASRN:	81777-89-1
DTXSID:	DTXSID1032355
Use:	Herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.000079

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
3	no adverse effects	9	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	5000	no adverse effects identified	general population	OPP	2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.39567	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Clomazone

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.84	mg/kg/day	OPP 2018	Morrow 1983	no effects identified at loael selected as pod	general population	33.8	4970	[398]	
Cancer Classification (CC)	NL		OPP 2018						[398]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	30	mg/L	EPA HHBP	
Acute PAD	1	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	5.4	mg/L	EPA HHBP	
Population-Adjusted Dose (PAD)	0.84	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1369	mg/kg	NIH HSDB	min
LD50	2077	mg/kg	NIH HSDB	max
LOAEL	100	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	300	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	100	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	50	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	5.13	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	273	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	160.9	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0025942	mol/kg	TEST QSAR	
Ames mutagenicity test	1.078	no units	TEST QSAR	
Developmental toxin test	0.592	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Clomazone
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	14	1	Sites	7.14	0.01	0.0659	0.396	0.537	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	14	1	Sites	7.14	0.01	0.0659	0.396	0.537	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	33	1,039,399	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	5	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	132	33	Sites	25	0.0022	0.0476	1.45	19.4	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	135	33	Sites	24	0.0022	0.0476	1.45	19.4	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	221	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	216	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	5	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	414	129	Sites	31	0.0045	0.288	2.82	12	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	2	Sites	5.26	0.0064	0.467	0.835	0.9271	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		7.58E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.33433	days	
Boiling point	OPERA QSAR	279.519	degree C	
Boiling point	TEST QSAR	310.651	degree C	
Vapor pressure	OPERA QSAR	0.000103082	mmHg	
Vapor pressure	TEST QSAR	0.0000329	mmHg	
Solubility in water	OPERA QSAR	0.00482471	mol/L	
Solubility in water	TEST QSAR	0.00106414	mol/L	
Bioconcentration factor	OPERA QSAR	37.6372	no units	
Bioconcentration factor	TEST QSAR			
Henry's Law constant	OPERA QSAR	3.33E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.35315	no units	

Clomazone

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
398	USEPA. 2018. Clomazone: Human Health Risk Assessment for Proposed (1) New Uses on Cilantro, Dill, and Rapeseed Subgroup 20A; (2) Tolerance Revisions of Cucurbit Vegetable Group 9; (3) Tolerance Expansions of Representative Commodities to (i) Cottonseed Subgroup 20C, (ii) Stalk and Stem Vegetable Subgroup 22A, except Kohlrabi, (iii) Dry Bean, and (iv) Succulent Bean; and (4) Tolerance Conversions from Crop Subgroup 5A (Head and Stem Brassica) to Crop Group 5-16 (Brassica Head and Stem Vegetable), Chinese Broccoli and Kohlrabi. EPA-HQ-OPP-2017-0372-0008. DP No. D445140.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Clopyralid

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Clopyralid
CASRN:	1702-17-6
DTXSID:	DTXSID9029221
Use:	Herbicide, food additive
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.00015

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	non-cancer effects	5	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	900	increased epithelial hyperplasia and thickening of the limiting ridge of the stomach	general population	OPP	2019

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.132	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Clopyralid

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.15	mg/kg/day	OPP 2019	Barna-Lloyd et al. 1985 and 1986	increased epithelial hyperplasia and thickening of the limiting ridge of the stomach	general population	33.8	888	[415]	
Cancer Classification (CC)	NL		OPP 2019						[415]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Chronic Human Health Benchmark	0.96	mg/L	EPA HHBP	
Health-Based Screening Level	0.96	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.15	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	4300	mg/kg	NIH HSDB	min
LD50	5000	mg/kg	NIH HSDB	max
LOAEL	150	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	2000	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	15	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	500	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	2.38	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	5000	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	2000	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0099541	mol/kg	TEST QSAR	
Ames mutagenicity test	0.114	no units	TEST QSAR	
Developmental toxin test	0.26	no units	TEST QSAR	

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Clopyralid
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	6,464	34	Sites	0.53	0.01	0.04	0.132	0.53	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	969	30	Sites	3.1	0.01	0.04	0.136	0.53	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	5,495	4	Sites	0.07	0.01	0.015	0.02	0.02	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	46	2,037,895	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	6	Sites	35	0.0057	0.012	0.0474	0.684	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	198	0	Sites	0						
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	542	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	740	0	Sites	0						
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	9	Sites	3.93	0.005661	0.012	0.036	0.36	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	218	5	Sites	2.29	0.005661	0.00566	0.0227	0.024	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	4	Sites	33	0.0057	0.012	0.036	0.36	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	182	0	Sites	0						
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	106	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		1.17E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.53754	days	
Boiling point	OPERA QSAR	286.1	degree C	
Boiling point	TEST QSAR	293.982	degree C	
Vapor pressure	OPERA QSAR	0.0000209	mmHg	
Vapor pressure	TEST QSAR	0.0000647	mmHg	
Solubility in water	OPERA QSAR	0.00334275	mol/L	
Solubility in water	TEST QSAR	0.0301995	mol/L	
Bioconcentration factor	OPERA QSAR	3.76695	no units	
Bioconcentration factor	TEST QSAR	2.5527	no units	
Henry's Law constant	OPERA QSAR	4.79E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.19217	no units	

Clopyralid

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
415	USEPA. 2019. Clopyralid. Draft Human Health Risk Assessment for Registration Review of the Herbicide. EPA-HQ-OPP-2014-0167-0031. DP No. D442247. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Clothianidin

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Clothianidin
CASRN:	210880-92-5
DTXSID:	DTXSID2034465
Use:	Insecticide used on food crops
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.000017

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	reproductive and developmental effects	10	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	100	decreased body weight gain, delayed sexual maturation, decreased thymus weights in F1 pups, increased stillbirths in F1 and F2	bottle-fed infants	OPP	2019

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.0017	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.098	mg/kg/day	OPP 2019	Freshwater and Astroff 2000	decreased body weight gain, delayed sexual maturation, decreased thymus weights in F1 pups, increased stillbirths in F1 and F2	bottle-fed infants	151	130	[416]	
Cancer Classification (CC)	NL		OPP 2019						[416]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Health-Based Guidance Value	0.2	mg/L	MN DOH	
Acute Human Health Benchmark	1.7	mg/L	EPA HHBP	
Acute PAD	0.25	mg/kg/day	EPA HHBP	
Chronic Health-Based Guidance Value	0.2	mg/L	MN DOH	
Chronic Human Health Benchmark	0.63	mg/L	EPA HHBP	
Health-Based Screening Level	0.63	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.098	mg/kg/day	EPA HHBP	
Short-Term/Subchronic Health-Based Guidance Value	0.2	mg/L	MN DOH	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	389	mg/kg	NIH HSDB	min
LD50	5000	mg/kg	NIH HSDB	max
LOAEL	215.89999	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	31.200001	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	10	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	65.1	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	1.94	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	202	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic LOAEL	40.900002	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	21.2	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	34	mg/kg/day	EPA Toxicity Reference Database	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0023933	mol/kg	TEST QSAR	
Ames mutagenicity test	0.998	no units	TEST QSAR	
Developmental toxin test	0.597	no units	TEST QSAR	

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Clothianidin
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	5	1	Sites	20	9.00E - 04	0.0014	0.0017	0.0019	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	5	1	Sites	20	9.00E - 04	0.0014	0.0017	0.0019	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	31	163,492	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	10	3	Sites	30	0.008	0.008	0.0102	0.018	ug/L	
Klarich et al. 2017 (Finished) [117]	2016	20	16	Sites	80	0.00389	0.0119	0.0291	0.03346	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	131	55	Sites	42	9.00E - 04	0.0092	0.0783	1.34	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	12	4	Sites	33	0.0123	0.0274	0.0491	0.0555	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	143	59	Sites	41	9.00E - 04	0.0094	0.0777	1.34	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	227	3	Sites	1.32	0.008	0.008	0.0265	0.045	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	218	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	10	3	Sites	30	0.008	0.008	0.0265	0.045	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	279	5	Sites	1.79	0.0311	0.0462	0.0645	0.0675	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	9	Sites	24	0.0026	0.0113	0.0438	0.0663	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		9.22E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.55019	days	
Boiling point	OPERA QSAR	326.625	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.000000197	mmHg	
Vapor pressure	TEST QSAR			
Solubility in water	OPERA QSAR	0.00076435	mol/L	
Solubility in water	TEST QSAR	0.00200447	mol/L	
Bioconcentration factor	OPERA QSAR	9.38346	no units	
Bioconcentration factor	TEST QSAR			
Henry's Law constant	OPERA QSAR	1.82E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	0.762847	no units	

Clothianidin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
117	Klarich, K.L., Pflug, N.C., DeWald, E.M., Hladik, M.L., Kolpin, D.W., Cwiertny, D.M. and LeFevre, G.H., 2017. Occurrence of neonicotinoid insecticides in finished drinking water and fate during drinking water treatment. <i>Environmental Science & Technology Letters</i> , 4(5), pp.168-173.
416	USEPA. 2019. Clothianidin. Human Health Risk Assessment to Address Residues from New/Amended Uses of Thiamethoxam. EPA-HQ-OPP-2018-0779-0004. DP No. D446686. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Cobalt

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Cobalt
CASRN:	7440-48-4
DTXSID:	DTXSID1031040
Use:	Use data are for cobaltous chloride: Formerly in medicines; as germicide; naturally-occurring
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	2.6

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	reproductive and developmental effects	9	7

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	2	"decreased iodine uptake in humans"	women of childbearing age	PPRTV	2008

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
5.198	90th Percentile	Finished Water	UCMR3	2013-2015

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
		X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Cobalt

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0003	mg/kg/day	PPRTV 2008	Roche and Layrisse 1956	"decreased iodine uptake in humans"	women of childbearing age	35.4	1.69	[294]	
			ATSDR 2004						[20]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Hematologic, Systemic	10	Nejad, 2014	Immune	10	Nejad, 2014	2007-08-01	2019-10-22	6161	13	287	2

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Chronic inhalation Minimal Risk Level (MRL)	0.0001	mg/m ³	CDC ATSDR	
Inhalation Unit Risk (IUR)	9	ug/m ³	EPA PPRTV	
Intermediate Minimal Risk Level (MRL)	0.01	mg/kg/day	CDC ATSDR	
Reference Concentration (RfC)	0.000006	mg/m ³	EPA PPRTV	
Subchronic Provisional RfD	0.003	mg/kg/day	EPA PPRTV	
Subchronic RfC	0.00002	mg/m ³	EPA PPRTV	
Cancer Classification (CC)	2B	no units	WHO IARC	
Cancer Classification (CC)	2B	no units	WHO IARC	
Cancer Classification (CC)	Female.Mice P	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats P	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice P	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats P	no units	HHS NTP	

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	6171	mg/kg	NIH HSDB	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity test			TEST QSAR	
Developmental toxin test			TEST QSAR	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Cobalt
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015	4,922	247	Sites	5.02	1	1.8	5.2	1097.099	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986	989	3	Sites	0.3	6	10	10	11	ug/L	
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	7,630	5,028	Sites	66	0.007	0.151	1.55	684	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	466	137	Sites	29	0.02	0.167	1.03	53.2	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	7,164	4,891	Sites	68	0.007	0.147	1.64	684	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)	38	240,271	Chemical Data Reporting (CDR) Results (EPA) (2016)	10M - 50M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	70	33	Sites	47	0.002	0.108	0.3	1.07	ug/L	
Bradley et al. 2018 (Finished) [53]	2016	26	12	Sites	46	0.04	0.11	0.147	0.18	ug/L	
Community Water System Survey (CWSS) (Finished) [178]	2006	1	NA	Sites							
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	139	47	Sites	34	0.009	0.166	2.1	29	ug/L	
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	1,272	1,167	Sites	92	0.005	0.21	1.5	508	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	4,565	2,769	Sites	61	0.007	0.129	2.88	1230	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	5,825	3,934	Sites	68	0.005	0.19	1.95	1230	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	757	602	Sites	80	0.022	0.0775	0.881	52.4	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)	0.28	ug/l	
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Cobalt

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
20	ATSDR. 2004. Toxicological Profile for Cobalt. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. Environmental science & technology, 52(23), 13972-13985.
178	USEPA (US Environmental Protection Agency). (2009). 2006 Community Water System Survey. Overview, 57.
294	USEPA. 2008. Provisional Peer Reviewed Toxicity Values for Cobalt (CASRN 7440-48-4). EPA/690/R-08/008F. U.S. Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment, Superfund Health Risk Technical Support Center, Cincinnati, OH.

Cotinine

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Cotinine
CASRN:	486-56-6
DTXSID:	DTXSID1047576
Use:	Urinary metabolite of nicotine
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
		9	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.1058	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Cotinine
CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
										NOTE: No health assessments found

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
							2020-04-06	4070	9	129	0

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Percent of active toxcast in vitro assays tested	0.6	percent	EPA Chemistry Dashboard	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0026363	mol/kg	TEST QSAR	
Ames mutagenicity test	0.336	no units	TEST QSAR	
Developmental toxin test	0.642	no units	TEST QSAR	

Cotinine
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	1,142	64	Sites	5.6	0.00027	0.0117	0.106	0.38	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	144	63	Sites	44	0.00027	0.012	0.106	0.38	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	998	1	Sites	0.1	0.00506	0.00506	0.00506	0.00506	ug/L	
Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data			Number of States	Amount Released (lbs/year)	Chemical Production Data		Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)					Chemical Data Reporting (CDR) Results (EPA) (2016)		

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Bradley et al. 2018 (Finished) [53]	2016	26	4	Sites	15	0.0010904	0.00166	0.00235	0.0025508	ug/L	
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	8		0.011		0.01581	ug/L	
Padhye et al. 2013 (Finished) [155]	2009 - 2010	8	1	Samples	12	0	0		4e-07 +/- 4e-07	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
IL EPA (2008) via Uslu et al. (2013) (Finished) [433]	2008	NA	NA						0.006	ug/L	
Ambient Water											
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	8		0.0153		0.01886	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	23	Sites	61	0.0011136	0.0173	0.0489	0.0680997	ug/L	
Padhye et al. 2013 (Ambient) [155]	2009 - 2010	8	2	Samples	25	0	0		2.7e-06 +/- 4e-07	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
IL EPA (2008) via Uslu et al. (2013) (Ambient) [433]	2008	NA	NA						0.012	ug/L	
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	21	Sites	100	0.0111602	0.042	0.192	0.2647215	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.000000117	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)	0.388	ng/ml	
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.34908	days	
Boiling point	OPERA QSAR	280.912	degree C	
Boiling point	TEST QSAR	279.705	degree C	
Vapor pressure	OPERA QSAR	0.000289385	mmHg	
Vapor pressure	TEST QSAR	0.000944061	mmHg	
Solubility in water	OPERA QSAR	0.252783	mol/L	
Solubility in water	TEST QSAR	0.0369828	mol/L	
Bioconcentration factor	OPERA QSAR	3.16285	no units	
Bioconcentration factor	TEST QSAR	2.46604	no units	
Henry's Law constant	OPERA QSAR	0.000000115	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	0.190328	no units	

Cotinine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. <i>Environmental science & technology</i> , 52(23), 13972-13985.
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
155	Padhye, L.P., Yao, H., Kung'u, F.T., and Huang, C.H. Year-long evaluation on the occurrence and fate of pharmaceuticals, personal care products, and endocrine disrupting chemicals in an urban drinking water treatment plant. 2014. <i>Water Research</i> 51 (2014) 266-276.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
433	Uslu, M., Jasim, S., Arvai, A., Bewtra, J. and Biswas, N., 2013. A Survey of Occurrence and Risk Assessment of Pharmaceutical Substances in the Great Lakes Basin. <i>Ozone: Science & Engineering</i> , 35(4), pp.249-262.

Cumene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Cumene
CASRN:	98-82-8
DTXSID:	DTXSID1021827
Use:	
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	X
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0054

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	non-cancer effects	4	6

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	600	increased average kidney weights	general population	IRIS	1997

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
3.24	90th Percentile	Finished Water	UCM1	1988-1992

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Cumene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.1	mg/kg/day	IRIS 1997	Wolf et al. 1956	increased average kidney weight	general population	33.8	592	[225]	
Reference Dose (RfD) or Equivalent	0.1	mg/kg/day	WHO 1999	Wolf et al. 1956	increased average kidney weight	general population	33.8	592	[436]	
Cancer Classification (CC)	D		IRIS 1997						[225]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
						2001-09-01	2020-04-14	480	0	4	

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	11	mg/L	EPA DWSHA 2018	
Chronic Health-Based Guidance Value	0.3	mg/L	MN DOH	
Reference Concentration (RFC)	0.4	mg/m ³	EPA IRIS	
Cancer Classification (CC)	2B	no units	WHO IARC	
Cancer Classification (CC)	Female.Mice P	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats SE	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice CE	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats CE	no units	HHS NTP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1400	mg/kg	NIH HSDB	min
LD50	2910	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	5.96	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.020893	mol/kg	TEST QSAR	
Ames mutagenicity test	0.04	no units	TEST QSAR	
Developmental toxin test	0.5	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Cumene
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997	22,995	56	Sites	0.24	0.1	0.6	2.58	15	ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992	12,771	35	Sites	0.27	0.01	0.9	3.24	6	ug/L	
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	6,831	75	Sites	1.1	0.005	0.03	3.5	27	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	277	14	Sites	5.05	0.005	0.2	3.5	3.8	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	6,554	61	Sites	0.93	0.005	0.0285	3.76	27	ug/L	
Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data			Number of States	Amount Released (lbs/year)	Chemical Production Data		Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			41	924,489	Chemical Data Reporting (CDR) Results (EPA) (2016)		5B - 10B

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	9	NA	Sites	0					ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	846	17	Sites	2.01	0.01	0.01	0.09	1.77	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3,434	34	Sites	0.99	0.01	0.0355	0.83	39.6	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	4,277	51	Sites	1.19	0.01	0.0245	0.8	39.6	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	9	NA	Sites	0					ug/L	
Arnold et al. 2016 (Unfiltered) [7]	2012 - 2013	158	1	Sites	0.63	0.064	0.064	0.064	0.064	ug/L	
Southeast Stream Quality Assessment (SESQA) (Ambient) [102]	2014	1	0	Sites	0						
Southeast Stream Quality Assessment (SESQA) (Ambient) [102]	2014	2	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	1	Sites	50						
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	0	Sites	0						
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.000106	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)	< LOD	ng/ml	
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	12.7811	days	
Boiling point	OPERA QSAR	157.394	degree C	
Boiling point	TEST QSAR	160.61	degree C	
Vapor pressure	OPERA QSAR	3.23017	mmHg	
Vapor pressure	TEST QSAR	2.95121	mmHg	
Solubility in water	OPERA QSAR	0.000517581	mol/L	
Solubility in water	TEST QSAR	0.000954993	mol/L	
Bioconcentration factor	OPERA QSAR	48.173	no units	
Bioconcentration factor	TEST QSAR	239.43	no units	
Henry's Law constant	OPERA QSAR	0.00860044	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.82156	no units	

Cumene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. Science of The Total Environment. v581-582, (909-922).
102	https://webapps.usgs.gov/rsqa/#!/region/SESQA
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. Science of the Total Environment, 636, 69-79.
225	USEPA. 1997. Chemical Assessment Summary, Cumene. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, D.C.
436	WHO. 1999. Concise International Chemical Assessment Document 18, Cumene. World Health Organization (WHO), Geneva, Switzerland.

Cycloate

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Cycloate
CASRN:	1134-23-2
DTXSID:	DTXSID6032356
Use:	Herbicide for annual grasses, nutgrass, many broadleafweeds in sugar beets, table beets, spinach
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.038

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	non-cancer effects	2	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	3	spinal nerve axonal atrophy and femoral nerve alterations in females	general population	OPP	2015

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.1139	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Cycloate

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0005	mg/kg/day	OPP 2015	Sprague et al. 1984	spinal nerve axonal atrophy and femoral nerve alterations in females	general population	33.8	2.96	[339]	
Cancer Classification (CC)	NL		OPP 2015						[339]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.45	mg/L	EPA HHBP	
Acute PAD	0.067	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.03	mg/L	EPA HHBP	
Health-Based Screening Level	0.03	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.005	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1275	mg/kg	NIH HSDB	min
LD50	4175	mg/kg	NIH HSDB	max
LOAEL	175	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	3.0999999	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	0.5	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	75	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	2.32	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0067608	mol/kg	TEST QSAR	
Ames mutagenicity test	0.352	no units	TEST QSAR	
Developmental toxin test	0.445	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Cycloate
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	2,751	4	Sites	0.15	0.009	0.02	0.114	0.48	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	221	4	Sites	1.81	0.009	0.02	0.114	0.48	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	2,530	0	Sites	0						
Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data			Number of States	Amount Released (lbs/year)	Chemical Production Data		
Estimated Annual Agricultural Pesticide Use (USGS)	2	48,166	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			1	10	Chemical Data Reporting (CDR) Results (EPA) (2016)		
Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	3	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	13	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	16	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	363	2	Sites	0.55	0.0016	0.03	0.0986	0.128	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	621	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	984	2	Sites	0.2	0.0016	0.03	0.0986	0.128	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	121	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	114	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	8	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	180	31	Sites	17	0.0136	0.105	0.306	0.601	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	1	Sites	2.63	0.0287	0.0287	0.0287	0.0287	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	106	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Expocast exposure		8.41E-08	
Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	2.66986	days	
Boiling point	OPERA QSAR	253.174	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.0017037	mmHg	
Vapor pressure	TEST QSAR	0.00480839	mmHg	
Solubility in water	OPERA QSAR	0.000321829	mol/L	
Solubility in water	TEST QSAR	0.00052723	mol/L	
Bioconcentration factor	OPERA QSAR	44.9671	no units	
Bioconcentration factor	TEST QSAR	27.1019	no units	
Henry's Law constant	OPERA QSAR	0.000000169	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.79283	no units	

Cycloate

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
339	USEPA. 2015. Cycloate. Human Health Scoping Document in Support of Registration Review. EPA-HQ-OPP-2015-0288-0008. DP No. D424437. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Cyfluthrin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Cyfluthrin
CASRN:	68359-37-5
DTXSID:	DTXSID5035957
Use:	Insecticide; medication
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.74

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	reproductive and developmental effects	1	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	5	reduced motor activity	bottle-fed infants	OPP	2017

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
3.677		EDWC SW (acute)	OPP	2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Cyfluthrin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0039	mg/kg/day	OPP 2017	Wolansky et al. 2006	reduced motor activity	bottle-fed infants	151	5.17	[379]	
Cancer Classification (CC)	NL		OPP 2017						[379]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.1	mg/L	EPA HHBP	
Acute Human Health Benchmark	0.1	mg/L	EPA HHBP	
Acute PAD	0.02	mg/kg/day	EPA HHBP	
Acute PAD	0.02	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.15	mg/L	EPA HHBP	
Chronic Human Health Benchmark	0.15	mg/L	EPA HHBP	
Health-Based Screening Level	0.15	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.024	mg/kg/day	EPA HHBP	
Population-Adjusted Dose (PAD)	0.024	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Inhalation LOAEL	0.14	mg/L	EPA Toxicity Reference Database	max
Inhalation LOAEL	0.0011013	mg/L	EPA Toxicity Reference Database	min
Inhalation NOAEL	0.0011013	mg/L	EPA Toxicity Reference Database	min
Inhalation NOAEL	0.0259	mg/L	EPA Toxicity Reference Database	max
LD50	140	mg/kg	NIH HSDB	min
LD50	500	mg/kg	NIH HSDB	max
LOAEL	114.8	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	9	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	3	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	38.4	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	8.29	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	13.9	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	38.900002	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	10.9	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	2.5	mg/kg/day	EPA Toxicity Reference Database	min

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0015311	mol/kg	TEST QSAR	
Ames mutagenicity test	0.002	no units	TEST QSAR	
Developmental toxin test	0.873	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

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EPA - Office of Water

Cyfluthrin
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	3,675	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	383	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	3,292	0	Sites	0						
Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data			Number of States	Amount Released (lbs/year)	Chemical Production Data		Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	48	279,251	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			2	21	Chemical Data Reporting (CDR) Results (EPA) (2016)		

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	576	1	Sites	0.17	0.098	0.098	0.098	0.098	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	2,014	1	Sites	0.05	0.015	0.015	0.015	0.015	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	2,589	2	Sites	0.08	0.015	0.0565	0.0814	0.098	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	201	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	190	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	4,669	343	Sites	7.35	0.000838	0.0082	0.0322	3.4	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	7	Sites	18	0.000263	0.000548	0.000831	0.000964	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	106	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					
Estimated Drinking Water Concentration (EDWC) in Surface Water (acute)	2017	OPP	3.677	ug/L	Tier I, FOQA Index Reservoir Screening Tool (FIRST) Model (alfalfa)	The critical effect of reduced motor activity was based on an acute population adjusted dose and is considered a less-than-chronic response. To account for this, the modeled surface water acute concentration found in the most recent available EPA OPP health assessment was selected as the occurrence concentration for cyfluthrin.					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.0000019	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.35028	days	
Boiling point	OPERA QSAR	424.382	degree C	
Boiling point	TEST QSAR	442.743	degree C	
Vapor pressure	OPERA QSAR	3.81E-10	mmHg	
Vapor pressure	TEST QSAR	6.1E-10	mmHg	
Solubility in water	OPERA QSAR	0.000000029	mol/L	
Solubility in water	TEST QSAR	5.37E-08	mol/L	
Bioconcentration factor	OPERA QSAR	414.928	no units	
Bioconcentration factor	TEST QSAR	928.966	no units	
Henry's Law constant	OPERA QSAR	4.42E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	6.08154	no units	

Cyfluthrin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
379	USEPA. 2017. Cyfluthrin and Beta-Cyfluthrin: Acute and Chronic Aggregate Dietary (Food and Drinking Water) Exposure and Risk Assessment for Registration Review. EPA-HQ-OPP-2010-0684-0101. DP No. D435057. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Cyhalothrin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Cyhalothrin
CASRN:	68085-85-8
DTXSID:	DTXSID6023997
Use:	Insecticide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	X
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	reproductive and developmental effects		

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	1	reduced motor activity	bottle-fed infants	OPP	2017

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Cyhalothrin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.00093	mg/kg/day	OPP 2017	Moser et al. 2016	reduced motor activity	bottle-fed infants	151	1.23	[385]	
Cancer Classification (CC)	NL		OPP 2017						[385]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.03	mg/L	EPA HHBP	
Acute PAD	0.005	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.006	mg/L	EPA HHBP	
Health-Based Screening Level	0.006	mg/L	Health-based screening levels from USGS	
Intermediate Minimal Risk Level (MRL)	0.01	mg/kg/day	CDC ATSDR	
Population-Adjusted Dose (PAD)	0.001	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	20	mg/kg	NIH HSDB	min
LD50	5000	mg/kg	NIH HSDB	max
LOAEL	5	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	75	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	1.5	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	15	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	13.19	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	12.5	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic LOAEL	2.5	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	1	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	2.5	mg/kg/day	EPA Toxicity Reference Database	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity test			TEST QSAR	
Developmental toxin test			TEST QSAR	

Cyhalothrin
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	10	0	Sites	0						
Ambient Water											
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	123	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	113	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	10	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					
Limit of solubility as a surrogate for occurrence concentration, Surface Water, Peak	2017	OPP	5	ug/L		Cyhalothrin is very insoluble in water and residues in drinking water are expected to be very low. Therefore, the limit of solubility of cyhalothrin (5 ppb) reported in the most recent EPA OPP health assessment was used as the occurrence concentration for cyhalothrin.					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exposure exposure		0.000000177	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.54201	days	
Boiling point	OPERA QSAR	422.672	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	4.02E-09	mmHg	
Vapor pressure	TEST QSAR			
Solubility in water	OPERA QSAR	1.97E-08	mol/L	
Solubility in water	TEST QSAR			
Bioconcentration factor	OPERA QSAR	133.673	no units	
Bioconcentration factor	TEST QSAR			
Henry's Law constant	OPERA QSAR	0.000000012	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	6.63514	no units	

Cyhalothrin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
385	USEPA. 2017. Lambda- & Gamma-Cyhalothrin: Human Health Draft Risk Assessment for Registration Review. EPA-HQ-OPP-2010-0480-0299. DP No. 426321. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.

Cypermethrin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Cypermethrin
CASRN:	52315-07-8
DTXSID:	DTXSID1023998
Use:	Insecticide; veterinary medication
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	X
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	X

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.00052

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	reproductive and developmental effects	2	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	30	reduced motor activity	bottle-fed infants	OPP	2017

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.0155	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Cypermethrin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.024	mg/kg/day	OPP 2017	Wolansky et al. 2006	reduced motor activity	bottle-fed infants	151	31.8	[380]	
Cancer Classification (CC)	C		OPP 2017						[380]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.15	mg/L	EPA HHBP	
Acute Human Health Benchmark	0.15	mg/L	EPA HHBP	
Acute Human Health Benchmark	0.15	mg/L	EPA HHBP	
Acute PAD	0.023	mg/kg/day	EPA HHBP	
Acute PAD	0.023	mg/kg/day	EPA HHBP	
Acute PAD	0.023	mg/kg/day	EPA HHBP	
Health-Based Screening Level	0.15	mg/L	Health-based screening levels from USGS	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	14.9	mg/kg	NIH HSDB	min
LD50	7180	mg/kg	NIH HSDB	max
LOAEL	450	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	5	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	1	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	100	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	10.78	percent	EPA Chemistry Dashboard	max
Percent of active toxcast in vitro assays tested	5.96	percent	EPA Chemistry Dashboard	min
Subchronic LOAEL	28.200001	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	37	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	16.3	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	34.3	mg/kg/day	EPA Toxicity Reference Database	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0017298	mol/kg	TEST QSAR	
Ames mutagenicity test	0.163	no units	TEST QSAR	
Developmental toxin test	0.877	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Cypermethrin
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	3,675	5	Sites	0.14	0.006	0.009	0.0155	0.018	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	383	4	Sites	1.04	0.006	0.011	0.016	0.018	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	3,292	1	Sites	0.03	0.009	0.009	0.009	0.009	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	14	23,804	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	15	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	123	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	113	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	10	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	1,129	84	Sites	7.44	0.0017	0.0107	0.0392	0.357	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	3,711	112	Sites	3.02	0.000516	0.00825	0.0479	1.25293	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	106	0	Sites	0						
Southeast Stream Quality Assessment (SESQA) (Ambient) [102]	2014	1	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
USGS, McKenzie River, Oregon, 2012 (Ambient) [158]	2002 - 2010	71	1	Samples	1.4				0.014	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.00000162	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.34971	days	
Boiling point	OPERA QSAR	424.351	degree C	
Boiling point	TEST QSAR	445.159	degree C	
Vapor pressure	OPERA QSAR	4.74E-09	mmHg	
Vapor pressure	TEST QSAR	1.12E-09	mmHg	
Solubility in water	OPERA QSAR	0.000000368	mol/L	
Solubility in water	TEST QSAR	6.27E-08	mol/L	
Bioconcentration factor	OPERA QSAR	349.137	no units	
Bioconcentration factor	TEST QSAR	741.31	no units	
Henry's Law constant	OPERA QSAR	1.99E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	6.47753	no units	

Cypermethrin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
102	https://webapps.usgs.gov/rsqa/#!/region/SESQA
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
158	Reconnaissance of Land-Use Sources of Pesticides in Drinking Water, McKenzie River, Oregon. U.S. Geological Survey Scientific Investigations Report 2012–5091, 46 p. plus appendixes.
380	USEPA. 2017. Cypermethrin, Zeta-cypermethrin, and Alpha-cypermethrin. Draft Human Health Risk Assessment for Registration Review. EPA-HQ-OPP-2012-0167-0116. DP No. D425964. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Cyprodinil

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Cyprodinil
CASRN:	121552-61-2
DTXSID:	DTXSID1032359
Use:	Fungicide used on fruits and vegetables
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.000043

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	non-cancer effects	10	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	200	histopathological alterations in the liver (spongiosis hepatitis) in males	general population	OPP	2015

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.00868	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis
Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.027	mg/kg/day	OPP 2015	Frankhauser 1994	histopathological alterations in the liver (spongiosis hepatitis) in males	general population	33.8	160	[340]	
Cancer Classification (CC)	NL		OPP 2015						[340]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	10	mg/L	EPA HHBP	
Acute PAD	2	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.17	mg/L	EPA HHBP	
Health-Based Screening Level	0.17	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.027	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	2000	mg/kg	NIH HSDB	
LOAEL	1000	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	35.599998	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	200	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	3.22	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	23.88	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	18.950001	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	559.65997	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	231.93	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	3.24	mg/kg/day	EPA Toxicity Reference Database	min

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0048865	mol/kg	TEST QSAR	
Ames mutagenicity test	0.679	no units	TEST QSAR	
Developmental toxin test	0.516	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Cyprodinil
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	14	2	Sites	14	0.0066	0.0079	0.00868	0.0092	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	14	2	Sites	14	0.0066	0.0079	0.00868	0.0092	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	31	271,518	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	132	16	Sites	12	2.00E - 04	0.0092	0.0764	0.111	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	135	16	Sites	12	2.00E - 04	0.0092	0.0764	0.111	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	259	15	Sites	5.79	0.0091	0.034	0.125	0.144	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	1	Sites	2.63	0.0334	0.0334	0.0334	0.0334	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		1.36E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	2.93362	days	
Boiling point	OPERA QSAR	320.755	degree C	
Boiling point	TEST QSAR	345.205	degree C	
Vapor pressure	OPERA QSAR	0.0000023	mmHg	
Vapor pressure	TEST QSAR	0.00000114	mmHg	
Solubility in water	OPERA QSAR	0.0000588	mol/L	
Solubility in water	TEST QSAR	0.000378443	mol/L	
Bioconcentration factor	OPERA QSAR	29.7556	no units	
Bioconcentration factor	TEST QSAR	40.5509	no units	
Henry's Law constant	OPERA QSAR	0.000000025	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.88086	no units	

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Reference Number	Full Reference
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
340	USEPA. 2015. Cyprodinil. Human Health Risk Assessment for the Expansion of Existing Crop Group/Representative Commodity Uses to Stone Fruit Group 12-12, and Adding New Uses on the Artichoke, Guava, Pomegranate, Passionfruit, Feijoa, Jaboticaba, Wax Jambu, Starfruit, and Acerola and Amended Uses on Greenhouse Cucumbers and Small Tomatoes. EPA-HQ-OPP-2014-0506-0013. DP No. D425998. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Desethylatrazine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Desethylatrazine
CASRN:	6190-65-4
DTXSID:	DTXSID5037494
Use:	Degradation product of atrazine
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.0004

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	reproductive and developmental effects	10	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	400	attenuation of LH surge in females ages 13-49 (estrous cycle disruption)	women of childbearing age	OPP	2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.16	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X	X		

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Desethylatrazine

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.076	mg/kg/day	OPP 2018	Cooper et al. 2010	attenuation of LH surge in females ages 13-49 (estrous cycle disruption)	women of childbearing age	35.4	429	[395]	
Cancer Classification (CC)	NL		OPP 2018						[395]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Maximum Allowable Daily Level	100	ug/day	CalEPA OEHHA Chemical Database	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LOAEL	100	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	25	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	25	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	5	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	1.53	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	35.099998	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	3.3	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0072444	mol/kg	TEST QSAR	
Ames mutagenicity test	0.194	no units	TEST QSAR	
Developmental toxin test	0.582	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
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Desethylatrazine

CCL 5 Contaminant Information Sheet

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	11,386	4,408	Sites	39	0.00068	0.023	0.16	6.08	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	2,318	1,703	Sites	73	0.00068	0.025	0.16	6.08	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	9,069	2,705	Sites	30	0.001	0.013	0.165	2.6	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	9	Sites	53	0.00072	0.0413	0.157	0.928	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	1	Sites	100	0.006	0.008	0.0216	0.032	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	990	688	Sites	69	0.00104	0.04	0.254	3.63	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3,239	940	Sites	29	0.00075	0.023	0.18	2.34	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	4,228	1,628	Sites	39	0.00075	0.0351	0.215	3.63	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	155	Sites	68	0.000716	0.031	0.21	1.55	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	149	Sites	68	0.000716	0.0208	0.156	1.55	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	7	Sites	58	0.00072	0.041	0.219	1.3	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	26	Sites	68	0.0047	0.0179	0.14	0.851	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	115	Sites	17	0.002	0.0276	0.157	0.802	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	2	Sites	100	0.008	0.024	0.0664	0.114	ug/L	
USGS, McKenzie River, Oregon, 2012 (Ambient) [158]	2002 - 2010	134	21	Samples	16				0.013	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Expcast exposure		6.61E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)	< LOD	ug/l	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.36178	days	
Boiling point	OPERA QSAR	330.895	degree C	
Boiling point	TEST QSAR	323.062	degree C	
Vapor pressure	OPERA QSAR	6.42E-09	mmHg	
Vapor pressure	TEST QSAR	0.000000337	mmHg	
Solubility in water	OPERA QSAR	0.00132007	mol/L	
Solubility in water	TEST QSAR	0.0100925	mol/L	
Bioconcentration factor	OPERA QSAR	10.3224	no units	
Bioconcentration factor	TEST QSAR	3.41979	no units	
Henry's Law constant	OPERA QSAR	2.43E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.56449	no units	

Desethylatrazine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
158	Reconnaissance of Land-Use Sources of Pesticides in Drinking Water, McKenzie River, Oregon. U.S. Geological Survey Scientific Investigations Report 2012–5091, 46 p. plus appendixes.
395	USEPA. 2018. Atrazine. Draft Human Health Risk Assessment for Registration Review. EPQ-HQ-OPP-2013-0266-1159. DP No. D418316. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.

Desisopropylatrazine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Desisopropylatrazine
CASRN:	1007-28-9
DTXSID:	DTXSID0037495
Use:	Degradation product of atrazine
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.00058

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	reproductive and developmental effects	10	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	400	attenuation of LH surge in females ages 13-49 (estrous cycle disruption)	women of childbearing age	OPP	2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.2311	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis
Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Desisopropylatrazine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.076	mg/kg/day	OPP 2018	Cooper et al. 2010	attenuation of LH surge in females ages 13-49 (estrous cycle disruption)	women of childbearing age	35.4	429	[395]	
Cancer Classification (CC)	NL		OPP 2018						[395]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Maximum Allowable Daily Level	100	ug/day	CalEPA OEHHA Chemical Database	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LOAEL	25	mg/kg/day	EPA Toxicity Reference Database	
NOAEL	5	mg/kg/day	EPA Toxicity Reference Database	
Percent of active toxcast in vitro assays tested	2.65	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	18	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	3.8	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0071121	mol/kg	TEST QSAR	
Ames mutagenicity test	0.08	no units	TEST QSAR	
Developmental toxin test	0.372	no units	TEST QSAR	

Desisopropylatrazine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	4,489	802	Sites	18	0.001	0.0474	0.231	4.44	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	9	Sites	53	0.0027	0.0163	0.063	0.469	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	2,038	374	Sites	18	0	0.0441	0.17	2.66	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	68	Sites	30	0.0027	0.017	0.19	1.03	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	61	Sites	28	0.005162	0.083	0.105	1.03	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	7	Sites	58	0.0027	0.0163	0.199	0.776	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	61	Sites	8.84	0.0032	0.0224	0.212	0.489	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		6.57E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)	< LOD	ug/l	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.34468	days	
Boiling point	OPERA QSAR	328.615	degree C	
Boiling point	TEST QSAR	291.377	degree C	
Vapor pressure	OPERA QSAR	5.11E-09	mmHg	
Vapor pressure	TEST QSAR	0.000000149	mmHg	
Solubility in water	OPERA QSAR	0.00268187	mol/L	
Solubility in water	TEST QSAR	0.0161065	mol/L	
Bioconcentration factor	OPERA QSAR	10.1928	no units	
Bioconcentration factor	TEST QSAR	2.23357	no units	
Henry's Law constant	OPERA QSAR	1.02E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.26299	no units	

Desisopropylatrazine

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
395	USEPA. 2018. Atrazine. Draft Human Health Risk Assessment for Registration Review. EPQ-HQ-OPP-2013-0266-1159. DP No. D418316. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.

Desvenlafaxine

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EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Desvenlafaxine
CASRN:	93413-62-8
DTXSID:	DTXSID40869118
Use:	Medication used to treat depression
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.36

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	non-cancer effects	9	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	1	lowest therapeutic dose: inhibition of serotonin and norepinephrine reuptake/treatment of depressive disorder	bottle-fed infants	FDA; NIH	2018; 2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.361	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Desvenlafaxine

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0071	mg/kg/day	FDA 2018; NIH 2018	Wyeth Pharmaceuticals Inc. 2014b	lowest therapeutic dose -- Developmental (persistent pulmonary hypertension and nervous system effects), gastrointestinal system (nausea, constipation, decreased appetite, weight loss); male reproductive effects (erectile dysfunction, Desvenlafaxine ejaculation failure/disorder, decreased libido), nervous system (effects on serotonin hormone receptor interaction, abnormal dreams, sweating, dizziness, insomnia, mydriasis, blurred/abnormal vision, and neuroendocrine-mediated increases in blood pressure)	bottle-fed infants	151	9.40	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels
Reference Dose (RfD) or Equivalent	0.000208333	mg/kg/day	FDA 2018; NIH 2018	Alembic Pharmaceuticals Limited	lowest therapeutic dose: inhibition of serotonin and norepinephrine reuptake/treatment of depressive disorder	bottle-fed infants	151	1.40	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels
Reference Dose (RfD) or Equivalent	0.000208333	mg/kg/day	FDA 2018; NIH 2018	Alembic Pharmaceuticals Limited	lowest therapeutic dose: inhibition of serotonin and norepinephrine reuptake/treatment of depressive disorder	general population	33.8	4.90	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Health-Based Guidance Value	0.02	mg/L	MN DOH	
Acute Health-Based Guidance Value	0.02	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.02	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.02	mg/L	MN DOH	
Screening level for pharmaceutical - general population	0.004901961	mg/L	EPA Office of Water	
Screening level for pharmaceutical - infants	0.001388889	mg/L	EPA Office of Water	
Short-Term/Subchronic Health-Based Guidance Value	0.02	mg/L	MN DOH	
Short-Term/Subchronic Health-Based Guidance Value	0.02	mg/L	MN DOH	

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0027542	mol/kg	TEST QSAR	
Ames mutagenicity test	0.31	no units	TEST QSAR	
Developmental toxin test	0.652	no units	TEST QSAR	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Desvenlafaxine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	557	22	Sites	3.95	0.00072	0.0307	0.361	1.02	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	75	18	Sites	24	0.00072	0.035	0.378	1.02	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	482	4	Sites	0.83	0.00135	0.00633	0.0224	0.0307	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	205	87	Sites	42	0.00068	0.0141	0.228	2.09	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	401	6	Sites	1.5	0.00071	0.00918	0.78	0.91	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	606	93	Sites	15	0.00068	0.0138	0.332	2.09	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	16		0.0283		0.06043	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	22	Sites	58	0.0017892	0.0865	0.822	1.953482	ug/L	
Bexfield et al. 2019 (Groundwater) [49]	2013 - 2015	1,106	0	Sites	0						
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	19	Sites	90	0.0930062	0.693	1.14	4.4928736	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.65547	days	
Boiling point	OPERA QSAR	313.112	degree C	
Boiling point	TEST QSAR	327.611	degree C	
Vapor pressure	OPERA QSAR	5.09E-08	mmHg	
Vapor pressure	TEST QSAR	0.00000177	mmHg	
Solubility in water	OPERA QSAR	0.0207862	mol/L	
Solubility in water	TEST QSAR	0.000695024	mol/L	
Bioconcentration factor	OPERA QSAR	16.0501	no units	
Bioconcentration factor	TEST QSAR	73.6207	no units	
Henry's Law constant	OPERA QSAR	0.000000483	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.58575	no units	

Desvenlafaxine

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Reference Number	Full Reference
49	Bexfield, L.M., P.L. Toccalino, K. Belitz, W.T. Foreman, and E.T. Furlong. 2019. Hormones and pharmaceuticals in groundwater used as a source of drinking water across the United States. Environmental Science and Technology 53: 2950-2960.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. Environmental science & technology, 51(9), 4792-4802.
77	FDA. 2018. Drugs @ FDA: FDA Approved Drug Products. U.S. Food and Drug Administration (FDA). https://www.accessdata.fda.gov/scripts/cder/daf/ .
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. Science of The Total Environment. v581-582, (909-922).
150	NIH. 2018. DailyMed Database. U.S. National Library of Medicine, National Institutes of Health (NIH). https://dailymed.nlm.nih.gov/dailymed/ .
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. Science of the Total Environment, 636, 69-79.

Diazepam

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Diazepam
CASRN:	439-14-5
DTXSID:	DTXSID4020406
Use:	anxiolytic; skeletal muscle relaxant
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	X

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.01

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
8	non-cancer effects	4	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	0.1	lowest therapeutic dose: anxiolytic, sedative, muscle-relaxant, anticonvulsant and amnestic effects	bottle-fed infants	FDA; NIH	2018; 2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.001014	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Diazepam

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	1.66667E-05	mg/kg/day	FDA 2018; NIH 2018	Mayne Pharma	lowest therapeutic dose: anxiolytic, sedative, muscle-relaxant, anticonvulsant and amnesic effects	bottle-fed infants	151	0.110	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels
Reference Dose (RfD) or Equivalent	1.66667E-05	mg/kg/day	FDA 2018; NIH 2018	Mayne Pharma	lowest therapeutic dose: anxiolytic, sedative, muscle-relaxant, anticonvulsant and amnesic effects	general population	33.8	0.390	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Cancer Classification (CC)	3	no units	WHO IARC	
Maximum Recommended Daily Dose	0.667	mg/kg/day	FDA	
Screening level for pharmaceutical - general population	0.000392157	mg/L	EPA Office of Water	
Screening level for pharmaceutical - infants	0.000111111	mg/L	EPA Office of Water	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	48	mg/kg	NIH HSDB	min
LD50	710	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	12.77	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0059979	mol/kg	TEST QSAR	
Ames mutagenicity test	0.064	no units	TEST QSAR	
Developmental toxin test	0.731	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Diazepam
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	556	2	Sites	0.36	0.00047	0.00081	0.00101	0.00115	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	75	1	Sites	1.33	0.00047	0.00047	0.00047	0.00047	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	481	1	Sites	0.21	0.00115	0.00115	0.00115	0.00115	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	4		0.00085		0.00085	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	210	2	Sites	0.95	0.00035	0.0902	0.144	0.18	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	401	2	Sites	0.5	0.00463	0.00577	0.00645	0.00691	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	611	4	Sites	0.65	0.00035	0.00577	0.111	0.18	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	6	Sites	16	0.001681	0.00219	0.004	0.0047434	ug/L	
Bexfield et al. 2019 (Groundwater) [49]	2013 - 2015	1,106	0	Sites	0						
Benotti et al. (2009) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.00047	ug/L	
Vanderford et al. (2003) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.0013	ug/L	
Vanderford et al. (2006) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.0026	ug/L	
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	17	Sites	81	0.0005702	0.0032	0.124	4.77	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		3.22E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.35313	days	
Boiling point	OPERA QSAR	357.022	degree C	
Boiling point	TEST QSAR	349.282	degree C	
Vapor pressure	OPERA QSAR	2.09E-08	mmHg	
Vapor pressure	TEST QSAR	2.42E-08	mmHg	
Solubility in water	OPERA QSAR	0.000162557	mol/L	
Solubility in water	TEST QSAR	0.000107152	mol/L	
Bioconcentration factor	OPERA QSAR	68.2943	no units	
Bioconcentration factor	TEST QSAR	60.1174	no units	
Henry's Law constant	OPERA QSAR	2.19E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.87833	no units	

Diazepam

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Reference Number	Full Reference
49	Bexfield, L.M., P.L. Toccalino, K. Belitz, W.T. Foreman, and E.T. Furlong. 2019. Hormones and pharmaceuticals in groundwater used as a source of drinking water across the United States. <i>Environmental Science and Technology</i> 53: 2950-2960.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
77	FDA. 2018. Drugs @ FDA: FDA Approved Drug Products. U.S. Food and Drug Administration (FDA). https://www.accessdata.fda.gov/scripts/cder/daf/ .
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
127	Kostich, MS, et al., 2010. Predicting variability of aquatic concentrations of human pharmaceuticals. <i>Sci. Total Environ.</i> 408 (20), 4504e4510.
150	NIH. 2018. DailyMed Database. U.S. National Library of Medicine, National Institutes of Health (NIH). https://dailymed.nlm.nih.gov/dailymed/ .
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.

Diazinon

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Diazinon
CASRN:	333-41-5
DTXSID:	DTXSID9020407
Use:	Pesticide; veterinary medication
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	X
Human Neurotoxicants	X
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	X
Compounds with neurodev effects, Mundy et al 2015	X

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.18

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	reproductive and developmental effects	1	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.5	inhibition of red blood cell acetylcholinesterase in female pups	bottle-fed infants	OPP	2016

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.091	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X	X		

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Diazinon

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.00035	mg/kg/day	OPP 2016	Parker 2003	inhibition of red blood cell acetylcholinesterase in female pups	bottle-fed infants	151	0.464	[363]	NOTE: this compound is a organophosphate pesticide. EPA has created a cumulative risk assessment regarding the common mechanisms of organophosphate
Cancer Classification (CC)	NL		OPP 2016						[363]	NOTE: this compound is a organophosphate pesticide. EPA has created a cumulative risk assessment regarding the common mechanisms of organophosphate

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	0.02	mg/L	EPA DWSHA 2018	
Acute Minimal Risk Level (MRL)	0.006	mg/kg/day	CDC ATSDR	
Intermediate Inhalation Minimal Risk Level (MRL)	0.01	mg/m ³	CDC ATSDR	
Intermediate Minimal Risk Level (MRL)	0.002	mg/kg/day	CDC ATSDR	
Lifetime Health Advisory	0.001	mg/L	EPA DWSHA 2018	
Maximum Allowable Concentration (MAC)	0.02	mg/L	Canadian Drinking Water Guidelines	
Cancer Classification (CC)	2A	no units	WHO IARC	
Cancer Classification (CC)	Female.Mice	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats N	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice N	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats N	no units	HHS NTP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1340	mg/kg	NIH HSDB	max
LD50	2.8	mg/kg	NIH HSDB	min
LOAEL	0.02	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	100	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	25	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	0.0037	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	6.9	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	0.3	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	0.04	mg/kg/day	EPA Toxicity Reference Database	
TD50	20.4	mg/kg/day	NIH CPDB	min
TD50	6230	mg/kg/day	NIH CPDB	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0005861	mol/kg	TEST QSAR	
Ames mutagenicity test	0.26	no units	TEST QSAR	
Developmental toxin test	0.609	no units	TEST QSAR	

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Diazinon
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OCCURRENCE DATA

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Scoring Data											
Nationally Representative Water Data	Date	PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003	295	0	Sites	0					ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
		Prevalence				Magnitude					
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	11,244	995	Sites	8.85	7.00E - 05	0.0117	0.091	19	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	2,229	885	Sites	40	1.00E - 04	0.0118	0.0914	3.8	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	9,016	110	Sites	1.22	7.00E - 05	0.0082	0.0518	19	ug/L	
Pesticide Application Data				Toxic Release Data			Chemical Production Data		Production Volume (lbs/year)		
Number of States	Amount Applied (lbs/year)	Date		Number of States	Amount Released (lbs/year)						
Estimated Annual Agricultural Pesticide Use (USGS)	12	73,164	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)				

Non-Scoring Data											
Non-Nationally Representative Water Data	Date	PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	173	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	3	Sites	18	0.00999	0.0345	0.111	0.133	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
		Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	1,871	1	Sites	0.05	0.007	0.007	0.007	0.007	ug/L	
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	1,553	74	Sites	4.76	0.00014	0.008	0.218	1.97	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3,630	4	Sites	0.11	0.007	0.094	0.177	0.189	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	5,182	78	Sites	1.51	0.00014	0.00886	0.214	1.97	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	3	Sites	1.31	0.0164	0.0655	0.0943	0.1	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	2	Sites	0.91	0.05	0.0655	0.0779	0.081	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	1	Sites	8.33	0.0164	0.0582	0.0916	0.1	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	19,790	5,003	Sites	25	1e-05	0.042	0.43	331	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	3	Sites	7.89	0.0212	0.0342	0.228	0.276	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	1	Sites	0.14	1e-04	1e-04	1e-04	1e-04	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
USGS, McKenzie River, Oregon, 2012 (Ambient) [158]	2002 - 2010	133	18	Samples	14				0.115	ug/L	
Waste Water Effluent											
		Prevalence				Magnitude					
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	1	Sites	4.76						
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg- bw/day)	Notes
Expcast exposure		0.000000102	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.76627	days	
Boiling point	OPERA QSAR	340.43	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.0000812	mmHg	
Vapor pressure	TEST QSAR	0.0000769	mmHg	
Solubility in water	OPERA QSAR	0.00011245	mol/L	
Solubility in water	TEST QSAR	0.000074	mol/L	
Bioconcentration factor	OPERA QSAR	69.9796	no units	
Bioconcentration factor	TEST QSAR	94.189	no units	
Henry's Law constant	OPERA QSAR	0.000000144	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.71388	no units	

Diazinon

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
158	Reconnaissance of Land-Use Sources of Pesticides in Drinking Water, McKenzie River, Oregon. U.S. Geological Survey Scientific Investigations Report 2012–5091, 46 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
363	USEPA. 2016. Diazinon Draft Human Health Risk Assessment for Registration Review. EPA-HQ-OPP-2008-0351-0093. DP No. D419216. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Dicamba

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Dicamba
CASRN:	1918-00-9
DTXSID:	DTXSID4024018
Use:	Herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.032

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	reproductive and developmental effects	4	5

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	50	decreased pup weight	bottle-fed infants	OPP	2016

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
1.576	90th Percentile	Finished Water	UCM2	1993-1997

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Dicamba

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.04	mg/kg/day	OPP 2016	Masters 1993	decreased pup weight	bottle-fed infants	151	53.0	[364]	
Cancer Classification (CC)	NL		OPP 2016						[364]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Chronic Health-Based Guidance Value	0.2	mg/L	MN DOH	
Lifetime Health Advisory	4	mg/L	EPA DWSHA 2018	
Maximum Allowable Concentration (MAC)	0.12	mg/L	Canadian Drinking Water Guidelines	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	3000	mg/kg	NIH HSDB	max
LD50	757	mg/kg	NIH HSDB	min
LOAEL	122	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	419	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	160	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	30	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in	1.02	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0046452	mol/kg	TEST QSAR	
Ames mutagenicity test	0.143	no units	TEST QSAR	
Developmental toxin test	0.447	no units	TEST QSAR	

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EPA - Office of Water

Dicamba
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water				Prevalence				Magnitude			
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997	14,034	48	Sites	0.34	0.02	0.2	1.58	4.06	ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water				Prevalence				Magnitude			
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	7,759	133	Sites	1.71	0.01	0.15	0.998	9.97	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	1,208	116	Sites	9.6	0.01	0.15	0.979	9.97	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	6,551	17	Sites	0.26	0.01	0.14	1.15	4.03	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	48	9,773,162	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	12	103,082	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water				Prevalence				Magnitude			
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	185	0	Sites	0						
Drinking Water Monitoring Data - MA (Finished)	2006 - 2020	819	3	Sites	0.37	0.1	0.7	0.7	0.7	ug/L	
Drinking Water Monitoring Data - WA (Finished)	2006 - 2011	782	0	Sites	0						
Disinfection Byproducts ICR 1997-1998. (Finished)	1997 - 1998	291	273	Sites	94	1	11	26	114.4	ug/L	
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	12	2	Sites	17	0.025	0.068	0.0888	0.094	ug/L	
Community Water System Survey (CWSS) (Finished) [178]	2006	3	NA	Sites			50	50		ug/L	
Ambient Water				Prevalence				Magnitude			
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	1,936	5	Sites	0.26	0.21	2.7	2.92	3	ug/L	
Drinking Water Monitoring Data - MA (Source)	2006 - 2020	77	0	Sites	0						
Drinking Water Monitoring Data - PA (Source)	2006 - 2011	2	1	Sites	50	0.44	0.44	0.44	0.44	ug/L	
Drinking Water Monitoring Data - WA (Source)	2006 - 2011	968	0	Sites	0						
Drinking Water Monitoring Data - WI (Source)	2012-2019	117	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	480	26	Sites	5.42	0.01	0.165	1.24	16.6	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	1,059	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,539	26	Sites	1.69	0.01	0.165	1.24	16.6	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	6	Sites	2.62	0.0165	0.0705	0.112	0.112	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	218	3	Sites	1.38	0.0165	0.0165	0.0925	0.111555	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	3	Sites	25	0.025	0.091	0.111	0.112	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	1,058	286	Sites	27	0.05	0.117	0.517	14	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	1	Sites	2.63	0.1453	0.145	0.145	0.1453	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	1	Sites	0.14	0.474	0.474	0.474	0.474	ug/L	
USGS, McKenzie River, Oregon, 2012 (Ambient) [158]	2002 - 2010	126	1	Samples	0.8				0.58	ug/L	
Waste Water Effluent				Prevalence				Magnitude			
Estimated Concentration in Water	Date	Source	Value	Units	Model				Notes		

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Expcast exposure		1.26E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.51412	days	
Boiling point	OPERA QSAR	301.323	degree C	
Boiling point	TEST QSAR	314.148	degree C	
Vapor pressure	OPERA QSAR	0.0000115	mmHg	
Vapor pressure	TEST QSAR	0.0000306	mmHg	
Solubility in water	OPERA QSAR	0.0145152	mol/L	
Solubility in water	TEST QSAR	0.00726106	mol/L	
Bioconcentration factor	OPERA QSAR	3.37811	no units	
Bioconcentration factor	TEST QSAR	4.12098	no units	
Henry's Law constant	OPERA QSAR	9.42E-10	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.25754	no units	

Dicamba

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
158	Reconnaissance of Land-Use Sources of Pesticides in Drinking Water, McKenzie River, Oregon. U.S. Geological Survey Scientific Investigations Report 2012–5091, 46 p. plus appendixes.
178	USEPA (US Environmental Protection Agency). (2009). 2006 Community Water System Survey. Overview, 57.
364	USEPA. 2016. Dicamba and Dicamba BAPMA Salt: Human-Health Risk Assessment for Proposed Section 3 New Uses on Dicamba-tolerant Cotton and Soybean. EPA-HQ-OPP-2012-0841-0052. DP Nos. D378366 D404917 D402514 D421306. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Dichlorvos (DDVP)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Dichlorvos (DDVP)
CASRN:	62-73-7
DTXSID:	DTXSID5020449
Use:	Insecticide; veterinary medicine
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	X
Human Neurotoxics	X
PubMed Neurotoxics	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.03

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	non-cancer effects	7	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	3	red blood cell and plasma cholinesterase inhibition	general population	OPP	2006

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.09118	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Dichlorvos (DDVP)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0005	mg/kg/day	OPP 2006	Markiewicz, 1990	plasma and red blood cell cholinesterase inhibition	general population	33.8	2.96	[265]	
Cancer Classification (CC)	S		OPP 2006						[265]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.05	mg/L	EPA HHBP	
Acute Inhalation Minimal Risk Level (MRL)	0.002	ppm	CDC ATSDR	
Acute Minimal Risk Level (MRL)	0.004	mg/kg/day	CDC ATSDR	
Acute PAD	0.008	mg/kg/day	EPA HHBP	
Cancer Slope Factor (CSF)	0.29	(mg/kg/day) ⁻¹	CalEPA OEHHA Chemical Database	
Chronic Human Health Benchmark	0.003	mg/L	EPA HHBP	
Chronic inhalation Minimal Risk Level (MRL)	0.00006	ppm	CDC ATSDR	
Health-Based Screening Level	0.003	mg/L	Health-based screening levels from USGS	
Inhalation Unit Risk (IUR)	0.000083	ug/m ³	CalEPA OEHHA Chemical Database	
Intermediate Inhalation Minimal Risk Level (MRL)	0.0003	ppm	CDC ATSDR	
Intermediate Minimal Risk Level (MRL)	0.003	mg/kg/day	CDC ATSDR	
Population-Adjusted Dose (PAD)	0.0005	mg/kg/day	EPA HHBP	
Reference Concentration (RFC)	0.0005	mg/m ³	EPA IRIS	
Cancer Classification (CC)	2B	no units	WHO IARC	
Cancer Classification (CC)	Female.Mice N	no units	HHS NTP	
Cancer Classification (CC)	Female.Mice P	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats EE	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats N	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice N	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice SE	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats N	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats SE	no units	HHS NTP	

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Inhalation LOAEL	0.05532	mg/L	EPA Toxicity Reference Database	
Inhalation NOAEL	0.00553	mg/L	EPA Toxicity Reference Database	
LD50	140	mg/kg	NIH HSDB	max
LD50	6.51	mg/kg	NIH HSDB	min
LOAEL	1	mg/kg/day	EPA Toxicity Reference Database	
NOAEL	0.05	mg/kg/day	EPA Toxicity Reference Database	
Percent of active toxcast in vitro assays tested	7.13	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	1.5	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	0.1	mg/kg/day	EPA Toxicity Reference Database	
TD50	3.21	mg/kg/day	NIH CPDB	min
TD50	7850	mg/kg/day	NIH CPDB	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0000565	mol/kg	TEST QSAR	
Ames mutagenicity test	0.617	no units	TEST QSAR	
Developmental toxin test	0.71	no units	TEST QSAR	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.13846	days	
Boiling point	OPERA QSAR	226.392	degree C	
Boiling point	TEST QSAR	215.618	degree C	
Vapor pressure	OPERA QSAR	0.0189601	mmHg	
Vapor pressure	TEST QSAR	0.047863	mmHg	
Solubility in water	OPERA QSAR	0.0349528	mol/L	
Solubility in water	TEST QSAR	0.159221	mol/L	
Bioconcentration factor	OPERA QSAR	0.579336	no units	
Bioconcentration factor	TEST QSAR	3.75837	no units	
Henry's Law constant	OPERA QSAR	3.85E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.38464	no units	

Dichlorvos (DDVP)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
265	USEPA. 2006. Dichlorvos (DDVP) HED Chapter of the Reregistration Eligibility Decision Document (RED). EPA-HQ-OPP-2002-0302-0016. DP No. D330262. U.S. Environmental Protection Agency, Office of Prevention, Pesticides and Toxic Substances, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Dicrotophos

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Dicrotophos
CASRN:	141-66-2
DTXSID:	DTXSID9023914
Use:	Insecticide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	4.0

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
8	reproductive and developmental effects	6	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.04	inhibition of brain cholinesterase	bottle-fed infants	OPP	2015

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.158	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
		X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Dicrotophos

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.00003	mg/kg/day	OPP 2015	Allen 1998; Horner 1995	inhibition of brain cholinesterase in adult rat	bottle-fed infants	151	0.0397	[341]	
Cancer Classification (CC)	5		OPP 2015						[341]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.0005	mg/L	EPA HHBP	
Acute PAD	0.00007	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.0002	mg/L	EPA HHBP	
Health-Based Screening Level	0.0002	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.00003	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	21	mg/kg	NIH HSDB	max
LD50	9	mg/kg	NIH HSDB	min
LOAEL	0.02	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	1.58	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	0.5	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	0.025	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	1.14	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.00003	mol/kg	TEST QSAR	
Ames mutagenicity test	0.421	no units	TEST QSAR	
Developmental toxin test	0.694	no units	TEST QSAR	

Dicrotophos

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
341	USEPA. 2015. Dicrotophos: Revised Human Health Risk Assessment for Registration Review of Dicrotophos. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Dieldrin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Dieldrin
CASRN:	60-57-1
DTXSID:	DTXSID9020453
Use:	Restricted insecticide
Chemical Notes:	Canceled pesticide. Last end of use date: 5/15/1987.

Is the contaminant on any lists?	
CERCLA	X
FIFRA	X
Human Neurotoxics	X
PubMed Neurotoxics	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	X

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	380

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	carcinogen with linear MOA	1	5

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.002	liver carcinomas	general population	OW	2003

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.764	90th Percentile	Finished Water	UCM2	1993 - 1997

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X			

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
X	Not Applicable	Not Applicable
Basis		

Dieldrin may cause adverse health effects in humans, specifically neurotoxicity to the central nervous system [a,b,c]. However, its occurrence in drinking water at frequencies or concentrations significant for public health concern is low; occurrence estimates from a cross-section of States with UCM data are very low with only 0.06% of all samples and 0.1% of PWSs showing detections where the HRL is 0.002 ug/L [d,e]. Furthermore, occurrence of dieldrin in drinking water supplies in the is likely to decrease in the coming years, since the chemical is no longer produced or used commercially [f].

[a] Jager, 1970 [113]; [b] ACGIH, 1984 [6]; [c] ATSDR, 2000 [16]; [d] USEPA, 2001 [239]; [e] USEPA, 2001 [247]; [f] ATSDR, 1993 [2]; as cited in USEPA, 2001 [179]

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Dieldrin
CCL 5 Contaminant Information Sheet
HEALTH EFFECTS DATA

EPA-OGWOW and OST

July 2021

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.00005	mg/kg/day	IRIS 1988	Walker et al., 1969	liver lesions	general population	33.8	0.296	[198]	
Reference Dose (RfD) or Equivalent	0.00005	mg/kg/day	ATSDR 2002	Walker et al., 1969	increased liver weight, liver parenchymal cell changes, focal hyperplasia	general population	33.8	0.296	[18]	
Reference Dose (RfD) or Equivalent	0.00005	mg/kg/day	OW 2003	Walker et al., 1969	increased liver weight, liver parenchymal cell changes, focal hyperplasia	general population	33.8	0.296	[255]	NOTE: canceled registration, OPP does not provide a publicly-available health assessment for dieldrin; no new information has been published by EPA regarding health effects of dieldrin - refer to the 2003 RegDet supporting documentation
Cancer Slope Factor (CSF)	16	(mg/kg/day) ⁻¹	IRIS 1988	(Davis and Fitzhugh, 1962; Davis, 1965; Walker et al., 1972; Thorpe and Walker, 1973; NCI, 1978; Tennekkes et al., 1981; Meierhenry et al., 1983)	liver carcinoma	general population	33.8	0.00185	[198]	
Cancer Slope Factor (CSF)	16	(mg/kg/day) ⁻¹	OW 2003	Davis and Fitzhugh, 1962; Davis, 1965; Walker et al., 1972; Thorpe and Walker, 1973; NCI, 1978; Tennekkes et al., 1981; Meierhenry et al., 1983	liver carcinoma	general population	33.8	0.00185	[255]	NOTE: canceled registration, OPP does not provide a publicly-available health assessment for dieldrin; no new information has been published by EPA regarding health effects of dieldrin - refer to the 2003 RegDet supporting documentation
Cancer Classification (CC)	B2		IRIS 1988						[198]	
Cancer Classification (CC)	B2		OW 2003						[255]	NOTE: canceled registration, OPP does not provide a publicly-available health assessment for dieldrin; no new information has been published by EPA regarding health effects of dieldrin - refer to the 2003 RegDet supporting documentation
Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations										
OPP										

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References Identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	0.0005	mg/L	EPA DWSHA 2018	
Acute Health-Based Guidance Value	0.0002	mg/L	MN DOH	
Acute Health-Based Guidance Value	0.0002	mg/L	MN DOH	
Acute Health-Based Guidance Value	0.0002	mg/L	MN DOH	
Cancer Slope Factor (CSF)	16	(mg/kg/day) ⁻¹	CalEPA OEHH Chemical Database	
Chronic Health-Based Guidance Value	0.0002	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.0002	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.0000006	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.0000006	mg/L	MN DOH	
Drinking Water Guideline Value	0.00003	mg/L	WHO Drinking Water Quality Guidelines	
Human Health Ambient Water Quality Criteria	1.2E-09	mg/L	EPA Human Health Criteria for CWA	
Inhalation Unit Risk (IUR)	0.0046	(ug/m ³) ⁻¹	EPA IRIS	
Inhalation Unit Risk (IUR)	0.0046	ug/m ³	CalEPA OEHH Chemical Database	
Intermediate Minimal Risk Level (MRL)	0.0001	mg/kg/day	CDC ATSDR	
Lifetime Health Advisory	0.000002	mg/L	EPA DWSHA 2018	
Short-Term/Subchronic Health-Based Guidance Value	0.0002	mg/L	MN DOH	
Short-Term/Subchronic Health-Based Guidance Value	0.0002	mg/L	MN DOH	
Cancer Classification (CC)	Female.Mice N	no units	HHS NTP	
Cancer Classification (CC)	Female.Mice NT	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats N	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats N	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice F	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice NT	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats N	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats N	no units	HHS NTP	

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	3	mg/kg	NIH HSDB	min
LD50	37000	mg/kg	NIH HSDB	max
Percent of active toxicant in vitro assays tested	21.43	percent	EPA Chemistry Dashboard	
TD50	1.04	mg/kg/day	NIH CPDB	min
TD50	489	mg/kg/day	NIH CPDB	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0000284	mol/kg	TEST QSAR	
Ames mutagenicity test	0.019	no units	TEST QSAR	
Developmental toxin test	0.55	no units	TEST QSAR	

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
The full citation for the critical study is provided in the corresponding health assessment.
PECO = Population, Exposure, Comparator, Outcome.

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EPA 815-R-21-006
July 2021

EPA - Office of Water

Dieldrin
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997	11,788	11	Sites	0.09	0.02	0.15	0.764	1.36	ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	10,180	351	Sites	3.45	0.001	0.009	0.05	5.6	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	2,054	154	Sites	7.5	0.001	0.007	0.02	0.19	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	8,127	197	Sites	2.42	0.001	0.013	0.19	5.6	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	162	0	Sites	0						
Drinking Water Monitoring Data - MA (Finished)	2006 - 2020	822	2	Sites	0.24	0.037	0.0385	0.0397	0.04	ug/L	
Drinking Water Monitoring Data - WA (Finished)	2006 - 2011	825	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	13	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Hawaii Department of Health (Finished) [172]	2014	1	NA	Sites		0.01	0.01	0.01	0.01	ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	1,514	4	Sites	0.26	0.01	0.025	31.2	52	ug/L	
Drinking Water Monitoring Data - FL (Source)	2006 - 2011	1	0	Sites	0						
Drinking Water Monitoring Data - MA (Source)	2006 - 2020	77	0	Sites	0						
Drinking Water Monitoring Data - PA (Source)	2006 - 2011	3	1	Sites	33	0.044	0.044	0.044	0.044	ug/L	
Drinking Water Monitoring Data - WA (Source)	2006 - 2011	999	0	Sites	0						
Drinking Water Monitoring Data - WI (Source)	2012-2019	92	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	747	42	Sites	5.62	5.00E - 04	0.003	0.0166	0.13	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	2,630	69	Sites	2.62	0.001	0.0158	0.074	1.78	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	3,376	111	Sites	3.29	5.00E - 04	0.008	0.0686	1.78	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	8	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	2	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	6	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	604	45	Sites	7.45	0.003	0.011	0.197	0.38	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	28	Sites	74	6.78E-05	0.000774	0.00245	0.0128	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	106	2	Sites	1.89	0.002	0.003	0.0038	0.004	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Minnesota Department of Health (Ambient) [149]	1970 - 2016	NA	32	Samples		0.01			0.9	ug/L	
Village Creek, AL (Ambient) [75]	2015	4	NA	Sites		0.00096	0.0013	0.00142	0.0015	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model					Notes	

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Expcast exposure		0.00000129	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)	14.4	ng/g	
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	343.763	days	
Boiling point	OPERA QSAR	329.92	degree C	
Boiling point	TEST QSAR	384.804	degree C	
Vapor pressure	OPERA QSAR	0.00000411	mmHg	
Vapor pressure	TEST QSAR	0.00000224	mmHg	
Solubility in water	OPERA QSAR	0.00000419	mol/L	
Solubility in water	TEST QSAR	0.0000026	mol/L	
Bioconcentration factor	OPERA QSAR	6042.55	no units	
Bioconcentration factor	TEST QSAR	918.333	no units	
Henry's Law constant	OPERA QSAR	0.000013	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	5.43154	no units	

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Dieldrin

CCL 5 Contaminant Information Sheet

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July 2021

Reference Number	Full Reference
2	Agency for Toxic Substances and Disease Registry (ATSDR). 1993. Toxicological Profile for Aldrin/Dieldrin (update). Atlanta: Agency for Toxic Substances and Disease Registry. 184 pp.
6	American Conference of Governmental Industrial Hygienists (ACGIH). 1984. Documentation of the Threshold Limit Values for Substances in Workroom Air. Third Edition. Cincinnati, OH: ACGIH. 139 pp.
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
16	ATSDR. 2000. Toxicological Profile for Aldrin/Dieldrin (Update). Atlanta, GA: Agency for Toxic Substances and Disease Registry. 280 pp.
18	ATSDR. 2002. Toxicological Profile for Aldrin/Dieldrin. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. Environmental science & technology, 51(9), 4792-4802.
75	EPA Region 4. Village Creek Dieldrin Screening. June 2015. https://www.birminghamal.gov/wp-content/uploads/2017/08/15-0308-Village-Creek-Dieldrin-Screening-Final-Report-v081015.pdf
113	Jager, K.W. 1970. Aldrin, Dieldrin, Endrin and Telodrin: An Epidemiological and Toxicological Study of Long-Term Occupational Exposure. New York: Elsevier Publishing Company. 234 pp.
149	Minnesota Department of Health. Dieldrin and Drinking Water. October 2016. https://www.health.state.mn.us/communities/environment/risk/docs/guidance/gw/dieldrininfo.pdf
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
172	State of Hawaii Department of Health. Trace levels of dieldrin and bromacil in two Oahu Water Systems. January 2015. https://health.hawaii.gov/news/files/2013/05/TRACE-LEVELS-OF-DIELDRIN-AND-BROMACIL-DETECTED-IN-TWO-OAHU-WATER-SYSTEMS.pdf
179	USEPA, 2001. Regulatory Determination Support Document for Aldrin and Dieldrin. EPA 815 R-01-011.
198	USEPA. 1988. Chemical Assessment Summary, Dieldrin. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, DC.
239	USEPA. 2001. Analysis of National Occurrence of the 1998 Contaminant Candidate List Regulatory Determination Priority Contaminants in Public Water Systems. Office of Water. EPA report 815-D-01-002. 77 pp.
247	USEPA. 2001. Occurrence of Unregulated Contaminants in Public Water Systems: An Initial Assessment. Office of Water. EPA report 815-P-00-001. Office of Water. 50 pp.
255	USEPA. 2003. Contaminant Candidate List Regulatory Determination Support Document for Aldrin and Dieldrin. U.S. Environmental Protection Agency, Office of Water, Standards and Risk Management Division, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society

Diethyl phthalate

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Diethyl phthalate
CASRN:	84-66-2
DTXSID:	DTXSID7021780
Use:	Solvent for nitrocellulose and cellulose acetate, plasticizer, wetting agent; in plastics, perfumery as fixative and solvent, alcohol denaturant, plasticizer in solid rocket propellants.
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.00016

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
3	non-cancer effects	9	5

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	4000	decreased weight gain and kidney weight	general population	OW	1992

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.62	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Diethyl phthalate

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.8	mg/kg/day	IRIS 1987	Brown et al. 1978	decreased growth rate and food consumption and altered organ weights	general population	33.8	4730	[192]	
Reference Dose (RfD) or Equivalent	0.75	mg/kg/day	OW 1992	Brown et al. 1978	decreased weight gain and kidney weight	general population	33.8	4440	[218]	
Cancer Classification (CC)	D		IRIS 1987						[192]	
Cancer Classification (CC)	D		OW 1992						[218]	
			ATSDR 1995						[9]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Systemic, Reproductive, Hepatic	0.57	Pereira, 2008, Pereira, 2006	Reproductive	1470	Yamasaki, 2005	1994-06-01	2020-04-14	728	10	39	7

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Chronic Health-Based Guidance Value	6	mg/L	MN DOH	
Human Health Ambient Water Quality Criteria	0.6	mg/L	EPA Human Health Criteria for CWA	
Intermediate Minimal Risk Level (MRL)	6	mg/kg/day	CDC ATSDR	
Cancer Classification (CC)	Female.Mice EE	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats NE	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice EE	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats NE	no units	HHS NTP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1000	mg/kg	NIH HSDB	min
LD50	9200	mg/kg	NIH HSDB	max
LOAEL	1150	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	197	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	267	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	56	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	1.44	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0157036	mol/kg	TEST QSAR	
Ames mutagenicity test	0.16	no units	TEST QSAR	
Developmental toxin test	0.748	no units	TEST QSAR	

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OCCURRENCE DATA

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	46	3	Sites	6.52	0.1	0.2	0.62	0.8	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	37	3	Sites	8.11	0.1	0.2	0.62	0.8	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	9	0	Sites	0						

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	1M - 10M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	17	1	Sites	5.88	0.007	0.0435	5.5	6.2	ug/L	
Drinking Water Monitoring Data - WA (Finished)	2006 - 2011	483	1	Sites	0.21	4.9	4.9	4.9	4.9	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	1	Sites	100	0.1	0.1	0.1	0.1	ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	113	2	Sites	1.77	0.005	0.046	6.34	13.6	ug/L	
Drinking Water Monitoring Data - WA (Source)	2006 - 2011	638	2	Sites	0.31	0.421	0.76	1.03	1.1	ug/L	
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	631	137	Sites	22	0.09	0.2	0.588	5	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	605	52	Sites	8.6	0.06	0.2	1.3	60.4	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,236	189	Sites	15	0.06	0.2	0.6	60.4	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	2	Sites	5.26	0.128	0.135	0.141	0.142	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	1	Sites	50	0.1	0.1	0.1	0.1	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.0000694	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.31107	days	
Boiling point	OPERA QSAR	297.011	degree C	
Boiling point	TEST QSAR	312.231	degree C	
Vapor pressure	OPERA QSAR	0.00203233	mmHg	
Vapor pressure	TEST QSAR	0.00091622	mmHg	
Solubility in water	OPERA QSAR	0.00366221	mol/L	
Solubility in water	TEST QSAR	0.00165196	mol/L	
Bioconcentration factor	OPERA QSAR	7.15782	no units	
Bioconcentration factor	TEST QSAR	6.45654	no units	
Henry's Law constant	OPERA QSAR	2.38E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.36526	no units	

Diethyl phthalate

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Reference Number	Full Reference
9	ATSDR. 1995. Toxicological Profile for Diethyl Phthalate. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
192	USEPA. 1987. Chemical Assessment Summary, Diethyl Phthalate. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, DC.
218	USEPA. 1992. Drinking Water Criteria Document for Phthalic Acid Esters (PAEs). U.S. Environmental Protection Agency, Office of Health and Environmental Assessment, Environmental Criteria and Assessment Office, Cincinnati, OH.

Difenoconazole

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Difenoconazole
CASRN:	119446-68-3
DTXSID:	DTXSID4032372
Use:	Fungicide, insecticide, seed treatment/protectant.
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.00030

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	non-cancer effects	9	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	60	cumulative decreases in body weight gains	general population	OPP	2017

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.0182	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Difenoconazole

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.01	mg/kg/day	OPP 2017	Cox 1989	cumulative decreases in body weight gains	general population	33.8	59.2	[381]	
Cancer Classification (CC)	S		OPP 2017						[381]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	1.7	mg/L	EPA HHBP	
Acute PAD	0.25	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.06	mg/L	EPA HHBP	
Population-Adjusted Dose (PAD)	0.01	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1453	mg/kg	NIH HSDB	min
LD50	2150	mg/kg	NIH HSDB	max
LOAEL	12.5	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	171.25	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	1.25	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	84.525	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	32.36	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	10	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	75	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	1	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	25	mg/kg/day	EPA Toxicity Reference Database	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0025468	mol/kg	TEST QSAR	
Ames mutagenicity test	0.467	no units	TEST QSAR	
Developmental toxin test	0.413	no units	TEST QSAR	

Difenoconazole

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	14	1	Sites	7.14	0.0182	0.0182	0.0182	0.0182	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	14	1	Sites	7.14	0.0182	0.0182	0.0182	0.0182	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	47	400,757	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	15	1	Sites	6.67	0.0053	0.0053	0.0053	0.0053	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	132	4	Sites	3.03	0.0084	0.0296	0.168	0.249	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	135	4	Sites	2.96	0.0084	0.0296	0.168	0.249	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	227	1	Sites	0.44	0.0053	0.0053	0.0053	0.0053	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	218	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	10	1	Sites	10	0.0053	0.0053	0.0053	0.0053	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	123	1	Sites	0.81	0.0182	0.0182	0.0182	0.0182	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.000000137	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.36121	days	
Boiling point	OPERA QSAR	335.605	degree C	
Boiling point	TEST QSAR	413.931	degree C	
Vapor pressure	OPERA QSAR	6.17E-10	mmHg	
Vapor pressure	TEST QSAR	1.75E-09	mmHg	
Solubility in water	OPERA QSAR	0.0000202	mol/L	
Solubility in water	TEST QSAR	0.000014	mol/L	
Bioconcentration factor	OPERA QSAR	230.63	no units	
Bioconcentration factor	TEST QSAR	148.936	no units	
Henry's Law constant	OPERA QSAR	0.00000505	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	4.07726	no units	

Difenoconazole

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
381	USEPA. 2017. Difenoconazole: human health risk assessment for proposed new foliar uses on cotton, rice and wild rice. EPA-HQ-OPP-2016-0254-0010. DP No. D432211. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Dimethenamid

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Dimethenamid
CASRN:	87674-68-8
DTXSID:	DTXSID4032376
Use:	Herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.00034

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	non-cancer effects	9	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	300	decreased body weight gain and decreased body weight, increased microscopic hepatic lesions	general population	OPP	2014

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.103	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Dimethenamid

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.05	mg/kg/day	OPP 2014	Ruckman et al. 1990; Sandoz Crop Protection Corp. 1990	decreased body weight gain and decreased body weight, increased microscopic hepatic lesions, increased food conversion ratios in females	general population	33.8	296	[332]	
Cancer Classification (CC)	C		OPP 2014						[332]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Health-Based Guidance Value	0.6	mg/L	MN DOH	
Acute Human Health Benchmark	10	mg/L	EPA HHBP	
Acute PAD	2	mg/kg/day	EPA HHBP	
Chronic Health-Based Guidance Value	0.3	mg/L	MN DOH	
Chronic Human Health Benchmark	0.3	mg/L	EPA HHBP	
Health-Based Screening Level	0.3	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.05	mg/kg/day	EPA HHBP	
Short-Term/Subchronic Health-Based Guidance Value	0.6	mg/L	MN DOH	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	371	mg/kg	NIH HSDB	min
LD50	427	mg/kg	NIH HSDB	max
LOAEL	200	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	36	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	6.8	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	75	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	12.84	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	33.599998	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	98	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	4.98	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	40.1	mg/kg/day	EPA Toxicity Reference Database	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity test	0.443	no units	TEST QSAR	
Developmental toxin test	0.711	no units	TEST QSAR	

Dimethenamid

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	2,362	205	Sites	8.68	0.00012	0.00812	0.103	7	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	347	194	Sites	56	0.00012	0.00814	0.103	7	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	2,015	11	Sites	0.55	0.00031	0.00161	0.021	0.25	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	16	1,115,877	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	12	5	Sites	42	0.000999	0.0024	0.011	0.075	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	358	97	Sites	27	0.00018	0.0175	0.214	3.19	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	848	10	Sites	1.18	0.0017	0.07	0.754	0.842	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,206	107	Sites	8.87	0.00018	0.0187	0.237	3.19	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	6	Sites	2.62	0.000999	0.0042	0.0299	0.51	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	1	Sites	0.46	0.004162	0.00416	0.00416	0.004162	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	5	Sites	42	0.000999	0.0042	0.03	0.51	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	4	Sites	11	0.03	0.03	0.079	0.1	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	6	Sites	1.03	3e-04	0.0024	0.0152	0.0224	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		9.96E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.34757	days	
Boiling point	OPERA QSAR	294.303	degree C	
Boiling point	TEST QSAR	337.241	degree C	
Vapor pressure	OPERA QSAR	0.000122276	mmHg	
Vapor pressure	TEST QSAR	0.0000108	mmHg	
Solubility in water	OPERA QSAR	0.00253016	mol/L	
Solubility in water	TEST QSAR	0.000765597	mol/L	
Bioconcentration factor	OPERA QSAR	45.9219	no units	
Bioconcentration factor	TEST QSAR	17.8238	no units	
Henry's Law constant	OPERA QSAR	3.83E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.13166	no units	

Dimethenamid

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. Environmental science & technology, 51(9), 4792-4802.
332	USEPA. 2014. Dimethenamid/Dimethenamid-P. Human Health Risk Assessment for Proposed New Use on Cotton Subgroup 20C. EPA-HQ-OPP-2013-0670-0005. DP No. D418118. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.

Dimethenamid OA

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Dimethenamid OA
CASRN:	380412-59-9
DTXSID:	DTXSID4037530
Use:	Pesticide metabolite
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.00052

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	non-cancer effects	9	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	400	Decrease in body weight gain; liver effects (increased relative liver weight, bile duct hyperplasia)	general population	MDH	2013

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.209	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Dimethenamid OA

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.06	mg/kg/day	MDH 2013	Ruckman 1990	Decrease in body weight gain; liver effects (increased relative liver weight; bile duct hyperplasia)	general population	33.8	355	[135]	NOTE: MN DOH determined that the RfD determined for dimethenamid would be protective for Dimethenamid OXA. MN DOH states that there are insufficient data to calculate a unique RfD for this compound.

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Health-Based Guidance Value	0.6	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.3	mg/L	MN DOH	
Short-Term/Subchronic Health-Based Guidance Value	0.6	mg/L	MN DOH	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0005164	mol/kg	TEST QSAR	
Ames mutagenicity test	-0.084	no units	TEST QSAR	
Developmental toxin test	0.898	no units	TEST QSAR	

Dimethenamid OA

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	2,539	73	Sites	2.88	0.0126	0.0748	0.209	0.596	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	363	68	Sites	19	0.0126	0.0747	0.209	0.596	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	2,176	5	Sites	0.23	0.03	0.0843	0.183	0.216	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	12	5	Sites	42	0.00105	0.0022	0.0144	0.03	ug/L	
Ambient Water											
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	25	Sites	11	0.001049	0.0045	0.039	0.061	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	218	20	Sites	9.17	0.001049	0.0078	0.0311	0.0441	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	5	Sites	42	0.00105	0.00425	0.039	0.061	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	2	Sites	5.26	0.02	0.02	0.02	0.02	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.34519	days	
Boiling point	OPERA QSAR	306.88	degree C	
Boiling point	TEST QSAR	366.15	degree C	
Vapor pressure	OPERA QSAR	0.00000997	mmHg	
Vapor pressure	TEST QSAR	0.00000151	mmHg	
Solubility in water	OPERA QSAR	0.0182443	mol/L	
Solubility in water	TEST QSAR	0.0122462	mol/L	
Bioconcentration factor	OPERA QSAR	3.10149	no units	
Bioconcentration factor	TEST QSAR	0.92045	no units	
Henry's Law constant	OPERA QSAR	7.22E-10	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.82828	no units	

Dimethenamid OA

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
135	MDH. 2013. Dimethenamid Degradates: ESA and OXA. Health Based Guidance for Water. Minnesota Department of Health (MDH), Environmental Health Division, Health Risk Assessment Unit, St Paul, MN.

Dimethoate

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Dimethoate
CASRN:	60-51-5
DTXSID:	DTXSID7020479
Use:	Pesticide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	X
Human Neurotoxicants	X
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.16

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	reproductive and developmental effects	1	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.3	inhibition of brain acetylcholinesterase	bottle-fed infants	OPP	2015

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.04707	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
		X	

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	X
Basis		

Dimethoate has the potential to cause adverse health effects, including cholinesterase inhibition. However, dimethoate does not appear to occur in PWSs with a frequency and at levels of public health concern [a,b]. Dimethoate was not detected in a number UCMR 2 samples collected by PWSs at levels greater than the ½ HRL (7.7 µg/L), the HRL (15.4 µg/L), or the MRL (0.7 µg/L)[c,d]. EPA concludes that regulation of dimethoate does not represent a meaningful opportunity for health risk reduction for persons served by PWSs due to the relatively small number of people likely exposed to dimethoate through drinking water [c,d].

[a] USEPA, 2007 [284]; [b] USEPA, 2007 [283]; [c] USEPA, 2010 [310]; [d] USEPA, 2015 [350]; as cited in USEPA, 2014 [334]

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Dimethoate

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.00022	mg/kg/day	OPP 2015	US EPA OP CRA 2002 & 2006; American Cyanamid Company 1986	inhibition of brain acetylcholinesterase	bottle-fed infants	151	0.291	[360]	
Cancer Classification (CC)	C		OPP 2015						[360]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.087	mg/L	EPA HHBP	
Acute PAD	0.013	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.014	mg/L	EPA HHBP	
Drinking Water Guideline Value	0.006	mg/L	WHO Drinking Water Quality Guidelines	
Health-Based Screening Level	0.014	mg/L	Health-based screening levels from USGS	
Maximum Allowable Concentration (MAC)	0.02	mg/L	Canadian Drinking Water Guidelines	
Population-Adjusted Dose (PAD)	0.0022	mg/kg/day	EPA HHBP	
Cancer Classification (CC)	Female.Mice N	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats N	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice N	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats N	no units	HHS NTP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	50	mg/kg	NIH HSDB	min
LD50	600	mg/kg	NIH HSDB	max
LOAEL	0.25	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	18	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	0.05	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	6	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	3.15	percent	EPA Chemistry Dashboard	
TD50	222	mg/kg/day	NIH CPDB	max
TD50	92.4	mg/kg/day	NIH CPDB	min

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0004656	mol/kg	TEST QSAR	
Ames mutagenicity test	0.366	no units	TEST QSAR	
Developmental toxin test	0.724	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Dimethoate
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data											
Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010	4,140	0	Sites	0					ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	4,941	64	Sites	1.3	0.00034	0.009	0.0471	1.95	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	581	62	Sites	11	0.00034	0.009	0.0448	1.95	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	4,360	2	Sites	0.05	0.061	0.152	0.207	0.243	ug/L	
Pesticide Application Data				Toxic Release Data				Chemical Production Data			
Number of States	Amount Applied (lbs/year)	Date		Number of States	Amount Released (lbs/year)			Chemical Data Reporting (CDR) Results (EPA) (2016)	Production Volume (lbs/year)		
Estimated Annual Agricultural Pesticide Use (USGS)	41	1,419,642	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	2	42					

Non-Scoring Data											
Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	184	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	2	Sites	12	0.0075	0.0378	0.062	0.068	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	2,100	2	Sites	0.1	0.082	0.541	0.908	1	ug/L	
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	724	24	Sites	3.31	0.00045	0.0227	0.126	0.271	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	2,523	3	Sites	0.12	0.0036	0.133	0.824	1.12	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	3,246	27	Sites	0.83	0.00045	0.0228	0.133	1.12	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	1	Sites	0.44	0.0088	0.0088	0.0088	0.0088	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	1	Sites	8.33	0.0088	0.0088	0.0088	0.0088	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	12,194	762	Sites	6.25	0.007	0.219	1.34	16.4	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	2	Sites	5.26	0.133	0.184	0.226	0.236	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	1	Sites	0.14	0.061	0.061	0.061	0.061	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Expocast exposure		0.000000994	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)	< LOD	ug/l	

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	73.9608	days	
Boiling point	OPERA QSAR	308.683	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.0000177	mmHg	
Vapor pressure	TEST QSAR	0.0000248	mmHg	
Solubility in water	OPERA QSAR	0.104479	mol/L	
Solubility in water	TEST QSAR	0.0171002	mol/L	
Bioconcentration factor	OPERA QSAR	1.77267	no units	
Bioconcentration factor	TEST QSAR	3.70681	no units	
Henry's Law constant	OPERA QSAR	2.06E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	0.833231	no units	

Dimethoate

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
283	USEPA. 2007. Revised Interim Reregistration Decision for Dimethoate. Available on the Internet at: http://www.epa.gov/pesticides/reregistration/REDs/dimethoate_ired_revised.pdf .
284	USEPA. 2007. Unregulated Contaminant Monitoring Regulation (UCMR) for Public Water Systems Revisions. Federal Register. Vol. 72, No. 2, p. 367, January 4, 2007.
310	USEPA. 2010. Data Management and Analytical Plan for the Second Unregulated Contaminant Monitoring Regulation (UCMR 2) Data. June 2010 Draft Report Submitted to EPA.
334	USEPA. 2014. Regulatory Determinations 3 Support Document. April 2014. EPA Publication # 815-R14-003.
350	USEPA. 2015. Occurrence Data from the Second Unregulated Contaminant Monitoring Regulation (UCMR 2). Including Appendices A-C. EPA 815-R-15-013. December 2015.
360	USEPA. 2015. Dimethoate: Human Health Risk Assessment for Registration Review. EPA-HQ-OPP-2009-0059-0027. DP No. D416010. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Di-n-butyl phthalate

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Di-n-butyl phthalate
CASRN:	84-74-2
DTXSID:	DTXSID2021781
Use:	Plasticizer in nitrocellulose lacquers, elastomers, explosives, nail polish and solid rocket propellants; in perfumes; in textiles; in safety glass; insecticides; in printing inks; resin solvent; paper coatings; and adhesives.
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	X
Human Neurotoxicants	X
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	X
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.00063

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	reproductive and developmental effects	10	7

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	3000	"Increased incidence of retained areolas and nipple in the male offspring of rats"	women of childbearing age	ATSDR	2001

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
1.9	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Di-n-butyl phthalate

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.1	mg/kg/day	IRIS 1987	Smith 1953	increased mortality	general population	33.8	592	[188]	
Reference Dose (RfD) or Equivalent	0.1	mg/kg/day	OW 1991	Smith 1953	"absense of increased mortality and hemotological effects"	general population	33.8	592	[211]	
Reference Dose (RfD) or Equivalent	0.5	mg/kg/day	ATSDR 2001	Mylchreest et al. 2000	"Increased incidence of retained areolas and nipple in the male offspring of rats"	women of childbearing age	35.4	2820	[17]	
Cancer Classification (CC)	D		IRIS 1987						[188]	
Cancer Classification (CC)	D		OW 1991						[211]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Neurological	0.01	Hoshi, 2009	Developmental;	2000	Dobrzynska, 2011;	2000-09-01	2019-12-17	1867	80	64	50

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Health-Based Guidance Value	0.02	mg/L	MN DOH	
Acute Health-Based Guidance Value	0.02	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.02	mg/L	MN DOH	
Human Health Ambient Water Quality Criteria	0.02	mg/L	EPA Human Health Criteria for CWA	
Short-Term/Subchronic Health-Based Guidance Value	0.02	mg/L	MN DOH	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	10000	mg/kg	NIH HSDB	max
LD50	4840	mg/kg	NIH HSDB	min
Percent of active toxcast in vitro assays tested	9.76	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0436516	mol/kg	TEST QSAR	
Ames mutagenicity test	0.09	no units	TEST QSAR	
Developmental toxin test	0.71	no units	TEST QSAR	

Di-n-butyl phthalate

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	22	4	Sites	18	0.3	1.5	1.9	2	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	13	4	Sites	31	0.3	1.5	1.9	2	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	9	0	Sites	0						

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	1M - 10M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	26	1	Sites	3.85	0.002	0.034	0.129	0.137	ug/L	
Drinking Water Monitoring Data - WA (Finished)	2006 - 2011	483	2	Sites	0.41	0.637	1.3	14.2	26.4	ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	247	7	Sites	2.83	0.006	0.178	6.76	8.1	ug/L	
Drinking Water Monitoring Data - FL (Source)	2006 - 2011	1	1	Sites	100	1.1	1.1	1.1	1.1	ug/L	
Drinking Water Monitoring Data - WA (Source)	2006 - 2011	638	8	Sites	1.25	0.477	1.5	3.42	6	ug/L	
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	154	25	Sites	16	0.11	0.44	5	5	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	360	46	Sites	13	0.04	0.09	0.377	1.65	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	514	71	Sites	14	0.04	0.13	0.865	5	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.00008	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.33363	days	
Boiling point	OPERA QSAR	332.592	degree C	
Boiling point	TEST QSAR	348.35	degree C	
Vapor pressure	OPERA QSAR	0.0000243	mmHg	
Vapor pressure	TEST QSAR	0.0000263	mmHg	
Solubility in water	OPERA QSAR	0.0000362	mol/L	
Solubility in water	TEST QSAR	0.0000407	mol/L	
Bioconcentration factor	OPERA QSAR	134.136	no units	
Bioconcentration factor	TEST QSAR	11.17	no units	
Henry's Law constant	OPERA QSAR	0.0000012	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	4.5098	no units	

Di-n-butyl phthalate

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
17	ATSDR. 2001. Toxicological Profile for Di-n-Butyl Phthalate. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
188	USEPA. 1987. Chemical Assessment Summary di-n-butyl phthalate. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, DC.
211	USEPA. 1991. Drinking Water Criteria Document for Phthalic Acid Esters (PAES). U.S. Environmental Protection Agency, Office of Water, Health and Ecological Criteria Division, Washington, DC.

Diuron

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Diuron
CASRN:	330-54-1
DTXSID:	DTXSID0020446
Use:	Herbicide (HSD8)
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	1.1

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	carcinogen with linear MOA	4	7

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	2	urinary bladder carcinomas	general population	OPP	2015

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
2.1	90th Percentile	Finished Water	UCMR1	2001-2003

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X	X	X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Diuron
CCL 5 Contaminant Information Sheet
HEALTH EFFECTS DATA
EPA-OGWDW and OST
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Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.001	mg/kg/day	OPP 2015	Schmidt, 1985; Rossberg & Wirnitzer, 1985; Rossberg, 1995; Malek, 1997	hemolytic anemia and compensatory hematopoiesis	general population	33.8	5.92	[342]	
Cancer Slope Factor (CSF)	0.0191	(mg/kg/day)^-1	OPP 2015	Schmidt 1985; Rossberg and Wirnitzer, 1985; Rossberg, 1995; Malek 1997; Eiben, 1983	urinary bladder carcinomas	general population	33.8	1.55	[342]	
Cancer Classification (CC)	L		OPP 2015						[342]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	1	mg/L	EPA DWSHA 2018	
Lifetime Health Advisory	0.002	mg/L	EPA DWSHA 2018	
Maximum Allowable Concentration (MAC)	0.15	mg/L	Canadian Drinking Water Guidelines	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1017	mg/kg	NIH HSDB	min
LD50	3400	mg/kg	NIH HSDB	max
LOAEL	1	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	640.13	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	10	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	77.5	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	7.46	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0047098	mol/kg	TEST QSAR	
Ames mutagenicity test	0.027	no units	TEST QSAR	
Developmental toxin test	0.759	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Diuron
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003	293	1	Sites	0.34	2.1	2.1	2.1	2.1	ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	7,756	698	Sites	9	0.00021	0.0256	0.24	27.7	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	1,199	452	Sites	38	0.00021	0.0253	0.24	27.7	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	6,557	246	Sites	3.75	0.00054	0.03	0.25	5.53	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	47	3,410,787	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	9	37,175	Chemical Data Reporting (CDR) Results (EPA) (2016)	100K - 500K

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	26	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	15	10	Sites	67	0.0027	0.0072	0.057	1.3	ug/L	
Bradley et al. 2018 (Finished) [53]	2016	26	1	Sites	3.85	0.0041	0.0041	0.0041	0.0041	ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	213	9	Sites	4.23	1.2	3.5	3.5	3.5	ug/L	
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	560	255	Sites	46	0.00102	0.0208	0.138	25	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	1,240	47	Sites	3.79	0.00266	0.02	0.105	0.487	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,800	302	Sites	17	0.00102	0.0206	0.135	25	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	227	37	Sites	16	0.0027	0.013	0.06	1.2	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	29	Sites	13	0.0027	0.0141	0.0589	0.134	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	10	8	Sites	80	0.0027	0.012	0.06	1.2	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	8,018	1,811	Sites	23	0.0032	0.41	4.2	860	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	20	Sites	53	0.0024	0.0256	0.193	1.362	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	19	Sites	2.75	5e-04	0.0225	0.0758	0.121	ug/L	
USGS, McKenzie River, Oregon, 2012 (Ambient) [158]	2002 - 2010	126	21	Samples	17				6.07	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		1.31E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.55395	days	
Boiling point	OPERA QSAR	323.013	degree C	
Boiling point	TEST QSAR	298.055	degree C	
Vapor pressure	OPERA QSAR	8.24E-08	mmHg	
Vapor pressure	TEST QSAR	0.00000828	mmHg	
Solubility in water	OPERA QSAR	0.000238919	mol/L	
Solubility in water	TEST QSAR	0.00027227	mol/L	
Bioconcentration factor	OPERA QSAR	15.9255	no units	
Bioconcentration factor	TEST QSAR	22.9087	no units	
Henry's Law constant	OPERA QSAR	1.06E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.55186	no units	

Diuron

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. <i>Environmental science & technology</i> , 52(23), 13972-13985.
158	Reconnaissance of Land-Use Sources of Pesticides in Drinking Water, McKenzie River, Oregon. U.S. Geological Survey Scientific Investigations Report 2012–5091, 46 p. plus appendixes.
342	USEPA. 2015. Diuron. Human Health Assessment Scoping Document in Support of Registration Review. EPA-HQ-OPP-2015-0077-0004. DP No. D423231. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

EPTC

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	EPTC
CASRN:	759-94-4
DTXSID:	DTXSID1024091
Use:	Herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.00024

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	non-cancer effects	1	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	300	decreased body weight and increased incidences of myocardial and neuromuscular lesions	general population	OPP	2017

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.0724	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X	X		

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	X	Not Applicable

Basis

EPTC does not appear to occur at health levels of concern in PWSs and EPA has made a determination that terbacil does not present a meaningful opportunity for health risk reduction. While EPTC has been found in ambient waters at levels less than the HRL of 175 µg (as well as ½ the HRL) [a,b], it was not found in the UCMR 1 survey of public water supplies [c].

[a] Kolpin & Martin, 2003 [123]; [b] Martin, Crawford, & Larson, 2003 [134]; [c] USEPA, 2008 [297]; as cited in USEPA, 2008 [296]

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

EPTC
CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.05	mg/kg/day	OPP 2017	Warner 1983	decreased body weight and increased incidences of myocardial and neuromuscular lesions	general population	33.8	296	[382]	
Cancer Classification (CC)	NL		OPP 2017						[382]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Health-Based Guidance Value	0.3	mg/L	MN DOH	
Acute Health-Based Guidance Value	0.3	mg/L	MN DOH	
Acute Human Health Benchmark	1	mg/L	EPA HHBP	
Acute PAD	0.2	mg/kg/day	EPA HHBP	
Chronic Health-Based Guidance Value	0.04	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.2	mg/L	MN DOH	
Chronic Human Health Benchmark	0.3	mg/L	EPA HHBP	
Health-Based Screening Level	0.3	mg/L	Health-based screening levels from USGS	
Maximum Allowable Daily Level	700	ug/day	CalEPA OEHHA Chemical Database	
Population-Adjusted Dose (PAD)	0.05	mg/kg/day	EPA HHBP	
Short-Term/Subchronic Health-Based Guidance Value	0.09	mg/L	MN DOH	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	112	mg/kg	NIH HSDB	min
LD50	2550	mg/kg	NIH HSDB	max
LOAEL	300	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	8	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	1	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	100	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	3.64	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	15	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	45	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	15	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	3	mg/kg/day	EPA Toxicity Reference Database	min

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0048753	mol/kg	TEST QSAR	
Ames mutagenicity test	0.356	no units	TEST QSAR	
Developmental toxin test	0.59	no units	TEST QSAR	

EPTC
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003	3,873	0	Sites	0					ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	10,705	423	Sites	3.95	4.00E - 04	0.008	0.0724	40	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	2,055	369	Sites	18	4.00E - 04	0.008	0.0722	40	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	8,650	54	Sites	0.62	0.001	0.0047	0.0607	0.952	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	29	3,047,799	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	1	170	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	58	0	Sites	0						
Drinking Water Monitoring Data - WA (Finished)	2006 - 2011	482	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	1	Sites	5.88	0.017	0.028	0.06	0.068	ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	315	0	Sites	0						
Drinking Water Monitoring Data - WA (Source)	2006 - 2011	634	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	936	32	Sites	3.42	4.00E - 04	0.0061	0.0474	0.838	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	2,019	16	Sites	0.79	0.0017	0.0115	0.103	0.168	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	2,954	48	Sites	1.62	4.00E - 04	0.00705	0.0637	0.838	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	2	Sites	0.87	0.008	0.028	0.137	0.2	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	2	Sites	17	0.008	0.028	0.137	0.2	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	3,722	391	Sites	11	0.002	0.0228	0.5	23	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	4	Sites	11	0.0116	0.0708	0.196	0.224	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	1	Sites	0.14	0.016	0.016	0.016	0.016	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		5.95E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.73295	days	
Boiling point	OPERA QSAR	215.91	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.0226925	mmHg	
Vapor pressure	TEST QSAR	0.011508	mmHg	
Solubility in water	OPERA QSAR	0.00143197	mol/L	
Solubility in water	TEST QSAR	0.00174582	mol/L	
Bioconcentration factor	OPERA QSAR	23.7326	no units	
Bioconcentration factor	TEST QSAR	14.6893	no units	
Henry's Law constant	OPERA QSAR	0.00000125	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.21713	no units	

EPTC

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
123	Kolpin, D.W. and J.D. Martin. 2003. Pesticides in Ground Water: Summary Statistics; Preliminary Results from Cycle I of the National Water Quality Assessment Program (NAWQA), 1992-2001. Available on the Internet at: http://ca.water.usgs.gov/pnsp/pestgw/Pest-GW_2001_Text.html .
134	Martin, J.D., C.G. Crawford, and S.J. Larson. 2003. Pesticides in Streams: Summary Statistics; Preliminary Results from Cycle I of the National Water Quality Assessment Program (NAWQA), 1992-2001. Available on the Internet at: http://ca.water.usgs.gov/pnsp/pestsw/Pest-SW_2001_Text.html .
296	USEPA. 2008. Regulatory Determinations Support Document for Selected Contaminants from the Second Drinking Water Contaminant Candidate List (CCL 2). EPA Report 815-R-08-012. June 2008.
297	USEPA. 2008. The Analysis of Occurrence Data from the First Unregulated Contaminant Monitoring Regulation (UCMR 1) in Support of Regulatory Determinations for the Second Drinking Water Contaminant Candidate List. EPA 815-R-08-013. June.
382	USEPA. 2017. EPTC: (S-Ethyl dipropylthiocarbamate) Acute and Chronic Aggregate Dietary (Food and Drinking Water), Exposure and Risk Assessments for Registration Review. EPA-HQ-OPP-2012-0720-0019. DP No. D439764. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Esfenvalerate

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Esfenvalerate
CASRN:	66230-04-4
DTXSID:	DTXSID4032667
Use:	Insecticide; medication
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	1.5

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	reproductive and developmental effects	1	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	5	reduced locomotor activity	bottle-fed infants	OPP	2017

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
7.54		EDWC SW (acute)	OPP	2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Esfenvalerate

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0037	mg/kg/day	OPP 2017	Wolansky et al. 2006	reduced locomotor activity	bottle-fed infants	151	4.90	[383]	
Cancer Classification (CC)	E		OPP 2017						[383]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.012	mg/L	EPA HHBP	
Acute PAD	0.0018	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.012	mg/L	EPA HHBP	
Health-Based Screening Level	0.012	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.0018	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute LOAEL	7.5	mg/kg/day	EPA Toxicity Reference Database	
Acute NOAEL	2.5	mg/kg/day	EPA Toxicity Reference Database	
LD50	325	mg/kg	NIH HSDB	max
LD50	88	mg/kg	NIH HSDB	min
LOAEL	2.5	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	3	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	11.45	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	7.5	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	75	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	2.5	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	22.5	mg/kg/day	EPA Toxicity Reference Database	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0006934	mol/kg	TEST QSAR	
Ames mutagenicity test	0.3	no units	TEST QSAR	
Developmental toxin test	0.75	no units	TEST QSAR	

Esfenvalerate

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	2,965	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	645	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	2,320	0	Sites	0						

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	47	157,875	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	15	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	140	0	Sites	0						
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	143	0	Sites	0						
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	119	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	111	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	8	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	4,983	152	Sites	3.05	0.000335	0.015	0.134	3.48	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					
Estimated Drinking Water Concentration (EDWC) in Surface Water (acute)	2017	OPP	7.54	ug/L	Tier I, FQPA Index Reservoir Screening Tool (FIRST) Model	The critical effect of reduced locomotor activity was based on an acute population adjusted dose and is considered a less-than-chronic response. To account for this, the modeled surface water acute concentration was selected as the occurrence concentration for esfenvalerate.					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.0000017	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.35348	days	
Boiling point	OPERA QSAR	434.894	degree C	
Boiling point	TEST QSAR	456.288	degree C	
Vapor pressure	OPERA QSAR	1.64E-09	mmHg	
Vapor pressure	TEST QSAR	1.31E-09	mmHg	
Solubility in water	OPERA QSAR	0.000000197	mol/L	
Solubility in water	TEST QSAR	0.000000282	mol/L	
Bioconcentration factor	OPERA QSAR	646.164	no units	
Bioconcentration factor	TEST QSAR	240.991	no units	
Henry's Law constant	OPERA QSAR	7.95E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	6.17889	no units	

Esfenvalerate

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
383	USEPA. 2017. Esfenvalerate. Draft Human Health Risk Assessment for Registration Review. EPA-HQ-OPP-2009-0301-0074. DP No. D414149. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Ethalfuralin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Ethalfuralin
CASRN:	55283-68-6
DTXSID:	DTXSID8032386
Use:	Herbicide used on used on beans, watermelons, sunflowers, cantaloupes, and cucumbers
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.25

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	carcinogen with linear MOA	6	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.3	mammary gland fibro-adenomas and combined adenomas/fibro-adenomas	general population	OPP	2016

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.0751	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis
Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Ethalfuralin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.04	mg/kg/day	OPP 2016	Adams 1985	increased urinary bilirubin, variations in erythrocyte morphology, increased thrombocyte count, increased erythroid series of the bone marrow	general population	33.8	237	[365]	
Cancer Slope Factor (CSF)	0.089	(mg/kg/day) ⁻¹	OPP 2016	Adams et al. 1981; Adams 1981	mammary gland fibro-adenomas and combined adenomas/fibro-adenomas	general population	33.8	0.332	[365]	
Cancer Classification (CC)	C		OPP 2016						[365]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	21	mg/L	EPA HHBP	
Acute PAD	0.75	mg/kg/day	EPA HHBP	
Cancer Slope Factor (CSF)	0.089	(mg/kg/day) ⁻¹	EPA HHBP	
Chronic Human Health Benchmark	0.3	mg/L	EPA HHBP	
Chronic Human Health Benchmark	0.00036	mg/L	EPA HHBP	
Health-Based Screening Level	0.3	mg/L	Health-based screening levels from USGS	
Health-Based Screening Level	0.00036	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.04	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	5000	mg/kg	NIH HSDB	
LOAEL	20	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	250	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	4	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	50	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	7.89	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	125	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	27.5	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0147571	mol/kg	TEST QSAR	
Ames mutagenicity test	0.628	no units	TEST QSAR	
Developmental toxin test	1.214	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Ethalfuralin
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	8,238	59	Sites	0.72	0.001	0.014	0.0751	0.768	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	1,828	54	Sites	2.95	0.001	0.014	0.0742	0.768	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	6,410	5	Sites	0.08	0.004	0.005	0.048	0.09	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	45	1,391,050	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	15	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	333	2	Sites	0.6	0.0016	0.0044	0.00762	0.009	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	615	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	948	2	Sites	0.21	0.0016	0.0044	0.00762	0.009	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	225	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	218	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	8	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	1,348	24	Sites	1.78	0.005	0.031	0.0751	0.13	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.000000105	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.53726	days	
Boiling point	OPERA QSAR	350.978	degree C	
Boiling point	TEST QSAR	350.199	degree C	
Vapor pressure	OPERA QSAR	0.0000691	mmHg	
Vapor pressure	TEST QSAR	0.00000379	mmHg	
Solubility in water	OPERA QSAR	0.000000666	mol/L	
Solubility in water	TEST QSAR	0.00000234	mol/L	
Bioconcentration factor	OPERA QSAR	199.31	no units	
Bioconcentration factor	TEST QSAR	184.502	no units	
Henry's Law constant	OPERA QSAR	0.000000345	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	5.13595	no units	

Ethalfuralin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
365	USEPA. 2016. Ethalfuralin: Human Health Draft Risk Assessment for Registration Review. EPA-HQ-OPP-2011-0094-0016. DP No. D429844. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Ethion

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Ethion
CASRN:	563-12-2
DTXSID:	DTXSID2024086
Use:	Insecticide
Chemical Notes:	Canceled pesticide. Last end of use date: 12/31/2004.

Is the contaminant on any lists?	
CERCLA	X
FIFRA	X
Human Neurotoxicants	X
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0029

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	non-cancer effects	2	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	3	plasma, red blood cell, and brain cholinesterase inhibition	general population	OPP	2001

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.0088	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Ethion

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0005	mg/kg/day	OPP 2001	Bailey 1989	plasma, red blood cell, and brain cholinesterase inhibition	general population	33.8	2.96	[245]	NOTE: canceled registration

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Minimal Risk Level (MRL)	0.002	mg/kg/day	CDC ATSDR	
Intermediate Minimal Risk Level (MRL)	0.002	mg/kg/day	CDC ATSDR	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	208	mg/kg	NIH HSDB	max
LD50	24.4	mg/kg	NIH HSDB	min
LOAEL	0.049	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	9.6000004	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	2.4	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	0.028	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	10.88	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0000755	mol/kg	TEST QSAR	
Ames mutagenicity test	0.338	no units	TEST QSAR	
Developmental toxin test			TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
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EPA - Office of Water

Ethion
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	3,699	6	Sites	0.16	0.003	0.0065	0.0088	0.01	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	402	3	Sites	0.75	0.004	0.008	0.0094	0.01	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	3,297	3	Sites	0.09	0.003	0.005	0.0071	0.008	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	1	0.661	2015	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	15	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	470	1	Sites	0.21	0.108	0.108	0.108	0.108	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	2,012	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	2,481	1	Sites	0.04	0.108	0.108	0.108	0.108	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	123	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	114	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	10	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	614	2	Sites	0.33	0.01	0.03	0.046	0.05	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	106	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.000000118	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	526.103	days	
Boiling point	OPERA QSAR	395.284	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.00000179	mmHg	
Vapor pressure	TEST QSAR	0.00000561	mmHg	
Solubility in water	OPERA QSAR	0.00000621	mol/L	
Solubility in water	TEST QSAR	0.0000151	mol/L	
Bioconcentration factor	OPERA QSAR	242.157	no units	
Bioconcentration factor	TEST QSAR	58.3445	no units	
Henry's Law constant	OPERA QSAR	0.000000452	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	4.72384	no units	

Ethion

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
245	USEPA. 2001. Ethion RED. U.S. Environmental Protection Agency, Office of Prevention, Pesticides and Toxic Substances, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Ethoprop

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Ethoprop
CASRN:	13194-48-4
DTXSID:	DTXSID4032611
Use:	Insecticide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	X
Human Neurotoxicants	X
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.063

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	reproductive and developmental effects	2	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.9	inhibition of red blood cell cholinesterase in pups	bottle-fed infants	OPP	2015

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.0563	90th Percentile	Finished Water	UCMR4	2018-2019

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
		X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Ethoprop

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.00065	mg/kg/day	OPP 2015	Chartier et al. 2005	inhibition of red blood cell cholinesterase in pups	bottle-fed infants	151	0.861	[343]	
Cancer Slope Factor (CSF)	0.0281	(mg/kg/day)^-1	OPP 2015	Williams 1992	malignant adrenal pheochromocytomas in males	general population	33.8	1.05	[343]	
Cancer Classification (CC)	L		OPP 2015						[343]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.051	mg/L	EPA HHBP	
Acute PAD	0.0076	mg/kg/day	EPA HHBP	
Cancer Slope Factor (CSF)	0.0281	(mg/kg/day)^-1	EPA HHBP	
Chronic Human Health Benchmark	0.00114	mg/L	EPA HHBP	
Chronic Human Health Benchmark	0.009	mg/L	EPA HHBP	
Health-Based Screening Level	0.00114	mg/L	Health-based screening levels from USGS	
Health-Based Screening Level	0.009	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.0014	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	216	mg/kg	NIH HSDB	max
LD50	5.62	mg/kg	NIH HSDB	min
LOAEL	0.254	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	24	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	13	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	0.032	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	3.88	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	0.025	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	0.01	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0001291	mol/kg	TEST QSAR	
Ames mutagenicity test	-0.038	no units	TEST QSAR	
Developmental toxin test	0.477	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
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EPA - Office of Water

Ethioprop
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019	3,648	4	Sites	0.11	0.0326	0.0485	0.0563	0.059	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	10,705	104	Sites	0.97	2.00E - 04	0.011	0.0796	5.75	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	2,055	100	Sites	4.87	2.00E - 04	0.011	0.0795	5.75	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	8,650	4	Sites	0.05	0.006	0.009	0.149	0.243	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	14	883,037	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	2	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	15	1	Sites	6.67	0.027	0.027	0.027	0.027	ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	11	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	841	17	Sites	2.02	0.00094	0.00334	0.148	0.268	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	2,018	1	Sites	0.05	0.00114	0.00114	0.00114	0.00114	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	2,858	18	Sites	0.63	0.00094	0.0032	0.147	0.268	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	123	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	114	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	10	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	6,608	29	Sites	0.44	0.003	0.112	0.729	5.4094	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	1	Sites	2.63	0.122	0.122	0.122	0.122	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		8.62E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	74.8059	days	
Boiling point	OPERA QSAR	286.424	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.000409034	mmHg	
Vapor pressure	TEST QSAR	0.000234963	mmHg	
Solubility in water	OPERA QSAR	0.00240073	mol/L	
Solubility in water	TEST QSAR	0.00295121	mol/L	
Bioconcentration factor	OPERA QSAR	20.4104	no units	
Bioconcentration factor	TEST QSAR	33.4965	no units	
Henry's Law constant	OPERA QSAR	0.00000701	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.42685	no units	

Ethoprop

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
343	USEPA. 2015. Ethoprop. Preliminary Occupational and Residential Exposure/Risk Assessment for Registration Review. EPA-HQ-OPP-2008-0560-0056. DP No. D421954. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Ethyl citrate

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Ethyl citrate
CASRN:	77-93-0
DTXSID:	DTXSID0040701
Use:	Solvent and plasticizer for nitrocellulose and natural resins, softener, paint removers, agglutinant, perfume base, food additive
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0000095

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
3	no adverse effects	9	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	20000	no adverse effect level	general population		

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.19	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Ethyl citrate
CCL 5 Contaminant Information Sheet
HEALTH EFFECTS DATA

EPA-OGWDW and OST

July 2021

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	4	mg/kg/day		Finkelstein and Gold, 1959	no adverse effect level	general population	33.8	23700	[78]	NOTE: No health assessments found; NOAEL/UF used in place of the RfD, NOAEL obtained from a study identified by the rapid systematic literature review

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
			Endocrine, Systemic, Renal, Immunological, Hepatic, Gastrointestinal, Respiratory, Cardiovascular, Hematological	4000	Finkelstein, 1959		2020-04-14	83	2	0	1

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
The full citation for the critical study is provided in the corresponding health assessment.
PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	3200	mg/kg	NIH HSDB	min
LD50	35000	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	1.2	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0146893	mol/kg	TEST QSAR	
Ames mutagenicity test	0.349	no units	TEST QSAR	
Developmental toxin test	0.701	no units	TEST QSAR	

Ethyl citrate
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	567	17	Sites	3	0.01	0.04	0.19	0.48	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	88	16	Sites	18	0.01	0.04	0.186	0.43	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	479	1	Sites	0.21	0.48	0.48	0.48	0.48	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	1M - 10M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	4		0.013		0.013	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	715	197	Sites	28	0.01	0.06	14.2	334	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	689	10	Sites	1.45	0.01	0.02	0.04	0.09	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,404	207	Sites	15	0.01	0.06	14	334	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	15	Sites	39	0.0266	0.11	0.462	0.694	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	1	Sites	50						
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	19	Sites	90	0.14	0.47	1.28	2	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.0000592	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.81755	days	
Boiling point	OPERA QSAR	292.74	degree C	
Boiling point	TEST QSAR	316.611	degree C	
Vapor pressure	OPERA QSAR	0.000485688	mmHg	
Vapor pressure	TEST QSAR	0.0000562	mmHg	
Solubility in water	OPERA QSAR	0.229189	mol/L	
Solubility in water	TEST QSAR	0.0166725	mol/L	
Bioconcentration factor	OPERA QSAR	3.52492	no units	
Bioconcentration factor	TEST QSAR	1.36144	no units	
Henry's Law constant	OPERA QSAR	2.49E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	0.512786	no units	

Ethyl citrate

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
78	Finkelstein M. and Gold, H. 1959. Toxicology of the citric acid esters: tributyl citrate, acetyl tributyl citrate, triethyl citrate, and acetyl triethyl citrate. <i>Toxicology and applied pharmacology</i> . 1(283-98).
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.

Famoxadone

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Famoxadone
CASRN:	131807-57-3
DTXSID:	DTXSID8034588
Use:	Fungicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.00074

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	non-cancer effects	1	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	8	microscopic lens lesions (cataracts)	general population	OPP	2015

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.0059	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Famoxadone

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0014	mg/kg/day	OPP 2015	Tompkins 1995; Salik 1995	microscopic lens lesions (cataracts)	general population	33.8	8.28	[344]	
Cancer Classification (CC)	NL		OPP 2015						[344]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Chronic Human Health Benchmark	0.009	mg/L	EPA HHBP	
Health-Based Screening Level	0.009	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.0014	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	5000	mg/kg	NIH HSDB	
LOAEL	1000	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	8.8000002	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	1.2	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	350	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	26.49	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	10	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	534	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	1.3	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	79.9	mg/kg/day	EPA Toxicity Reference Database	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0038548	mol/kg	TEST QSAR	
Ames mutagenicity test	0.201	no units	TEST QSAR	
Developmental toxin test	0.803	no units	TEST QSAR	

Famoxadone

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	1,348	1	Sites	0.07	0.0059	0.0059	0.0059	0.0059	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	290	1	Sites	0.34	0.0059	0.0059	0.0059	0.0059	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	1,058	0	Sites	0						

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	36	56,460	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	273	1	Sites	0.37	0.0091	0.016	0.0196	0.0216	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	153	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	426	1	Sites	0.23	0.0091	0.016	0.0196	0.0216	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	134	4	Sites	2.99	0.0091	0.016	0.0201	0.0216	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exposure exposure		0.000000023	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.54781	days	
Boiling point	OPERA QSAR	408.651	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	6.94E-09	mmHg	
Vapor pressure	TEST QSAR	1.3E-10	mmHg	
Solubility in water	OPERA QSAR	0.000000238	mol/L	
Solubility in water	TEST QSAR	0.00000161	mol/L	
Bioconcentration factor	OPERA QSAR	83.2068	no units	
Bioconcentration factor	TEST QSAR	38.5478	no units	
Henry's Law constant	OPERA QSAR	5.34E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	4.59956	no units	

Famoxadone

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
344	USEPA. 2015. Famoxadone. Human Health Assessment Scoping Document in Support of Registration Review. EPA-HQ-OPP-2015-0094-0002. DP No. D423286. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Fenbuconazole

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Fenbuconazole
CASRN:	114369-43-6
DTXSID:	DTXSID8032548
Use:	Fungicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	1.5

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
3	carcinogen with linear MOA	1	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	8	hepatocellular adenomas and carcinomas in mice; thyroid follicular adenomas and combined adenomas/carcinomas in rats	general population	OPP	2019

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
11.7		EDWC SW (chronic,	OPP	2019

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		
Not Applicable		

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Fenbuconazole

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.03	mg/kg/day	OPP 2019	Wolfe 1990	decreased body weight gain, increased thyroid weight, histopathological lesions in liver and thyroid gland	general population	33.8	178	[417]	
Cancer Slope Factor (CSF)	0.00359	(mg/kg/day)^-1	OPP 2019	Wolfe 1990 and 1991a and b	hepatocellular adenomas and carcinomas in mice; thyroid follicular adenomas and combined adenomas/carcinomas in rats	general population	33.8	8.24	[417]	
Cancer Classification (CC)	C		OPP 2019						[417]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	8	mg/L	EPA HHBP	
Acute PAD	0.3	mg/kg/day	EPA HHBP	
Cancer Slope Factor (CSF)	0.00359	(mg/kg/day)^-1	EPA HHBP	
Chronic Human Health Benchmark	0.2	mg/L	EPA HHBP	
Chronic Human Health Benchmark	0.00891	mg/L	EPA HHBP	
Population-Adjusted Dose (PAD)	0.03	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LOAEL	3.75	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	75	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	0.38	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	30	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	17.11	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	13.27	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic LOAEL	5.0999999	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	1.5	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	5.7	mg/kg/day	EPA Toxicity Reference Database	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0034834	mol/kg	TEST QSAR	
Ames mutagenicity test	0.752	no units	TEST QSAR	
Developmental toxin test	0.488	no units	TEST QSAR	

Fenbuconazole

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	14	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	14	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	30	46,778	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	13	1	Sites	7.69	0.057	0.057	0.057	0.057	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	132	0	Sites	0						
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	135	0	Sites	0						
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	121	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	114	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	8	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	99	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					
Estimated Drinking Water Concentration (EDWC) in Surface Water (chronic, cancer)	2019	OPP	11.7	ug/L	Tier II Pesticide Root Zone Model (PRZM) - Exposure Analysis Modeling System (EXAMS)	The modeled surface water chronic, cancer concentration provided by the most recent available EPA OPP health assessment was selected as the occurrence concentration for fenbuconazole. This value coincides with the critical effects of thyroid and liver adenomas and carcinomas provided within the health effects report.					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
ExpoCast exposure		0.000000133	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.3514	days	
Boiling point	OPERA QSAR	335.634	degree C	
Boiling point	TEST QSAR	445.687	degree C	
Vapor pressure	OPERA QSAR	4.42E-08	mmHg	
Vapor pressure	TEST QSAR	5.66E-09	mmHg	
Solubility in water	OPERA QSAR	0.0000013	mol/L	
Solubility in water	TEST QSAR	0.0000166	mol/L	
Bioconcentration factor	OPERA QSAR	281.827	no units	
Bioconcentration factor	TEST QSAR	132.739	no units	
Henry's Law constant	OPERA QSAR	0.00000424	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.14361	no units	

Fenbuconazole

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
417	USEPA. 2019. Fenbuconazole: Human Health Risk Assessment for Proposed Use on Imported Tea. EPA-HQ-OPP-2018-0300-0004. DP No. D446940. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Fenitrothion

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Fenitrothion
CASRN:	122-14-5
DTXSID:	DTXSID4032613
Use:	Insecticide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	X
PubMed Neurotoxics	X
Neurodev. Disruptors	
Androgen Receptors in vitro	X
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.39

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	reproductive and developmental effects		

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.2	plasma cholinesterase inhibition and histopathology of lymph nodes	bottle-fed infants	OPP	2010

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.078	90th Percentile	Ambient (SW) Water	SURF	1990-2018

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Fenitrothion

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.000125	mg/kg/day	OPP 2010	Spicer 1986	plasma cholinesterase inhibition and histopathology of lymph nodes	bottle-fed infants	151	0.166	[313]	
Cancer Classification (CC)	E		OPP 2010						[313]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.0017	mg/L	EPA HHBP	
Acute PAD	0.00025	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.0008	mg/L	EPA HHBP	
Population-Adjusted Dose (PAD)	0.000125	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1720	mg/kg	NIH HSDB	max
LD50	500	mg/kg	NIH HSDB	min
LOAEL	0.25	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	30	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	0.125	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	10	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	15.77	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	1.5	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	0.5	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0001122	mol/kg	TEST QSAR	
Ames mutagenicity test	0.548	no units	TEST QSAR	
Developmental toxin test	0.713	no units	TEST QSAR	

Fenitrothion

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	0	Sites	0						
Ambient Water											
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	201	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	191	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	2,406	1	Sites	0.04	0.078	0.078	0.078	0.078	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					
	2010	OPP		ug/L		No modeled concentrations were provided by OPP because "it is highly unlikely that fenitrothion will reach drinking water resources..." due to its selective uses in bait traps. "The only route of [oral] exposure ... is in the diet from imported wheat."					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.000000078	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.49784	days	
Boiling point	OPERA QSAR	353.148	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.0000185	mmHg	
Vapor pressure	TEST QSAR	0.000016	mmHg	
Solubility in water	OPERA QSAR	0.000156501	mol/L	
Solubility in water	TEST QSAR	0.0000621	mol/L	
Bioconcentration factor	OPERA QSAR	83.6872	no units	
Bioconcentration factor	TEST QSAR	57.1479	no units	
Henry's Law constant	OPERA QSAR	0.000000596	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.37577	no units	

Fenitrothion

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
313	USEPA. 2010. Fenitrothion. Risk Assessment to Support Final Registration Review Decision. EPA-HQ-OPP-2009-0172-0016. DP No. D383647. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Fenpropathrin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Fenpropathrin
CASRN:	39515-41-8
DTXSID:	DTXSID0024002
Use:	Insecticide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0016

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	reproductive and developmental effects	1	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	20	reduced motor activity	bottle-fed infants	OPP	2016

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.0324	90th Percentile	Ambient (SW) Water	CA SURF	1990-2018

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis
Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Fenpropathrin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.017	mg/kg/day	OPP 2016	Wolansky et al. 2006	reduced motor activity	bottle-fed infants	151	22.5	[366]	
Cancer Classification (CC)	NL		OPP 2016						[366]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.11	mg/L	EPA HHBP	
Acute PAD	0.017	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	66.7	mg/kg	NIH HSDB	min
LD50	70.6	mg/kg	NIH HSDB	max
LOAEL	19.450001	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	2	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	0.4	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	7.23	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	12.5	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	30	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic LOAEL	6.25	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	15	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0004742	mol/kg	TEST QSAR	
Ames mutagenicity test	0.248	no units	TEST QSAR	
Developmental toxin test	0.825	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Fenpropathrin

CCL 5 Contaminant Information Sheet

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	14	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	14	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	24	185,210	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	13	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	140	0	Sites	0						
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	143	0	Sites	0						
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	121	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	114	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	8	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	2,562	29	Sites	1.13	0.001092	0.005	0.0324	2.979733	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					
Limit of solubility surrogate for occurrence concentration, Surface Water Peak	2016	OPP	10.3	ug/L		Fenpropathrin is very insoluble in water and residues in drinking water are expected to be very low. Therefore, no modeling of estimated occurrence was conducted and the limit of solubility of fenpropathrin (10.3 ppb) reported in the most recent EPA OPP health assessment was used as a surrogate for the peak expected occurrence concentration.					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.0000001	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.53866	days	
Boiling point	OPERA QSAR	370.491	degree C	
Boiling point	TEST QSAR	414.903	degree C	
Vapor pressure	OPERA QSAR	0.00000331	mmHg	
Vapor pressure	TEST QSAR	0.000000011	mmHg	
Solubility in water	OPERA QSAR	0.0000003	mol/L	
Solubility in water	TEST QSAR	0.000000228	mol/L	
Bioconcentration factor	OPERA QSAR	217.595	no units	
Bioconcentration factor	TEST QSAR	744.732	no units	
Henry's Law constant	OPERA QSAR	9.96E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	5.47445	no units	

Fenpropathrin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
366	USEPA. 2016. Fenpropathrin. Draft Human Health Risk Assessment for Registration Review. EPA-HQ-OPP-2010-0422-0017. DP No. D425768. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Fenthion

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Fenthion
CASRN:	55-38-9
DTXSID:	DTXSID8020620
Use:	Insecticide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	X
PubMed Neurotoxics	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.48

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	non-cancer effects	1	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.4	plasma cholinesterase inhibition	general population	OPP	2001

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.19		EEC SW 56-day average (chronic)	OPP	2001

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		
Not Applicable		

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Fenthion

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.00007	mg/kg/day	OPP 2001	Rosenblum 1980	plasma cholinesterase inhibition	general population	33.8	0.414	[246]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.005	mg/L	EPA HHBP	
Acute PAD	0.0007	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.0004	mg/L	EPA HHBP	
Health-Based Screening Level	0.0004	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.00007	mg/kg/day	EPA HHBP	
Cancer Classification (CC)	Female.Mice N	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats N	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice E	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats N	no units	HHS NTP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	150	mg/kg	NIH HSDB	min
LD50	245	mg/kg	NIH HSDB	max
LOAEL	18	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	0.03	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	0.056	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	6	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	11.56	percent	EPA Chemistry Dashboard	
TD50	1.03	mg/kg/day	NIH CPDB	min
TD50	29.4	mg/kg/day	NIH CPDB	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0002965	mol/kg	TEST QSAR	
Ames mutagenicity test	0.214	no units	TEST QSAR	
Developmental toxin test	0.588	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Fenthion
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	336	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	36	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	300	0	Sites	0						

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	1	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	15	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	3	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	59	0	Sites	0						
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	1	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	60	0	Sites	0						
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	123	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	114	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	10	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	4,579	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					
Estimated Environmental Concentration (EEC) in Surface Water, 56-day Average (chronic)	2001	OPP	0.19	ug/L	GENeric Estimated Environmental Concentration (GENEEC) Model	The estimated environmental concentration provided by the most recent available EPA OPP health assessment was selected as the occurrence value for fenthion. The 56-day concentration in surface water was the only value available as an estimate of chronic exposure.					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		8.99E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.47178	days	
Boiling point	OPERA QSAR	361.38	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.0000182	mmHg	
Vapor pressure	TEST QSAR	0.0000659	mmHg	
Solubility in water	OPERA QSAR	0.0000218	mol/L	
Solubility in water	TEST QSAR	0.0000212	mol/L	
Bioconcentration factor	OPERA QSAR	285.803	no units	
Bioconcentration factor	TEST QSAR	130.317	no units	
Henry's Law constant	OPERA QSAR	0.00000106	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	4.07281	no units	

Fenthion

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
246	USEPA. 2001. Interim Reregistration Eligibility Decision for Fenthion. EPA 738-R-00-013. U.S. Environmental Protection Agency, Office of Prevention, Pesticides and Toxic Substances, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Fexofenadine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Fexofenadine
CASRN:	83799-24-0
DTXSID:	DTXSID00861411
Use:	Antihistaminic
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.47

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	non-cancer effects	9	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	3	lowest therapeutic dose: anxiolytic, sedative, muscle-relaxant, anticonvulsant and amnestic effects	bottle-fed infants	FDA; NIH	2018; 2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
1.4	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Fexofenadine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0005	mg/kg/day	FDA 2018; NIH 2018	Major Pharmaceuticals	lowest therapeutic dose: anxiolytic, sedative, muscle-relaxant, anticonvulsant and amnesic effects	bottle-fed infants	151	3.30	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels
Reference Dose (RfD) or Equivalent	0.0005	mg/kg/day	FDA 2018; NIH 2018	Major Pharmaceuticals	lowest therapeutic dose: anxiolytic, sedative, muscle-relaxant, anticonvulsant and amnesic effects	general population	33.8	12.0	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Screening level for pharmaceutical - general population	0.011764706	mg/L	EPA Office of Water	
Screening level for pharmaceutical - infants	0.003333333	mg/L	EPA Office of Water	

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0019634	mol/kg	TEST QSAR	
Ames mutagenicity test	0.02	no units	TEST QSAR	
Developmental toxin test	0.836	no units	TEST QSAR	

Fexofenadine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	557	24	Sites	4.31	0.00197	0.0348	1.4	3.89	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	75	24	Sites	32	0.00197	0.0348	1.4	3.89	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	482	0	Sites	0						

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Ambient Water											
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	8		0.112		0.16309	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	16	Sites	42	0.010424	0.576	1.74	2.047397	ug/L	
Bexfield et al. 2019 (Groundwater) [49]	2013 - 2015	1,106	0	Sites	0						
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	20	Sites	95	0.015476	1.13	2.79	17.37626	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exposure exposure			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	26.1502	days	
Boiling point	OPERA QSAR	422.926	degree C	
Boiling point	TEST QSAR	514.695	degree C	
Vapor pressure	OPERA QSAR	2.56E-09	mmHg	
Vapor pressure	TEST QSAR	1.45E-11	mmHg	
Solubility in water	OPERA QSAR	0.0000028	mol/L	
Solubility in water	TEST QSAR	0.0000137	mol/L	
Bioconcentration factor	OPERA QSAR	13.808	no units	
Bioconcentration factor	TEST QSAR	15.9956	no units	
Henry's Law constant	OPERA QSAR	2.51E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	4.63629	no units	

Fexofenadine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
49	Bexfield, L.M., P.L. Toccalino, K. Belitz, W.T. Foreman, and E.T. Furlong. 2019. Hormones and pharmaceuticals in groundwater used as a source of drinking water across the United States. Environmental Science and Technology 53: 2950-2960.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. Environmental science & technology, 51(9), 4792-4802.
77	FDA. 2018. Drugs @ FDA: FDA Approved Drug Products. U.S. Food and Drug Administration (FDA). https://www.accessdata.fda.gov/scripts/cder/daf/ .
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. Science of The Total Environment. v581-582, (909-922).
150	NIH. 2018. DailyMed Database. U.S. National Library of Medicine, National Institutes of Health (NIH). https://dailymed.nlm.nih.gov/dailymed/ .
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. Science of the Total Environment, 636, 69-79.

Fipronil

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Fipronil
CASRN:	120068-37-3
DTXSID:	DTXSID4034609
Use:	insecticide, seed treatment/protectant
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.02

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
9	reduced longevity	9	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	1	increased incidence of seizures and death, changes in clinical chemistry (protein), increased TSH, decreased T4	women of childbearing age	OPP	2011

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.02	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Fipronil

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0002	mg/kg/day	OPP 2011	Aughton 1993	increased incidence of seizures and death, alterations in clinical chemistry (protein), increased TSH, decreased T4	women of childbearing age	35.4	1.13	[319]	
Cancer Classification (CC)	C		OPP 2011						[319]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.17	mg/L	EPA HHBP	
Acute PAD	0.025	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.001	mg/L	EPA HHBP	
Health-Based Screening Level	0.001	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.0002	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	103	mg/kg	NIH HSDB	max
LD50	91	mg/kg	NIH HSDB	min
LOAEL	26.299999	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	0.059	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	0.025	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	4	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	26.37	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	0.32	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	3.2	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	0.11	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	1.72	mg/kg/day	EPA Toxicity Reference Database	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity test			TEST QSAR	
Developmental toxin test			TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
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EPA - Office of Water

Fipronil
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OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	5,307	402	Sites	7.57	0.00014	0.0063	0.02	6.41	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	634	326	Sites	51	0.00014	0.00619	0.019	6.41	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	4,673	76	Sites	1.63	0.00096	0.008	0.0503	0.43	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	12	7,124	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	8	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	1,001	321	Sites	32	0.00022	0.0067	0.035	0.181	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3,062	46	Sites	1.5	0.001	0.005	0.0168	0.035	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	4,062	367	Sites	9.03	0.00022	0.0065	0.033	0.181	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	121	15	Sites	12	0.00058	0.00058	0.00226	0.013	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	114	11	Sites	9.65	0.00058	0.0014	0.00531	0.013	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	8	4	Sites	50	0.00058	0.00058	0.00132	0.0028	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	1,135	513	Sites	45	0.00031	0.051	0.203	2.11	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	17	Sites	45	0.0066	0.0238	0.0948	0.153	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	4	Sites	0.58	0.001	0.0014	0.00255	0.003	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	1	Sites	50	0.001	0.001	0.001	0.001	ug/L	
USGS, McKenzie River, Oregon, 2012 (Ambient) [158]	2002 - 2010	119	5	Samples	4.2				0.041	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		2.65E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.54048	days	
Boiling point	OPERA QSAR	323.014	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	2.17E-09	mmHg	
Vapor pressure	TEST QSAR			
Solubility in water	OPERA QSAR	0.00000538	mol/L	
Solubility in water	TEST QSAR	0.000065	mol/L	
Bioconcentration factor	OPERA QSAR	5.12606	no units	
Bioconcentration factor	TEST QSAR			
Henry's Law constant	OPERA QSAR	9.05E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.93502	no units	

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
158	Reconnaissance of Land-Use Sources of Pesticides in Drinking Water, McKenzie River, Oregon. U.S. Geological Survey Scientific Investigations Report 2012–5091, 46 p. plus appendixes.
319	USEPA. 2011. Fipronil. Human Health Assessment Scoping Document in Support of Registration Review. EPA-HQ-OPP-2011-0448-0004. DP No. D387318. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Fluconazole
CASRN:	86386-73-4
DTXSID:	DTXSID3020627
Use:	Antifungal
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.36

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	non-cancer effects	9	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	1	lowest therapeutic dose: treatment of vaginal candidiasis (vaginal yeast infections due to Candida), oropharyngeal and esophageal candidiasis, cryptococcal meningitis	bottle-fed infants	FDA; NIH	2018; 2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.357	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		
Not Applicable		

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Fluconazole

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.000208333	mg/kg/day	FDA 2018; NIH 2018	Teva Pharmaceuticals USA, Inc.	lowest therapeutic dose: treatment of vaginal candidiasis (vaginal yeast infections due to Candida), oropharyngeal and esophageal candidiasis, cryptococcal meningitis	bottle-fed infants	151	1.40	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels
Reference Dose (RfD) or Equivalent	0.000208333	mg/kg/day	FDA 2018; NIH 2018	Teva Pharmaceuticals USA, Inc.	lowest therapeutic dose: treatment of vaginal candidiasis (vaginal yeast infections due to Candida), oropharyngeal and esophageal candidiasis, cryptococcal meningitis	general population	33.8	4.90	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
							2020-01-28	5574			

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Screening level for pharmaceutical - general population	0.004901961	mg/L	EPA Office of Water	
Screening level for pharmaceutical - infants	0.001388889	mg/L	EPA Office of Water	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Percent of active toxcast in vitro assays tested	0.45	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0021727	mol/kg	TEST QSAR	
Ames mutagenicity test	0.828	no units	TEST QSAR	
Developmental toxin test			TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
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Fluconazole
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	557	14	Sites	2.51	0.00139	0.025	0.357	0.482	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	75	12	Sites	16	0.00139	0.025	0.395	0.482	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	482	2	Sites	0.41	0.00501	0.0895	0.14	0.174	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Ambient Water											
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	4		0.0337		0.03367	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	14	Sites	37	0.0053864	0.108	0.196	0.2324315	ug/L	
Bexfield et al. 2019 (Groundwater) [49]	2013 - 2015	1,106	1	Sites	0.09	0.0507747	0.0508	0.0508	0.0507747	ug/L	
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	21	Sites	100	0.0700863	0.146	0.497	555	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exposure exposure		0.000000221	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.46378	days	
Boiling point	OPERA QSAR	293.089	degree C	
Boiling point	TEST QSAR	408.078	degree C	
Vapor pressure	OPERA QSAR	2.39E-09	mmHg	
Vapor pressure	TEST QSAR	2.99E-08	mmHg	
Solubility in water	OPERA QSAR	0.0101826	mol/L	
Solubility in water	TEST QSAR	0.00134586	mol/L	
Bioconcentration factor	OPERA QSAR	6.95881	no units	
Bioconcentration factor	TEST QSAR	20.797	no units	
Henry's Law constant	OPERA QSAR	7.12E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	0.62128	no units	

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Reference Number	Full Reference
49	Bexfield, L.M., P.L. Toccalino, K. Belitz, W.T. Foreman, and E.T. Furlong. 2019. Hormones and pharmaceuticals in groundwater used as a source of drinking water across the United States. Environmental Science and Technology 53: 2950-2960.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. Environmental science & technology, 51(9), 4792-4802.
77	FDA. 2018. Drugs @ FDA: FDA Approved Drug Products. U.S. Food and Drug Administration (FDA). https://www.accessdata.fda.gov/scripts/cder/daf/ .
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. Science of The Total Environment. v581-582, (909-922).
150	NIH. 2018. DailyMed Database. U.S. National Library of Medicine, National Institutes of Health (NIH). https://dailymed.nlm.nih.gov/dailymed/ .
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. Science of the Total Environment, 636, 69-79.

Flufenacet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Flufenacet
CASRN:	142459-58-3
DTXSID:	DTXSID2032552
Use:	Preemergent herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.11

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	reproductive and developmental effects	8	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	2	decreased pup body weight, delayed eye opening, delayed preputial separation, decreased caudate putamen size	bottle-fed infants	OPP	2015

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.228	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Flufenacet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0017	mg/kg/day	OPP 2015	Hoberman 2000	decreased pup body weight, delayed eye opening, delayed preputial separation, decreased caudate putamen size	bottle-fed infants	151	2.25	[345]	
Cancer Classification (CC)	NL		OPP 2015						[345]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.011	mg/L	EPA HHBP	
Acute PAD	0.0017	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.011	mg/L	EPA HHBP	
Health-Based Screening Level	0.011	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.0017	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	2347	mg/kg	NIH HSDB	max
LD50	371	mg/kg	NIH HSDB	min
LOAEL	1.2	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	1000	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	1.29	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	25	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	12.4	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	6	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	64.199997	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	1.7	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	24.5	mg/kg/day	EPA Toxicity Reference Database	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0039995	mol/kg	TEST QSAR	
Ames mutagenicity test	0.556	no units	TEST QSAR	
Developmental toxin test	0.742	no units	TEST QSAR	

Flufenacet

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	973	15	Sites	1.54	0.02	0.03	0.228	0.44	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	69	12	Sites	17	0.02	0.03	0.252	0.44	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	904	3	Sites	0.33	0.02	0.04	0.047	0.05	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	14	115,383	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	4	1	Sites	25	0.075	0.075	0.075	0.075	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	113	3	Sites	2.65	0.02	0.03	0.065	0.08	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	342	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	455	3	Sites	0.66	0.02	0.03	0.065	0.08	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	4	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	4	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.00000012	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.53831	days	
Boiling point	OPERA QSAR	350.468	degree C	
Boiling point	TEST QSAR	362.085	degree C	
Vapor pressure	OPERA QSAR	0.000000773	mmHg	
Vapor pressure	TEST QSAR	0.000000151	mmHg	
Solubility in water	OPERA QSAR	0.000125919	mol/L	
Solubility in water	TEST QSAR	0.0000364	mol/L	
Bioconcentration factor	OPERA QSAR	10.967	no units	
Bioconcentration factor	TEST QSAR	51.9996	no units	
Henry's Law constant	OPERA QSAR	7.92E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.14459	no units	

Flufenacet

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
345	USEPA. 2015. Flufenacet: Human Health Draft Risk Assessment for Registration Review. EPA-HQ-OPP-2010-0863-0017. DP No. D416546. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.

Fluometuron

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Fluometuron
CASRN:	2164-17-2
DTXSID:	DTXSID8020628
Use:	Herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.56

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	carcinogen with linear MOA	9	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	2	combined adenomas/carcinomas in the lung of males and malignant lymphocytic lymphomas in females	general population	OPP	2016

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
1.116	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		
Not Applicable		

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Fluometuron

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.005	mg/kg/day	OPP 2016	Burdock et al. 1982	decreased body weight gain, increased splenic hemosiderin pigment deposition	general population	33.8	29.6	[367]	
Cancer Slope Factor (CSF)	0.018	(mg/kg/day)^-1	OPP 2016	Burdock et al. 1982	combined adenomas/carcinomas in the lung of males and malignant lymphocytic lymphomas in females	general population	33.8	1.64	[367]	
Cancer Classification (CC)	C		OPP 2016						[367]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	2	mg/L	EPA DWSHA 2018	
Cancer Classification (CC)	3	no units	WHO IARC	
Lifetime Health Advisory	0.09	mg/L	EPA DWSHA 2018	
Cancer Classification (CC)	Female.Mice N	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats N	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice E	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats N	no units	HHS NTP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	6416	mg/kg	NIH HSDB	max
LD50	810	mg/kg	NIH HSDB	min
LOAEL	100	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	260.20001	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	10	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	83.9	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	3.04	percent	EPA Chemistry Dashboard	
TD50	1420	mg/kg/day	NIH CPDB	max
TD50	55.4	mg/kg/day	NIH CPDB	min

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0031915	mol/kg	TEST QSAR	
Ames mutagenicity test	0.047	no units	TEST QSAR	
Developmental toxin test	0.851	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Fluometuron

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	7,813	242	Sites	3.1	0.00011	0.07	1.12	31.5	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	1,222	136	Sites	11	0.00011	0.06	1.09	31.5	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	6,591	106	Sites	1.61	0.00035	0.17	1.27	2.26	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	15	1,023,468	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	3	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	15	6	Sites	40	0.001998	0.007	0.007	0.042	ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	24	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	495	26	Sites	5.25	0.00424	0.03	0.108	0.79	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	1,249	14	Sites	1.12	0.00938	0.106	0.316	2.71	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,744	40	Sites	2.29	0.00424	0.04	0.27	2.71	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	227	14	Sites	6.17	0.001998	0.007	0.083	0.229	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	8	Sites	3.65	0.006993	0.083	0.22	0.229	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	10	6	Sites	60	0.001998	0.007	0.007	0.1	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	393	1	Sites	0.25	3	3	3	3	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	3	Sites	7.89	0.0086	0.014	0.0168	0.0175	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	7	Sites	1.01	3e-04	0.0011	0.0315	0.0514	ug/L	
USGS, McKenzie River, Oregon, 2012 (Ambient) [158]	2002 - 2010	126	2	Samples	1.6				0.02	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		7.92E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.65653	days	
Boiling point	OPERA QSAR	302.918	degree C	
Boiling point	TEST QSAR	280.864	degree C	
Vapor pressure	OPERA QSAR	0.00000113	mmHg	
Vapor pressure	TEST QSAR	0.000000807	mmHg	
Solubility in water	OPERA QSAR	0.000355964	mol/L	
Solubility in water	TEST QSAR	0.000616595	mol/L	
Bioconcentration factor	OPERA QSAR	10.1821	no units	
Bioconcentration factor	TEST QSAR	28.774	no units	
Henry's Law constant	OPERA QSAR	8.44E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.43892	no units	

Fluometuron

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
158	Reconnaissance of Land-Use Sources of Pesticides in Drinking Water, McKenzie River, Oregon. U.S. Geological Survey Scientific Investigations Report 2012–5091, 46 p. plus appendixes.
367	USEPA. 2016. Fluometuron. Human Health Assessment Scoping Document in Support of Registration Review. EPA-HQ-OPP-2015-0746-0009. DP No. D430248; D391415. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Fluoranthene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Fluoranthene
CASRN:	206-44-0
DTXSID:	DTXSID3024104
Use:	Polycyclic aromatic hydrocarbon; occurs as a result of incomplete burning
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.00028

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	non-cancer effects	9	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	200	nephropathy, increased liver weights, hematological alterations, and clinical effects	general population	IRIS	1990

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.056	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Fluoranthene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.04	mg/kg/day	IRIS 1990	USEPA 1988	nephropathy, increased liver weights, hematological alterations, and clinical effects	general population	33.8	237	[207]	
Reference Dose (RfD) or Equivalent	0.0125	mg/kg/day	WHO 2003	USEPA 1988	nephropathy, increased liver weights, hematological alterations, and clinical effects	general population	33.8	74.0	[438]	
Cancer Classification (CC)	I		PPRTV 2012						[327]	
Cancer Classification (CC)	D		IRIS 1990						[207]	
			ATSDR 1995						[10]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
						2011-12-01	2020-03-13	818	0	7	

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Cancer Classification (CC)	3	no units	WHO IARC	
Chronic Health-Based Guidance Value	0.3	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.07	mg/L	MN DOH	
Human Health Ambient Water Quality Criteria	0.02	mg/L	EPA Human Health Criteria for CWA	
Intermediate Minimal Risk Level (MRL)	0.4	mg/kg/day	CDC ATSDR	
Short-Term/Subchronic Health-Based Guidance Value	0.1	mg/L	MN DOH	
Subchronic Provisional RfD	0.1	mg/kg/day	EPA PPRTV	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	2000	mg/kg	NIH HSDB	
Percent of active toxcast in vitro assays tested	10.62	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0049091	mol/kg	TEST QSAR	
Ames mutagenicity test	0.836	no units	TEST QSAR	
Developmental toxin test	0.74	no units	TEST QSAR	

Fluoranthene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	589	42	Sites	7.13	0.003	0.01	0.056	0.15	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	101	34	Sites	34	0.003	0.0105	0.064	0.15	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	488	8	Sites	1.64	0.005	0.01	0.0323	0.044	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	500K - 1M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	20	1	Sites	5	0.002	0.002	0.002	0.002	ug/L	
Drinking Water Monitoring Data - WA (Finished)	2006 - 2011	481	0	Sites	0						
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	90	1	Sites	1.11	0.034	0.034	0.034	0.034	ug/L	
Drinking Water Monitoring Data - WA (Source)	2006 - 2011	634	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	865	283	Sites	33	0.002	0.03	0.425	25.6	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	1,096	62	Sites	5.66	0.003	0.02	0.195	6	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,961	345	Sites	18	0.002	0.03	0.41	25.6	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	15	Sites	39	0.0045	0.0122	0.0339	0.0564	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	5	Sites	24						
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exposure exposure		0.000000955	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	162.696	days	
Boiling point	OPERA QSAR	392.038	degree C	
Boiling point	TEST QSAR	378.496	degree C	
Vapor pressure	OPERA QSAR	0.00000386	mmHg	
Vapor pressure	TEST QSAR	0.000000371	mmHg	
Solubility in water	OPERA QSAR	0.000000668	mol/L	
Solubility in water	TEST QSAR	0.000000318	mol/L	
Bioconcentration factor	OPERA QSAR	2457.49	no units	
Bioconcentration factor	TEST QSAR	480.839	no units	
Henry's Law constant	OPERA QSAR	0.0000109	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	5.17848	no units	

Fluoranthene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
10	ATSDR. 1995. Toxicological Profile for Polycyclic Aromatic Hydrocarbons. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
207	USEPA. 1990. Chemical Assessment Summary, Fluoranthene. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, D.C.
327	USEPA. 2012. Provisional Peer-Reviewed Toxicity Values for Fluoranthene. U.S. Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment, Superfund Health Risk Technical Support Center, Cincinnati, OH.
438	WHO. 2003. Guidelines for Drinking Water Quality: Polynuclear Aromatic Hydrocarbons (PAHs). World Health Organization (WHO), Geneva, Switzerland.

Fluoxetine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Fluoxetine
CASRN:	54910-89-3
DTXSID:	DTXSID7023067
Use:	antidepressant
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	X

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.024

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	non-cancer effects	5	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	0.6	lowest therapeutic dose: treatment of major depressive disorder/bulimia nervosa/OCD/Panic disorder	bottle-fed infants	FDA; NIH	2018; 2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.014322	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination
X

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Fluoxetine

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	8.33333E-05	mg/kg/day	FDA 2018; NIH 2018	McKesson Packaging Services Business Unit of McKesson Corporation	lowest therapeutic dose: treatment of major depressive disorder/bulimia nervosa/OCD/Panic disorder	bottle-fed infants	151	0.560	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels
Reference Dose (RfD) or Equivalent	8.33333E-05	mg/kg/day	FDA 2018; NIH 2018	McKesson Packaging Services Business Unit of McKesson Corporation	lowest therapeutic dose: treatment of major depressive disorder/bulimia nervosa/OCD/Panic disorder	general population	33.8	2.00	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Maximum Recommended Daily Dose	1.33	mg/kg/day	FDA	
Screening level for pharmaceutical - general population	0.001960784	mg/L	EPA Office of Water	
Screening level for pharmaceutical - infants	0.000555556	mg/L	EPA Office of Water	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Percent of active toxcast in vitro assays tested	34.04	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0034514	mol/kg	TEST QSAR	
Ames mutagenicity test	0.158	no units	TEST QSAR	
Developmental toxin test	0.795	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Fluoxetine
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	557	3	Sites	0.54	0.00585	0.00784	0.0143	0.0171	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	75	2	Sites	2.67	0.00585	0.00684	0.00744	0.00784	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	482	1	Sites	0.21	0.0171	0.0171	0.0171	0.0171	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Furlong et al 2017 (Finished) [83]	2007 - 2012	NA	NA	Sites	0					ug/L	
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	9	NA	Sites	0					ug/L	
Padhye et al. 2013 (Finished) [155]	2009 - 2010	8	1	Samples	12	0	0		1.92e-05 +/- 7e-07	ug/L	
IL EPA (2008) via Uslu et al. (2013) (Finished) [433]	2008	NA	NA						0.001	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	206	4	Sites	1.94	0.002	0.0522	0.0896	0.169	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	401	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	607	4	Sites	0.66	0.002	0.0522	0.0896	0.169	ug/L	
Furlong et al 2017 (Ambient) [83]	2007 - 2012	NA	NA	Sites	0					ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	9	NA	Sites	11		0.00053		0.00053	ug/L	
Batt et al. 2016 (Ambient) [46]	2008 - 2009	182	10	Sites	5.49	9e-04	0.00465	0.0133	0.0248	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	3	Sites	7.89	0.0065174	0.0136	0.0224	0.0246002	ug/L	
Bexfield et al. 2019 (Groundwater) [49]	2013 - 2015	1,106	1	Sites	0.09	0.0170815	0.0171	0.0171	0.0170815	ug/L	
Padhye et al. 2013 (Ambient) [155]	2009 - 2010	8	3	Samples	38	0	0		9e-07 +/- 1e-07	ug/L	
Rahman et al. (2010) via Uslu et al. (2013) (Ambient) [433]	2010	NA	NA						0.0475	ug/L	
IL EPA (2008) via Uslu et al. (2013) (Ambient) [433]	2008	NA	NA						0.002	ug/L	
Barnes et al. (2008) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.056	ug/L	
Benotti et al. (2009) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.0033	ug/L	
Conley et al. (2008) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.01	ug/L	
Kolpin et al. (2002) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.012	ug/L	
Vanderford et al. (2003) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.0055	ug/L	
Vanderford et al. (2006) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.0026	ug/L	
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	13	Sites	62	0.0025456	0.01	0.0333	0.0432505	ug/L	
Kostich et al. 2014 (Wastewater) [126]	not reported	48	18	Sites	38	0.0032	0.0199	0.0272	0.0312	ug/L	
Batt et al. (2008) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						0.073	ug/L	
Glassmeyer et al. (2005) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						0.021	ug/L	
Shultz et al. (2008) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						0.07	ug/L	
Vanderford et al. (2006) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						0.025	ug/L	

Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Expocast exposure		3.67E-08	
Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.54542	days	
Boiling point	OPERA QSAR	316.438	degree C	
Boiling point	TEST QSAR	343.305	degree C	
Vapor pressure	OPERA QSAR	0.000000398	mmHg	
Vapor pressure	TEST QSAR	0.00000143	mmHg	
Solubility in water	OPERA QSAR	0.0000392	mol/L	
Solubility in water	TEST QSAR	0.0000237	mol/L	
Bioconcentration factor	OPERA QSAR	125.272	no units	
Bioconcentration factor	TEST QSAR	171.791	no units	
Henry's Law constant	OPERA QSAR	0.000000144	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	4.13029	no units	

Fluoxetine

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
46	Batt, A. L., Kincaid, T. M., Kostich, M. S., Lazorchak, J. M., & Olsen, A. R. (2016). Evaluating the extent of pharmaceuticals in surface waters of the United States using a National-scale Rivers and Streams Assessment survey. <i>Environmental toxicology and chemistry</i> , 35(4), 874-881.
49	Bexfield, L.M., P.L. Toccalino, K. Belitz, W.T. Foreman, and E.T. Furlong. 2019. Hormones and pharmaceuticals in groundwater used as a source of drinking water across the United States. <i>Environmental Science and Technology</i> 53: 2950-2960.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
77	FDA. 2018. Drugs @ FDA: FDA Approved Drug Products. U.S. Food and Drug Administration (FDA). https://www.accessdata.fda.gov/scripts/cder/daf/ .
83	Furlong, E.T., Batt, A.L., Glassmeyer, S.T., Noriega, M.C., Kolpin, D.W., Mash, H., Schenck, K.M. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States: Pharmaceuticals. <i>Science of The Total Environment</i> . 579 (1629-1642).
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
126	Kostich MS, et al. 2014 Concentrations of prioritized pharmaceuticals in effluents from 50 large wastewater treatment plants in the US and implications for risk estimation. <i>Environ Pollut</i> . 2014 Jan;184:354-9. doi: 10.1016/j.envpol.2013.09.013. Epub 2013 Oct 3. PMID: 24095705.
127	Kostich, MS, et al., 2010. Predicting variability of aquatic concentrations of human pharmaceuticals. <i>Sci. Total Environ</i> . 408 (20), 4504e4510.
150	NIH. 2018. DailyMed Database. U.S. National Library of Medicine, National Institutes of Health (NIH). https://dailymed.nlm.nih.gov/dailymed/ .
155	Padhye, L.P., Yao, H., Kung'u, F.T., and Huang, C.H. Year-long evaluation on the occurrence and fate of pharmaceuticals, personal care products, and endocrine disrupting chemicals in an urban drinking water treatment plant. 2014. <i>Water Research</i> 51 (2014) 266-276.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
433	Uslu, M., Jasim, S., Arvai, A., Bewtra, J. and Biswas, N., 2013. A Survey of Occurrence and Risk Assessment of Pharmaceutical Substances in the Great Lakes Basin. <i>Ozone: Science & Engineering</i> , 35(4), pp.249-262.

Galaxolide

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Galaxolide
CASRN:	1222-05-5
DTXSID:	DTXSID8027373
Use:	Fragrance ingredient in perfumes, soaps, cosmetics, and detergents.
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.000009

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
3	no adverse effects	9	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	20000	no adverse effects seen at highest dose tested	general population	ECHA	2011

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.18	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis
Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Galaxolide

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	3.8	mg/kg/day	ECHA 2011	Api and Ford 1999	no adverse effects at the highest dose tested	general population	33.8	22500	[71]	NOTE: An ECHA Derived No Effect Level (DNEL) is used in place of the RfD

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Hepatic	5	Api, 1999	Respiratory, Reproductive,	150	Api, 1999		2020-04-06	385	2	0	2

Other Health Data

Data Element	Value	Units	Source	Notes
<i>Measured Data and Assessment Results</i>				

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
<i>Measured Data and Assessment Results</i>				
LD50	4640	mg/kg	NIH HSDB	
Percent of active toxcast in vitro assays tested	25	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
<i>Modeled Data</i>				
LD50	0.0032063	mol/kg	TEST QSAR	
Ames mutagenicity test	-0.048	no units	TEST QSAR	
Developmental toxin test	0.709	no units	TEST QSAR	

Galaxolide

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	570	52	Sites	9.12	0.007	0.057	0.18	2.4	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	87	40	Sites	46	0.007	0.065	0.2	2.4	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	483	12	Sites	2.48	0.008	0.017	0.0484	0.081	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	1M - 10M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	24		0.0365		0.061	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	717	279	Sites	39	0.005	0.04	0.23	4.6	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	692	38	Sites	5.49	0.004	0.0375	0.942	1.72	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,409	317	Sites	22	0.004	0.04	0.256	4.6	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	36		0.028		0.11	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	20	Sites	53	0.0076	0.285	1.03	1.4	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	1	Sites	50						
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	21	Sites	100	0.49	1.2	2	4.6	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exposure exposure			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	28.8833	days	
Boiling point	OPERA QSAR	323.86	degree C	
Boiling point	TEST QSAR	312.099	degree C	
Vapor pressure	OPERA QSAR	0.000374131	mmHg	
Vapor pressure	TEST QSAR	0.000385478	mmHg	
Solubility in water	OPERA QSAR	0.00000606	mol/L	
Solubility in water	TEST QSAR	0.000015	mol/L	
Bioconcentration factor	OPERA QSAR	788.097	no units	
Bioconcentration factor	TEST QSAR	1667.25	no units	
Henry's Law constant	OPERA QSAR	0.0000223	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	5.75078	no units	

Galaxolide

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Reference Number	Full Reference
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
71	ECHA. 2011. Registration Dossier: 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethylindeno[5,6-c]pyran. European Chemicals Agency (ECHA), Helsinki, Finland. https://echa.europa.eu/registration-dossier/-/registered-dossier/14504/1 . Accessed 03/03/2020
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.

Gemfibrozil

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Gemfibrozil
CASRN:	25812-30-0
DTXSID:	DTXSID0020652
Use:	antihyperlipoproteinemic
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0022

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	non-cancer effects		

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	30	lowest therapeutic dose: lipid regulation (decreases VLDL, increases HDL cholesterol)	bottle-fed infants	FDA; NIH	2018; 2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.06654	90th Percentile	Ambient Water	Batt et al.	2016

PUBLIC NOMINATION STATUS

Public Nomination
X

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis
Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Gemfibrozil

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.005	mg/kg/day	FDA 2018; NIH 2018	Watson Laboratories, Inc.	lowest therapeutic dose: lipid regulation (decreases VLDL, increases HDL cholesterol)	bottle-fed infants	151	33.0	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels
Reference Dose (RfD) or Equivalent	0.005	mg/kg/day	FDA 2018; NIH 2018	Watson Laboratories, Inc.	lowest therapeutic dose: lipid regulation (decreases VLDL, increases HDL cholesterol)	general population	33.8	120	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Cancer Classification (CC)	3	no units	WHO IARC	
Maximum Recommended Daily Dose	20	mg/kg/day	FDA	
Screening level for pharmaceutical - general population	0.117647059	mg/L	EPA Office of Water	
Screening level for pharmaceutical - infants	0.033333333	mg/L	EPA Office of Water	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	316	mg/kg	NIH HSDB	min
LD50	479	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	2.56	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.001875	mol/kg	TEST QSAR	
Ames mutagenicity test	0.229	no units	TEST QSAR	
Developmental toxin test	0.849	no units	TEST QSAR	

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Gemfibrozil

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water		Prevalence				Magnitude					
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water		Prevalence				Magnitude					
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water		Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	1	0	Sites	0						
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Kleywegt et al. (2011) via Uslu et al. (2013) (Finished) [433]	2011	NA	NA						0.004	ug/L	
Tabe et al. (2009) via Uslu et al. (2013) (Finished) [433]	2009	NA	NA						0.002	ug/L	
Kormos et al. (2007) via Uslu et al. (2013) (Finished) [433]	2007	NA	NA						0.003	ug/L	
IL EPA (2008) via Uslu et al. (2013) (Finished) [433]	2008	NA	NA						0.0106	ug/L	
Ambient Water		Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	2	0	Sites	0						
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Batt et al. 2016 (Ambient) [46]	2008 - 2009	182	27	Sites	15	0.0051	0.0225	0.0665	0.1125	ug/L	
Kleywegt et al. (2011) via Uslu et al. (2013) (Ambient) [433]	2011	NA	NA						0.009	ug/L	
Tabe et al. (2009) via Uslu et al. (2013) (Ambient) [433]	2009	NA	NA						0.004	ug/L	
Kormos et al. (2007) via Uslu et al. (2013) (Ambient) [433]	2007	NA	NA						0.006	ug/L	
IL EPA (2008) via Uslu et al. (2013) (Ambient) [433]	2008	NA	NA						0.0174	ug/L	
Benotti et al. (2009) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.024	ug/L	
Conkle et al. (2008) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.081	ug/L	
Fono et al. (2006) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.079	ug/L	
Gross et al. (2004) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.18	ug/L	
Kolpin et al. (2002) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.79	ug/L	
Lin et al. (2006) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.065	ug/L	
Spongberg et al. (2008) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.006	ug/L	
Trenholm et al. (2006) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.0048	ug/L	
Vanderford et al. (2003) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.056	ug/L	
Vanderford et al. (2006) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.17	ug/L	

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Waste Water Effluent											
		Prevalence				Magnitude					
Kostich et al. 2014 (Wastewater) [126]	not reported	50	38	Sites	76	0.0908	0.506	1.4	2.3396	ug/L	
Batt et al. (2008) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						1.22	ug/L	
Conkle et al. (2008) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						1.819	ug/L	
Drewes et al. (2002) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						1.235	ug/L	
Fono et al. (2006) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						0.234	ug/L	
Gross et al. (2004) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						0.158	ug/L	
Soliman et al. (2007) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						0.5	ug/L	
Spongberg et al. (2008) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						0.451	ug/L	
Trenholm et al. (2006) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						1.22	ug/L	
Vanderford et al. (2006) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						4.77	ug/L	
Yu et al. (2006) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						0.41	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Expocast exposure		0.000000193	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.52148	days	
Boiling point	OPERA QSAR	326.707	degree C	
Boiling point	TEST QSAR	349.352	degree C	
Vapor pressure	OPERA QSAR	0.00000936	mmHg	
Vapor pressure	TEST QSAR	0.00000172	mmHg	
Solubility in water	OPERA QSAR	0.000247743	mol/L	
Solubility in water	TEST QSAR	0.00000685	mol/L	
Bioconcentration factor	OPERA QSAR	3.16534	no units	
Bioconcentration factor	TEST QSAR	16.1065	no units	
Henry's Law constant	OPERA QSAR	8.62E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	4.42964	no units	

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46	Batt, A. L., Kincaid, T. M., Kostich, M. S., Lazorchak, J. M., & Olsen, A. R. (2016). Evaluating the extent of pharmaceuticals in surface waters of the United States using a National-scale Rivers and Streams Assessment survey. <i>Environmental toxicology and chemistry</i> , 35(4), 874-881.
77	FDA. 2018. Drugs @ FDA: FDA Approved Drug Products. U.S. Food and Drug Administration (FDA). https://www.accessdata.fda.gov/scripts/cder/daf/ .
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
126	Kostich MS, et al. 2014 Concentrations of prioritized pharmaceuticals in effluents from 50 large wastewater treatment plants in the US and implications for risk estimation. <i>Environ Pollut</i> . 2014 Jan;184:354-9. doi: 10.1016/j.envpol.2013.09.013. Epub 2013 Oct 3. PMID: 24095705.
127	Kostich, MS, et al., 2010. Predicting variability of aquatic concentrations of human pharmaceuticals. <i>Sci. Total Environ</i> . 408 (20), 4504e4510.
150	NIH. 2018. DailyMed Database. U.S. National Library of Medicine, National Institutes of Health (NIH). https://dailymed.nlm.nih.gov/dailymed/ .
433	Uslu, M., Jasim, S., Arvai, A., Bewtra, J. and Biswas, N., 2013. A Survey of Occurrence and Risk Assessment of Pharmaceutical Substances in the Great Lakes Basin. <i>Ozone: Science & Engineering</i> , 35(4), pp.249-262.

Halon 1011 (bromochloromethane)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Halon 1011 (bromochloromethane)
CASRN:	74-97-5
DTXSID:	DTXSID4021503
Use:	Fire extinguishing fluid; chemical intermediate
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
		9	5

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.3954	90th Percentile	Finished Water	UCMR3	2013-2015

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
		X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Halon 1011 (bromochloromethane)
CCL 5 Contaminant Information Sheet
HEALTH EFFECTS DATA

EPA-OGWDW and OST

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Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.013	mg/kg/day	OW 1989	Torkelson et al., 1960	increased liver to bodyweight ratio	general population	33.8	76.9	[202]	
Cancer Classification (CC)	D		OW 1989						[202]	
Cancer Classification (CC)	D		IRIS 1991						[210]	
Cancer Classification (CC)	I		PPRTV 2009						[302]	Note: No toxicity values have been derived for bromochloromethane

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
						2008-09-01	2020-04-14	6	0	0	

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	1	mg/L	EPA DWSHA 2018	
Lifetime Health Advisory	0.09	mg/L	EPA DWSHA 2018	
Subchronic RfC	0.1	mg/m ³	EPA PPRTV	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	4300	mg/kg	NIH HSDB	min
LD50	5000	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	0.85	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0023878	mol/kg	TEST QSAR	
Ames mutagenicity test	0.69	no units	TEST QSAR	
Developmental toxin test			TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
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EPA - Office of Water

Halon 1011 (bromochloromethane)
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015	4,916	309	Sites	6.29	0.06	0.11	0.395	5.17	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997	22,974	106	Sites	0.46	0.0023	1	6	33.4	ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992	12,881	65	Sites	0.5	0.05	1	10	210	ug/L	
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	7,734	19	Sites	0.25	0.01	0.14	0.445	1.15	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	264	4	Sites	1.52	0.01	0.38	0.441	0.45	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	7,470	15	Sites	0.2	0.02	0.075	0.384	1.15	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	401	11	Sites	2.74	0.5	0.805	3.65	6	ug/L	
Drinking Water Monitoring Data - MA (Finished)	2006 - 2020	888	29	Sites	3.27	0.5	2.4	6.26	18	ug/L	
Drinking Water Monitoring Data - WA (Finished)	2006 - 2011	1,188	1	Sites	0.08	0.66	0.66	0.66	0.66	ug/L	
Bradley et al. 2018 (Finished) [53]	2016	26	1	Sites	3.85	0.07637	0.0764	0.0764	0.07637	ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	4,242	23	Sites	0.54	0.4	1.15	3	8.9	ug/L	
Drinking Water Monitoring Data - MA (Source)	2006 - 2020	130	0	Sites	0						
Drinking Water Monitoring Data - PA (Source)	2006 - 2011	13	0	Sites	0						
Drinking Water Monitoring Data - WA (Source)	2006 - 2011	1,665	0	Sites	0						
Drinking Water Monitoring Data - WI (Source)	2012-2019	33	1	Sites	3.03	0.61	0.61	0.61	0.61	ug/L	
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	169	9	Sites	5.33	0.01	0.04	0.06	0.06	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3,487	8	Sites	0.23	0.02	0.035	0.09	0.17	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	3,653	17	Sites	0.47	0.01	0.04	0.07	0.17	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	5	Sites	13	0.02169	0.0357	0.0554	0.05931	ug/L	
Arnold et al. 2016 (Unfiltered) [7]	2012 - 2013	685	1	Sites	0.15	0.03	0.03	0.03	0.03	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		4.55E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	14.1519	days	
Boiling point	OPERA QSAR	64.2952	degree C	
Boiling point	TEST QSAR	66.832	degree C	
Vapor pressure	OPERA QSAR	181.807	mmHg	
Vapor pressure	TEST QSAR	231.206	mmHg	
Solubility in water	OPERA QSAR	0.0723047	mol/L	
Solubility in water	TEST QSAR	0.0625173	mol/L	
Bioconcentration factor	OPERA QSAR	5.65089	no units	
Bioconcentration factor	TEST QSAR	4.40555	no units	
Henry's Law constant	OPERA QSAR	0.0038283	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.45955	no units	

Halon 1011 (bromochloromethane)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. <i>Environmental science & technology</i> , 52(23), 13972-13985.
202	USEPA. 1989. Bromochloromethane Health Advisory. U.S. Environmental Protection Agency, Office of Water, Washington, D.C.
210	USEPA. 1991. Chemical Assessment Summary, Bromochloromethane. U.S. Environmental Protection Agency, National Center for Environmental Protection, Integrated Risk Information System (IRIS), Washington, D.C.
302	USEPA. 2009. Provisional Peer-Reviewed Toxicity Values for Bromochloromethane. U.S. Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment, Superfund Health Risk Technical Support Center, Cincinnati, OH.

HCFC-22

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	HCFC-22
CASRN:	75-45-6
DTXSID:	DTXSID6020301
Use:	Refrigerant; low-temperature solvent; fluorocarbon resins, especially tetrafluoroethylene polymers; gas
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
		9	5

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
1.2	90th Percentile	Finished Water	UCMR3	2013-2015

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
		X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

HCFC-22

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
			IRIS 1993						[221]	NOTE: HCFC-22 is highly volatile. No oral toxicity values were derived. No PECO-relevant studies were found in the rapid systematic literature review.

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
						2002-08-01	2020-03-25	130	0	2	

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Cancer Classification (CC)	3	no units	WHO IARC	
Reference Concentration (RfC)	50	mg/m ³	EPA IRIS	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity test	0.574	no units	TEST QSAR	
Developmental toxin test	0.57	no units	TEST QSAR	

HCFC-22

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015	4,916	286	Sites	5.82	0.08	0.22	1.2	250	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	1,411	55	Sites	3.9	0.02	0.08	0.895	15.6	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	51	3	Sites	5.88	0.07	0.095	0.224	0.35	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	1,360	52	Sites	3.82	0.02	0.07	0.907	15.6	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)	23	1,908,568	Chemical Data Reporting (CDR) Results (EPA) (2016)	100M - 250M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Bradley et al. 2018 (Finished) [53]	2016	26	1	Sites	3.85	0.04688	0.0469	0.0469	0.04688	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	47	2	Sites	4.26	0.03	0.3	0.57	0.57	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	824	39	Sites	4.73	0.03	0.175	1.71	4.02	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	871	41	Sites	4.71	0.03	0.175	1.71	4.02	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	2	Sites	5.26	0.03401	0.301	0.515	0.5687	ug/L	
Arnold et al. 2016 (Unfiltered) [7]	2012 - 2013	527	11	Sites	2.09	0.02	0.08	0.18	0.56	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exposure exposure		0.000000574	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	7.58302	days	
Boiling point	OPERA QSAR	-36.5186	degree C	
Boiling point	TEST QSAR	-10.361	degree C	
Vapor pressure	OPERA QSAR	5705.02	mmHg	
Vapor pressure	TEST QSAR	3273.41	mmHg	
Solubility in water	OPERA QSAR	0.0211658	mol/L	
Solubility in water	TEST QSAR	0.159221	mol/L	
Bioconcentration factor	OPERA QSAR	10.1839	no units	
Bioconcentration factor	TEST QSAR	4.19759	no units	
Henry's Law constant	OPERA QSAR	0.0424827	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.00459	no units	

HCFC-22

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. <i>Environmental science & technology</i> , 52(23), 13972-13985.
221	USEPA. 1993. Chemical Assessment Summary, Chlorodifluoromethane. U.S. Environmental Protection Agency, National Center for Environmental Protection, Integrated Risk Information System (IRIS), Washington, D.C.

Heroin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Heroin
CASRN:	561-27-3
DTXSID:	DTXSID6046761
Use:	Addictive substance of abuse; used for the relief of severe pain, especially in terminal illness
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date

PUBLIC NOMINATION STATUS

Public Nomination
X

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Heroin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
										NOTE: derivative of morphine; no health assessments found

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
<i>Measured Data and Assessment Results</i>				

Data Element	Value	Units	Source	Notes
<i>Measured Data and Assessment Results</i>				

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
<i>Modeled Data</i>				
LD50			TEST QSAR	
Ames mutagenicity test			TEST QSAR	
Developmental toxin test			TEST QSAR	

Heroin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Ambient Water											
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exposure exposure			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Heroin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference

Hexazinone

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Hexazinone
CASRN:	51235-04-2
DTXSID:	DTXSID4024145
Use:	Post emergence contact herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.00007

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	non-cancer effects	9	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	300	decreased body weight, hepatotoxicity (clinical chemical changes and microscopic lesions)	general population	OPP	2015

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.021	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Hexazinone

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.05	mg/kg/day	OPP 2015	Dalgard 1991	decreased body weight, hepatotoxicity (clinical chemical changes and microscopic lesions)	general population	33.8	296	[349]	NOTE: Though this compound is listed as having a D cancer classification in the OPP assessment, the document also states: "Hexazinone is classified as "Likely at high doses, but unlikely to be carcinogenic to humans at low doses." Therefore, a cancer dietary exposure analysis is not required."
Cancer Classification (CC)	D		OPP 2015						[349]	NOTE: Though this compound is listed as having a D cancer classification in the OPP assessment, the document also states: "Hexazinone is classified as "Likely at high doses, but unlikely to be carcinogenic to humans at low doses." Therefore, a cancer dietary exposure analysis is not required."

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	2	mg/L	EPA DWSHA 2018	
Lifetime Health Advisory	0.4	mg/L	EPA DWSHA 2018	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	3400	mg/kg	NIH HSDB	max
LD50	860	mg/kg	NIH HSDB	min
LOAEL	37.57	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	900	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	400	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	5	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	1.26	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	122.5	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	440.39999	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	31.6	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	87.3	mg/kg/day	EPA Toxicity Reference Database	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0074473	mol/kg	TEST QSAR	
Ames mutagenicity test	0.624	no units	TEST QSAR	
Developmental toxin test	1.093	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Hexazinone
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	4,886	375	Sites	7.67	1.00E - 04	0.00382	0.021	1.23	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	582	211	Sites	36	1.00E - 04	0.00361	0.019	1.23	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	4,304	164	Sites	3.81	0.00015	0.01	0.0871	1.13	ug/L	
Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data			Number of States	Amount Released (lbs/year)	Chemical Production Data		Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	27	483,326	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			3	1,574	Chemical Data Reporting (CDR) Results (EPA) (2016)		

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	1	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	10	3	Sites	30	8e-04	8e-04	0.0025	0.087	ug/L	
Bradley et al. 2018 (Finished) [53]	2016	26	2	Sites	7.69	0.0065	0.0076	0.00848	0.0087	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	1	0	Sites	0						
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	227	17	Sites	7.49	8e-04	8e-04	0.0115	0.11	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	218	14	Sites	6.42	8e-04	0.0046	0.0122	0.021	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	10	3	Sites	30	8e-04	8e-04	0.00425	0.11	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	1,615	347	Sites	21	0.0036	0.025	0.128	35	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	7	Sites	18	0.0029	0.0168	0.036	0.0466	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	39	Sites	5.65	3e-04	0.0016	0.00666	0.0929	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
USGS, McKenzie River, Oregon, 2012 (Ambient) [158]	2002 - 2010	71	19	Samples	27				0.097	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		7.69E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.72279	days	
Boiling point	OPERA QSAR	324.385	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.00000035	mmHg	
Vapor pressure	TEST QSAR	0.000000111	mmHg	
Solubility in water	OPERA QSAR	0.0801096	mol/L	
Solubility in water	TEST QSAR	0.00772681	mol/L	
Bioconcentration factor	OPERA QSAR	2.40816	no units	
Bioconcentration factor	TEST QSAR	5.98412	no units	
Henry's Law constant	OPERA QSAR	0.000000166	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.76651	no units	

Hexazinone

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. <i>Environmental science & technology</i> , 52(23), 13972-13985.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
158	Reconnaissance of Land-Use Sources of Pesticides in Drinking Water, McKenzie River, Oregon. U.S. Geological Survey Scientific Investigations Report 2012–5091, 46 p. plus appendixes.
349	USEPA. 2015. Hexazinone: Draft Human Health Risk Assessment for Registration Review. EPA-HQ-OPP-2009-0755-0019. DP No. D424526. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Imazalil

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Imazalil
CASRN:	35554-44-0
DTXSID:	DTXSID8024151
Use:	Fungicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.13

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	carcinogen with linear MOA	10	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.5	hepatocytic neoplasm	general population	OPP	2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.0654	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Imazalil

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.108	mg/kg/day	OPP 2018	Van Deun 1999	reductions in body weight and weight gain and macro and microscopic effects in the liver (male and female) and thyroid (male)	general population	33.8	639	[399]	
Cancer Slope Factor (CSF)	0.0611	(mg/kg/day)^-1	OPP 2018	Verstraeten 1993	hepatocytic neoplasm	general population	33.8	0.484	[399]	
Cancer Classification (CC)	L		OPP 2018						[399]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.47	mg/L	EPA HHBP	
Acute PAD	0.017	mg/kg/day	EPA HHBP	
Cancer Slope Factor (CSF)	0.0611	(mg/kg/day)^-1	EPA HHBP	
Chronic Human Health Benchmark	0.016	mg/L	EPA HHBP	
Chronic Human Health Benchmark	0.000524	mg/L	EPA HHBP	
Population-Adjusted Dose (PAD)	0.0025	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	227	mg/kg	NIH HSDB	min
LD50	640	mg/kg	NIH HSDB	max
LOAEL	120	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	20	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	2.5	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	40	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	32.93	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	20	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	37.900002	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	15	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	22.3	mg/kg/day	EPA Toxicity Reference Database	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0028973	mol/kg	TEST QSAR	
Ames mutagenicity test	0.541	no units	TEST QSAR	
Developmental toxin test	0.281	no units	TEST QSAR	

Imazalil
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	14	2	Sites	14	0.0534	0.0609	0.0654	0.0684	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	14	2	Sites	14	0.0534	0.0609	0.0654	0.0684	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	1	36,692	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	2	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	132	7	Sites	5.3	0.0116	0.0307	0.1	0.119	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	135	7	Sites	5.19	0.0116	0.0307	0.1	0.119	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	191	12	Sites	6.28	0.0116	0.03	0.0965	0.1189	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	3	Sites	7.89	0.0517	0.0521	0.221	0.2634	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		1.65E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.35613	days	
Boiling point	OPERA QSAR	346.361	degree C	
Boiling point	TEST QSAR	344.153	degree C	
Vapor pressure	OPERA QSAR	0.00000235	mmHg	
Vapor pressure	TEST QSAR	0.00000314	mmHg	
Solubility in water	OPERA QSAR	0.000551691	mol/L	
Solubility in water	TEST QSAR	0.000328095	mol/L	
Bioconcentration factor	OPERA QSAR	35.0705	no units	
Bioconcentration factor	TEST QSAR	168.655	no units	
Henry's Law constant	OPERA QSAR	0.000000522	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.66695	no units	

Imazalil

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
399	USEPA. 2018. Imazalil. Acute, Chronic, and Cancer Dietary (Food Only) Exposure and Risk Assessment in Support of the HED Draft Risk Assessment for Registration Review. EPA-HQ-OPP-2013-0305-0026. DP No. D446973. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Imazapyr

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Imazapyr
CASRN:	81334-34-1
DTXSID:	DTXSID8034665
Use:	Herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0079

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
3	no adverse effects	4	6

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	10000	no adverse effects identified	general population	OPP	2006

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
79		EDWC SW 30-Year mean (chronic, non-cancer)	OPP	2006

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Imazapyr
CCL 5 Contaminant Information Sheet
HEALTH EFFECTS DATA
EPA-OGWDW and OST
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Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	2.5	mg/kg/day	OPP 2006	Shellenberger 1987	no effects identified at loael selected as pod	general population	33.8	14800	[271]	
Cancer Classification (CC)	E		OPP 2006						[271]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Chronic Human Health Benchmark	16	mg/L	EPA HHBP	
Health-Based Screening Level	16	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	2.5	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	2000	mg/kg	NIH HSDB	min
LD50	5000	mg/kg	NIH HSDB	max
LOAEL	1000	mg/kg/day	EPA Toxicity Reference Database	
NOAEL	300	mg/kg/day	EPA Toxicity Reference Database	
Percent of active toxcast in vitro assays tested	1.48	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0046026	mol/kg	TEST QSAR	
Ames mutagenicity test	0.624	no units	TEST QSAR	
Developmental toxin test	0.879	no units	TEST QSAR	

Imazapyr

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	4	358,171	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	15	9	Sites	60	0.001498	0.002	0.0097	0.2	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	3	1	Sites	33	0.026	0.026	0.026	0.026	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	3	1	Sites	33	0.026	0.026	0.026	0.026	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	227	114	Sites	50	0.001498	0.0035	0.02	3.054	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	107	Sites	49	0.0015	0.0149	0.131	3.054	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	10	8	Sites	80	0.001498	0.002	0.01	0.21	ug/L	
USGS, McKenzie River, Oregon, 2012 (Ambient) [158]	2002 - 2010	52	7	Samples	14				0.209	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					
Estimated Drinking Water Concentration (EDWC) in Surface Water, 30-Year Mean (chronic, non-cancer)	2006	OPP	79	ug/L	Tier 1 FQPA Index Reservoir Screening Tool (FIRST)	The modeled surface water chronic, non-cancer concentration provided by the most recent available EPA OPP health assessment was selected as the occurrence concentration for imazapyr. This value coincides with the chronic health effects data which report no adverse effects seen after chronic exposures to imazapyr.					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		9.23E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.33907	days	
Boiling point	OPERA QSAR	276.309	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	1.73E-10	mmHg	
Vapor pressure	TEST QSAR	1.43E-08	mmHg	
Solubility in water	OPERA QSAR	0.0301436	mol/L	
Solubility in water	TEST QSAR	0.0043451	mol/L	
Bioconcentration factor	OPERA QSAR	5.19409	no units	
Bioconcentration factor	TEST QSAR	1.93197	no units	
Henry's Law constant	OPERA QSAR	3.08E-10	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	0.4738	no units	

Imazapyr

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
158	Reconnaissance of Land-Use Sources of Pesticides in Drinking Water, McKenzie River, Oregon. U.S. Geological Survey Scientific Investigations Report 2012–5091, 46 p. plus appendixes.
271	USEPA. 2006. Reregistration Eligibility Decision for Imazapyr. EPA-HQ-OPP-2005-0495-0031. OPP-2005-0495. U.S. Environmental Protection Agency, Office of Prevention, Pesticides and Toxic Substances, Washington, D.C.

Imazaquin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Imazaquin
CASRN:	81335-37-7
DTXSID:	DTXSID3024152
Use:	Herbicide used on broad leaved weeds in soya beans
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.00018

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	non-cancer effects	9	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	1000	decreased body weights (within 4 weeks of exposure), slight anemia, clinical chemistry/hematology changes, and evidence of skeletal muscle myopathy	general population	OPP	2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.18	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Imazaquin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.25	mg/kg/day	OPP 2018	American Cyanamid Company, 1984	decreased body weights (within first 4 weeks of exposure), slight anemia, clinical chemistry/hematology changes, and evidence of skeletal muscle myopathy	general population	33.8	1480	[400]	
Cancer Classification (CC)	E		OPP 2018						[400]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Chronic Human Health Benchmark	1.6	mg/L	EPA HHBP	
Health-Based Screening Level	1.6	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.25	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	2363	mg/kg	NIH HSDB	min
LD50	5000	mg/kg	NIH HSDB	max
LOAEL	125	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	600	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	25	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	250	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	1.65	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.011298	mol/kg	TEST QSAR	
Ames mutagenicity test	0.56	no units	TEST QSAR	
Developmental toxin test	0.945	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
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EPA - Office of Water

Imazaquin
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	4,148	170	Sites	4.1	0.00102	0.0154	0.18	5.9	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	472	114	Sites	24	0.00102	0.0151	0.18	5.9	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	3,676	56	Sites	1.52	0.00152	0.02	0.132	0.7	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	15	52,207	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	5	Sites	29	0.0018	0.004	0.0184	0.047	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	475	31	Sites	6.53	0.00159	0.0131	0.0792	0.255	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	1,051	27	Sites	2.57	0.00093	0.01	0.02	0.07	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,526	58	Sites	3.8	0.00093	0.01	0.056	0.255	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	17	Sites	7.42	0.0018	0.00735	0.0245	0.058	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	12	Sites	5.48	0.0018	0.008	0.0357	0.0458	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	5	Sites	42	0.0018	0.005	0.0228	0.058	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	3	Sites	7.89	0.0128	0.0133	0.0322	0.0369	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	6	Sites	0.87	0.0015	0.00305	0.0289	0.05	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		8.51E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.34801	days	
Boiling point	OPERA QSAR	288.545	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	1.27E-10	mmHg	
Vapor pressure	TEST QSAR	5.35E-10	mmHg	
Solubility in water	OPERA QSAR	0.000453923	mol/L	
Solubility in water	TEST QSAR	0.000450817	mol/L	
Bioconcentration factor	OPERA QSAR	2.886	no units	
Bioconcentration factor	TEST QSAR	3.4435	no units	
Henry's Law constant	OPERA QSAR	2.11E-10	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.87775	no units	

Imazaquin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
400	USEPA. 2018. Imazaquin: Draft Human Health Risk Assessment for Registration Review. EPA-HQ-OPP-2014-0224-0020. DP No. D445078. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.

Imazethapyr

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Imazethapyr
CASRN:	81335-77-5
DTXSID:	DTXSID3024287
Use:	Herbicide used on annual and perennial grass
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0000093

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
3	no adverse effects	9	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	10000	no effects identified at loael selected as pod	general population	OPP	2002

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.09264	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Imazethapyr

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	2.5	mg/kg/day	OPP 2002	American Cyanamid Co. 1987	no effects identified at loael selected as pod	general population	33.8	14800	[250]	
Cancer Classification (CC)	NL		OPP 2002						[250]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Chronic Human Health Benchmark	16	mg/L	EPA HHBP	
Health-Based Screening Level	16	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	2.5	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	5000	mg/kg	NIH HSDB	
LOAEL	125	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	1500	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	25	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	750	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	1.27	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.001349	mol/kg	TEST QSAR	
Ames mutagenicity test	0.639	no units	TEST QSAR	
Developmental toxin test	0.927	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
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Imazethapyr
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	4,118	232	Sites	5.63	4.00E - 05	0.0167	0.0926	2.71	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	472	174	Sites	37	4.00E - 05	0.0167	0.0938	2.71	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	3,646	58	Sites	1.59	0.00021	0.0131	0.07	0.242	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	43	641,374	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	5	Sites	29	0.002	0.004	0.018	0.063	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	475	71	Sites	15	0.00112	0.0172	0.0726	0.65	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	1,057	10	Sites	0.95	0.00674	0.01	0.0189	0.02	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,532	81	Sites	5.29	0.00112	0.0162	0.0686	0.65	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	52	Sites	23	0.001665	0.004	0.0157	0.137	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	47	Sites	21	0.001665	0.00255	0.00304	0.0082	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	5	Sites	42	0.002	0.004	0.0174	0.137	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	35	0	Sites	0						
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	14	Sites	2.03	0.000211	0.0037	0.0249	0.07	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		9.56E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.34063	days	
Boiling point	OPERA QSAR	277.233	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	1.57E-10	mmHg	
Vapor pressure	TEST QSAR	5.12E-09	mmHg	
Solubility in water	OPERA QSAR	0.00538382	mol/L	
Solubility in water	TEST QSAR	0.00181552	mol/L	
Bioconcentration factor	OPERA QSAR	4.52231	no units	
Bioconcentration factor	TEST QSAR	2.50611	no units	
Henry's Law constant	OPERA QSAR	9.25E-10	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.45322	no units	

Imazethapyr

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
250	USEPA. 2002. Health Effects Division (HED) Risk Assessment for Imazethapyr. EPA-HQ-OPP-2002-0189-0003. DP Nos. D232428 D269226 D277925. U.S. Environmental Protection Agency, Office of Prevention, Pesticides and Toxic Substances, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Imidacloprid

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Imidacloprid
CASRN:	138261-41-3
DTXSID:	DTXSID5032442
Use:	Insecticide used on pests on agricultural and nursery crops
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.00018

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	non-cancer effects	9	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	500	increased incidence of tremors	general population	OPP	2017

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.09098	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis
Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Imidacloprid

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.08	mg/kg/day	OPP 2017	Ruf 1990	increased incidence of tremors	general population	33.8	473	[384]	
Cancer Classification (CC)	NL		OPP 2017						[384]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.93	mg/L	EPA HHBP	
Acute PAD	0.14	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.36	mg/L	EPA HHBP	
Health-Based Screening Level	0.36	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.057	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	4870	mg/kg	NIH HSDB	max
LD50	98	mg/kg	NIH HSDB	min
LOAEL	16.9	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	414	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	274	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	7.6	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	0.84	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0012162	mol/kg	TEST QSAR	
Ames mutagenicity test	0.912	no units	TEST QSAR	
Developmental toxin test	0.805	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Imidacloprid
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	4,177	399	Sites	9.55	0.00066	0.0242	0.091	2.15	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	471	272	Sites	58	0.00066	0.0242	0.089	2.15	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	3,706	127	Sites	3.43	0.00151	0.0269	0.226	1.99	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	48	987,466	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	8	Sites	47	0.002498	0.0025	0.0106	0.099	ug/L	
Bradley et al. 2018 (Finished) [53]	2016	26	3	Sites	12	0.004	0.0072	0.00952	0.0101	ug/L	
Klarich et al. 2017 (Finished) [117]	2016	20	16	Sites	80	0.00122	0.00396	0.0162	0.02636	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	624	203	Sites	33	0.00071	0.0245	0.155	4.18	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	1,057	32	Sites	3.03	0.00351	0.03	0.282	4.48	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,681	235	Sites	14	0.00071	0.0245	0.158	4.48	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	23	Sites	10	0.002498	0.006	0.0264	0.202	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	18	Sites	8.22	0.0025	0.0103	0.031	0.124	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	5	Sites	42	0.002498	0.0025	0.0247	0.202	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	1,031	668	Sites	65	0.0201	0.222	1.23	12.7	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	14	Sites	37	0.0036	0.0275	0.0696	0.1428	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	14	Sites	2.03	0.0015	0.0126	0.0782	0.741	ug/L	
USGS, McKenzie River, Oregon, 2012 (Ambient) [158]	2002 - 2010	126	2	Samples	1.6				0.159	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Expcast exposure		1.54E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.541	days	
Boiling point	OPERA QSAR	322.953	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	1.19E-09	mmHg	
Vapor pressure	TEST QSAR			
Solubility in water	OPERA QSAR	0.00210815	mol/L	
Solubility in water	TEST QSAR	0.00205589	mol/L	
Bioconcentration factor	OPERA QSAR	9.64405	no units	
Bioconcentration factor	TEST QSAR			
Henry's Law constant	OPERA QSAR	2.56E-10	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	0.599499	no units	

Imidacloprid

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. <i>Environmental science & technology</i> , 52(23), 13972-13985.
117	Klarich, K.L., Pflug, N.C., DeWald, E.M., Hladik, M.L., Kolpin, D.W., Cwiertny, D.M. and LeFevre, G.H., 2017. Occurrence of neonicotinoid insecticides in finished drinking water and fate during drinking water treatment. <i>Environmental Science & Technology Letters</i> , 4(5), pp.168-173.
158	Reconnaissance of Land-Use Sources of Pesticides in Drinking Water, McKenzie River, Oregon. U.S. Geological Survey Scientific Investigations Report 2012–5091, 46 p. plus appendixes.
384	USEPA. 2017. Imidacloprid. Acute and Chronic Aggregate Dietary (Food and Drinking Water) Exposure and Risk Assessments for the Registration Review Risk Assessment. EPA-HQ-OPP-2008-0844-1236. DP Nos. D438392 D438433. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Indoxacarb

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Indoxacarb
CASRN:	173584-44-6
DTXSID:	DTXSID1032690
Use:	Broad spectrum insecticide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.00069

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	non-cancer effects	6	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	100	decreased body weight, body weight gain, food consumption, and food efficiency; decreased hematocrit, hemoglobin and red blood cells	general population	OPP	2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.069398	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Indoxacarb

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.02	mg/kg/day	OPP 2018	Long et al. 1998; Frame 1997; Breslin 1997	decreased body weight, body weight gain, food consumption, and food efficiency	general population	33.8	118	[401]	
Cancer Classification (CC)	NL		OPP 2018						[401]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.8	mg/L	EPA HHBP	
Acute PAD	0.12	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.1	mg/L	EPA HHBP	
Health-Based Screening Level	0.1	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.02	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1732	mg/kg	NIH HSDB	max
LD50	268	mg/kg	NIH HSDB	min
LOAEL	1000	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	2.1300001	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	1.114	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	500	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	18.17	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	3.78	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	30	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	16	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	3.09	mg/kg/day	EPA Toxicity Reference Database	min

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0007798	mol/kg	TEST QSAR	
Ames mutagenicity test	0.589	no units	TEST QSAR	
Developmental toxin test	1.1	no units	TEST QSAR	

Indoxacarb

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	1,761	12	Sites	0.68	0.00104	0.0017	0.0694	0.273	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	322	11	Sites	3.42	0.00104	0.00153	0.00338	0.0859	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	1,439	1	Sites	0.07	0.273	0.273	0.273	0.273	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	32	100,007	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	359	4	Sites	1.11	0.00195	0.107	0.169	0.187	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	528	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	887	4	Sites	0.45	0.00195	0.107	0.169	0.187	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	202	7	Sites	3.47	0.066	0.071	0.851	2.01	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exposure exposure		0.000000197	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	5.1378	days	
Boiling point	OPERA QSAR	349.98	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	2.38E-10	mmHg	
Vapor pressure	TEST QSAR	8.99E-11	mmHg	
Solubility in water	OPERA QSAR	0.0000344	mol/L	
Solubility in water	TEST QSAR	0.00000211	mol/L	
Bioconcentration factor	OPERA QSAR	4.57962	no units	
Bioconcentration factor	TEST QSAR	36.7282	no units	
Henry's Law constant	OPERA QSAR	0.000000022	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	4.33162	no units	

Indoxacarb

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
401	USEPA. 2018. Indoxacarb: Update to the Human Health Draft Risk Assessment for Indoxacarb to Support Registration Review and the Proposed New Use for Controlling Ants at Ornamental Nurseries, Sod Farms, and Livestock Corrals of non-Food Bearing Animals. EPA-HQ-OPP-2013-0367-0050. DP No. D445517. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Iprodione

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	iprodione
CASRN:	36734-19-7
DTXSID:	DTXSID3024154
Use:	Fungicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	X
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	3.2

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	carcinogen with linear MOA	7	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.7	leydig cell tumor	general population	OPP	2012

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
2.208	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Iprodione

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.05	mg/kg/day	OPP 2012	Blystone et al. 2007; Chambers et al. 1992; Larochelle 1993	reduced serum testosterone	general population	33.8	296	[325]	
Cancer Slope Factor (CSF)	0.0439	(mg/kg/day)^-1	OPP 2012	Chambers et al. 1992	leydig cell tumor	general population	33.8	0.674	[325]	
Cancer Classification (CC)	L		OPP 2012						[325]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	1	mg/L	EPA HHBP	
Acute PAD	0.05	mg/kg/day	EPA HHBP	
Cancer Slope Factor (CSF)	0.0439	(mg/kg/day)^-1	EPA HHBP	
Chronic Human Health Benchmark	0.3	mg/L	EPA HHBP	
Chronic Human Health Benchmark	0.000729	mg/L	EPA HHBP	
Health-Based Screening Level	0.3	mg/L	Health-based screening levels from USGS	
Health-Based Screening Level	0.000729	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.05	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	3500	mg/kg	NIH HSDB	min
LD50	4000	mg/kg	NIH HSDB	max
LOAEL	12.4	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	200	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	2.5	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	90	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	8.93	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	151	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	180	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	60	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	89	mg/kg/day	EPA Toxicity Reference Database	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0095719	mol/kg	TEST QSAR	
Ames mutagenicity test	0.085	no units	TEST QSAR	
Developmental toxin test	1.168	no units	TEST QSAR	

Nationally Representative Water Data

Non-Scoring Data												
Non-Nationally Representative Water Data		Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water			Prevalence				Magnitude					
USDA Pesticide Data Program (PDP) (Finished)		2001 - 2013	11	0	Sites	0						
Bradley et al. 2018 (Finished) [53]		2016	26	2	Sites	7.69	0.0174	0.0174	0.0174	0.0174	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]		2009 - 2010	1	0	Sites	0						
Ambient Water			Prevalence				Magnitude					
National Water Information System (USGS NWIS) (Surface Water)		2008 - 2017	569	33	Sites	5.8	0.006	0.0346	0.196	1.24	ug/L	
National Water Information System (USGS NWIS) (Groundwater)		2008 - 2017	2,014	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)		2008 - 2017	2,582	33	Sites	1.28	0.006	0.0346	0.196	1.24	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)		2001 - 2013	4	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)		2001 - 2013	4	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]		1990 - 2018	15	0	Sites	0						
Bradley et al. 2017 (Ambient) [52]		2012 - 2014	38	3	Sites	7.89	0.0246	0.0304	0.0745	0.0855	ug/L	
Arnold et al. 2016 (Filtered) [7]		2012 - 2013	106	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Ambient) [153]		2009 - 2010	2	0	Sites	0						
Waste Water Effluent			Prevalence				Magnitude					
Estimated Concentration in Water		Date	Source	Value	Units	Model	Notes					

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.35536	days	
Boiling point	OPERA QSAR	352.665	degree C	
Boiling point	TEST QSAR	428.894	degree C	
Vapor pressure	OPERA QSAR	5.56E-09	mmHg	
Vapor pressure	TEST QSAR	7.85E-10	mmHg	
Solubility in water	OPERA QSAR	0.0000573	mol/L	
Solubility in water	TEST QSAR	0.0000681	mol/L	
Bioconcentration factor	OPERA QSAR	210.915	no units	
Bioconcentration factor	TEST QSAR	15.3815	no units	
Henry's Law constant	OPERA QSAR	3.27E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.99477	no units	

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. <i>Environmental science & technology</i> , 52(23), 13972-13985.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
325	USEPA. 2012. Iprodione. Acute Probabilistic, Chronic and Cancer Aggregate (Food and Drinking Water) Dietary Exposure and Risk Assessments for Parent and 3,5-DCA to Support New Section 3 Registration Actions on Cucurbits (Crop Group 9) and Fruiting Vegetables (Crop Group 8-10) and to Support a Tolerance for Imported Canola. EPA-HQ-OPP-2012-0392-0008. DP No. D392706. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Isophorone

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Isophorone
CASRN:	78-59-1
DTXSID:	DTXSID8020759
Use:	Solvent mixtures for finishes, for polyvinyl and nitrocellulose resins, stoving lacquers
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	X
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0026

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
2	carcinogen with linear MOA	9	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	50	preputial gland carcinomas	general population	OPP	1999

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.129	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.2	mg/kg/day	IRIS 1989	Nor-Am Agricultural Products 1972	no adverse effects at highest dose tested	general population	33.8	1180	[204]	
Reference Dose (RfD) or Equivalent	0.15	mg/kg/day	OW 1992	Nor-Am Agricultural Products 1972	no adverse effects at highest dose tested	general population	33.8	888	[220]	
Reference Dose (RfD) or Equivalent	0.15	mg/kg/day	OPP 1999	Nor-Am Agricultural Products 1972	no adverse effects at highest dose tested	general population	33.8	888	[234]	
Reference Dose (RfD) or Equivalent	0.2	mg/kg/day	ATSDR 2018	NTP 1986	hepatic, renal, and gastrointestinal lesions	general population	33.8	1180	[36]	
Cancer Slope Factor (CSF)	0.00095	(mg/kg/day)^-1	IRIS 1989	NTP 1986	preputial gland carcinoma	general population	33.8	31.1	[204]	
Cancer Slope Factor (CSF)	0.004	(mg/kg/day)^-1	OW 1992	NTP 1986	renal tubular cell tumors and preputial gland carcinomas	general population	33.8	7.40	[220]	
Cancer Slope Factor (CSF)	0.000608	(mg/kg/day)^-1	OPP 1999	NTP 1986	preputial gland carcinoma	general population	33.8	48.7	[234]	
Cancer Classification (CC)	C		IRIS 1989						[204]	
Cancer Classification (CC)	C		OW 1992						[220]	
Cancer Classification (CC)	C		OPP 1999						[234]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
						2017-07-01	2020-02-13	25	0	2	

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	15	mg/L	EPA DWSHA 2018	
Chronic Health-Based Guidance Value	0.1	mg/L	MN DOH	
Human Health Ambient Water Quality Criteria	0.034	mg/L	EPA Human Health Criteria for CWA	
Intermediate Minimal Risk Level (MRL)	3	mg/kg/day	CDC ATSDR	
Lifetime Health Advisory	0.04	mg/L	EPA DWSHA 2018	
Lifetime Health Advisory	0.1	mg/L	EPA DWSHA 2018	
Reference Concentration (RfC)	2000	ug/m^3	CalEPA OEHHA Chemical Database	
Cancer Classification (CC)	Female.Mice NE	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats NE	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice EE	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats SE	no units	HHS NTP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1000	mg/kg	NIH HSDB	min
LD50	3200	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	2.72	percent	EPA Chemistry Dashboard	
TD50	16600	mg/kg/day	NIH CPDB	max
TD50	203	mg/kg/day	NIH CPDB	min

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0104954	mol/kg	TEST QSAR	
Ames mutagenicity test	0.25	no units	TEST QSAR	
Developmental toxin test	0.944	no units	TEST QSAR	

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OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
		Prevalence				Magnitude					
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	1,920	52	Sites	2.71	0.003	0.01	0.129	3.9	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	150	36	Sites	24	0.003	0.01	0.0991	3.9	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	1,770	16	Sites	0.9	0.005	0.0105	0.316	0.54	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	10M - 50M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	12	1	Sites	8.33	0.149	0.149	0.149	0.149	ug/L	
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	4		0.032		0.032	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
		Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	47	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	830	414	Sites	50	0.002	0.011	0.0437	18.2	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	1,871	99	Sites	5.29	0.002	0.013	0.0605	0.18	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	2,701	513	Sites	19	0.002	0.011	0.0452	18.2	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	24	Sites	63	0.0038	0.012	0.0267	0.0991	ug/L	
Arnold et al. 2016 (Unfiltered) [7]	2012 - 2013	527	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	1	Sites	50						
Waste Water Effluent											
		Prevalence				Magnitude					
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	14	Sites	67	0.017	0.03	0.0694	0.081	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.0000459	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.55543	days	
Boiling point	OPERA QSAR	210.791	degree C	
Boiling point	TEST QSAR	211.454	degree C	
Vapor pressure	OPERA QSAR	0.616548	mmHg	
Vapor pressure	TEST QSAR	0.429536	mmHg	
Solubility in water	OPERA QSAR	0.0353497	mol/L	
Solubility in water	TEST QSAR	0.0304088	mol/L	
Bioconcentration factor	OPERA QSAR	2.63961	no units	
Bioconcentration factor	TEST QSAR	8.27942	no units	
Henry's Law constant	OPERA QSAR	0.0000366	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.02537	no units	

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
36	ATSDR. 2018. Toxicological Profile for Isophorone. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
204	USEPA. 1989. Chemical Assessment Summary, Isophorone. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, D.C.
220	USEPA. 1992. Isophorone Drinking Water Health Advisory. U.S. Environmental Protection Agency, Office of Water, Washington, D.C.
234	USEPA. 1999. Isophorone - Report of the Hazard Identification Assessment Review Committee. U.S. Environmental Protection Agency, Office of Prevention, Pesticides, and Toxic Substances, Office of Pesticides Programs, Health Effects Division, Washington, D.C.

Isoxaflutole

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Isoxaflutole
CASRN:	141112-29-0
DTXSID:	DTXSID5034723
Use:	Herbicide; for use on corn fields
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.067

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	carcinogen with linear MOA	7	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	3	liver adenomas and carcinomas	general population	OPP	2011

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.1998	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

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Isoxaflutole

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.02	mg/kg/day	OPP 2011	Chase 1995	liver, thyroid, ocular, nervous system toxicity	general population	33.8	118	[320]	
Cancer Slope Factor (CSF)	0.0114	(mg/kg/day) ⁻¹	OPP 2011	Chase 1995	liver adenomas and carcinomas	general population	33.8	2.60	[320]	
Cancer Classification (CC)	L		OPP 2011						[320]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.6	mg/L	EPA HHBP	
Acute PAD	0.02	mg/kg/day	EPA HHBP	
Cancer Slope Factor (CSF)	0.0114	(mg/kg/day) ⁻¹	EPA HHBP	
Chronic Human Health Benchmark	0.1	mg/L	EPA HHBP	
Chronic Human Health Benchmark	0.00281	mg/L	EPA HHBP	
Health-Based Screening Level	0.1	mg/L	Health-based screening levels from USGS	
Health-Based Screening Level	0.00281	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.02	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	5000	mg/kg	NIH HSDB	
LOAEL	5	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	500	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	1.79	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	100	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	3.38	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0023388	mol/kg	TEST QSAR	
Ames mutagenicity test	0.62	no units	TEST QSAR	
Developmental toxin test	0.897	no units	TEST QSAR	

Isoxaflutole

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	1,699	22	Sites	1.29	0.0028	0.0257	0.2	0.66	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	322	21	Sites	6.52	0.0028	0.0219	0.141	0.66	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	1,377	1	Sites	0.07	0.261	0.261	0.261	0.261	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	35	717,004	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	13	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	302	2	Sites	0.66	0.178	0.178	0.178	0.178	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	528	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	830	2	Sites	0.24	0.178	0.178	0.178	0.178	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	221	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	216	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	5	0	Sites	0						
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		1.97E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.53704	days	
Boiling point	OPERA QSAR	371.042	degree C	
Boiling point	TEST QSAR	316.595	degree C	
Vapor pressure	OPERA QSAR	0.000000009	mmHg	
Vapor pressure	TEST QSAR	5.09E-08	mmHg	
Solubility in water	OPERA QSAR	0.0000252	mol/L	
Solubility in water	TEST QSAR	0.0000219	mol/L	
Bioconcentration factor	OPERA QSAR	4.99662	no units	
Bioconcentration factor	TEST QSAR	207.491	no units	
Henry's Law constant	OPERA QSAR	2.3E-10	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.47956	no units	

Isoxaflutole

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
320	USEPA. 2011. Isoxaflutole. Section 3 Registration for Use on Soybeans. Human Health Risk Assessment. EPA-HQ-OPP-2010-0845-0005. DP No. D382796. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.

Lactofen

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Lactofen
CASRN:	77501-63-4
DTXSID:	DTXSID7024160
Use:	Herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0046

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	non-cancer effects	2	5

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	50	increased incidence of proteinaceous casts in kidneys and decreases in thyroid and adrenal gland weights	general population	OPP	2007

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.2322	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Lactofen

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.008	mg/kg/day	OPP 2007	Tisdell et al. 1982	increased incidence of proteinaceous casts in kidneys and decreases in thyroid and adrenal gland weights	general population	33.8	47.3	[277]	
Cancer Classification (CC)	NL		OPP 2007						[277]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.47	mg/L	EPA HHBP	
Acute PAD	0.017	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.05	mg/L	EPA HHBP	
Health-Based Screening Level	0.05	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.008	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	5000	mg/kg	NIH HSDB	
LOAEL	1.4	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	150	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	0.79	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	50	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	13.87	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	73.699997	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	17	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0062661	mol/kg	TEST QSAR	
Ames mutagenicity test	0.466	no units	TEST QSAR	
Developmental toxin test	1.012	no units	TEST QSAR	

Lactofen

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	1,737	2	Sites	0.12	0.101	0.183	0.232	0.265	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	322	1	Sites	0.31	0.101	0.101	0.101	0.101	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	1,415	1	Sites	0.07	0.265	0.265	0.265	0.265	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	32	785,344	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	1	1,845	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	2	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	304	2	Sites	0.66	0.154	0.163	0.168	0.172	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	528	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	832	2	Sites	0.24	0.154	0.163	0.168	0.172	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.000000159	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.54533	days	
Boiling point	OPERA QSAR	378.705	degree C	
Boiling point	TEST QSAR	425.323	degree C	
Vapor pressure	OPERA QSAR	6.62E-08	mmHg	
Vapor pressure	TEST QSAR	2.29E-08	mmHg	
Solubility in water	OPERA QSAR	0.000000301	mol/L	
Solubility in water	TEST QSAR	0.000000822	mol/L	
Bioconcentration factor	OPERA QSAR	93.5153	no units	
Bioconcentration factor	TEST QSAR	30.4088	no units	
Henry's Law constant	OPERA QSAR	1.05E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	4.66713	no units	

Lactofen

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
277	USEPA. 2007. Lactofen: Revised Human Health Risk Assessment for Proposed Uses on Fruiting Vegetables and Okra. EPA-HQ-OPP-2006-0178-0008. DP No. D339011. U.S. Environmental Protection Agency, Office of Prevention, Pesticides and Toxic Substances, Washington, D.C.

lambda-Cyhalothrin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	lambda-Cyhalothrin
CASRN:	91465-08-6
DTXSID:	DTXSID7032559
Use:	Insecticide (HSD8 - data for cyhalothrin, CASRN 68085-85-8)
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	X
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision

Not List

Final Hazard Quotient (HQ)

0.024

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	reproductive and developmental effects	2	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	1	reduced motor activity	bottle-fed infants	OPP	2017

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.0236	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		
Not Applicable		

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

lambda-Cyhalothrin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.00093	mg/kg/day	OPP 2017	Moser et al. 2016	reduced motor activity	bottle-fed infants	151	1.23	[385]	
Cancer Classification (CC)	NL		OPP 2017						[385]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.03	mg/L	EPA HHBP	
Acute Minimal Risk Level (MRL)	0.01	mg/kg/day	CDC ATSDR	
Acute Minimal Risk Level (MRL)	0.02	mg/kg/day	CDC ATSDR	
Acute PAD	0.005	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.006	mg/L	EPA HHBP	
Health-Based Screening Level	0.006	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.001	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LOAEL	0.5	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	5	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	0.1	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	1.5	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	9.32	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	12.5	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	2.5	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0011776	mol/kg	TEST QSAR	
Ames mutagenicity test	-0.114	no units	TEST QSAR	
Developmental toxin test	0.956	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

lambda-Cyhalothrin
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	3,055	4	Sites	0.13	0.003	0.0075	0.0236	0.034	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	190	2	Sites	1.05	0.007	0.0075	0.0078	0.008	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	2,865	2	Sites	0.07	0.003	0.0185	0.0278	0.034	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	48	773,940	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	0	0	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	7	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	437	1	Sites	0.23	0.048	0.048	0.048	0.048	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	981	1	Sites	0.1	0.006	0.006	0.006	0.006	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,417	2	Sites	0.14	0.006	0.027	0.0396	0.048	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	118	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	111	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	7	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	4,815	237	Sites	4.92	7e-04	0.00511	0.0222	0.447	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	8	Sites	21	9.23e-05	0.000314	0.0018	0.0022	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	106	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.00000189	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.54201	days	
Boiling point	OPERA QSAR	422.672	degree C	
Boiling point	TEST QSAR	431.019	degree C	
Vapor pressure	OPERA QSAR	4.02E-09	mmHg	
Vapor pressure	TEST QSAR	2.05E-09	mmHg	
Solubility in water	OPERA QSAR	1.97E-08	mol/L	
Solubility in water	TEST QSAR	0.000000071	mol/L	
Bioconcentration factor	OPERA QSAR	133.673	no units	
Bioconcentration factor	TEST QSAR	342.768	no units	
Henry's Law constant	OPERA QSAR	0.000000012	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	6.63514	no units	

lambda-Cyhalothrin

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
385	USEPA. 2017. Lambda- & Gamma-Cyhalothrin: Human Health Draft Risk Assessment for Registration Review. EPA-HQ-OPP-2010-0480-0299. DP No. 426321. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Lidocaine

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Lidocaine
CASRN:	137-58-6
DTXSID:	DTXSID1045166
Use:	Anesthetic
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	X

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.004

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	non-cancer effects	10	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	8	lowest therapeutic dose:local anesthesia	bottle-fed infants	FDA; NIH	2018; 2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.0318	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Lidocaine

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.00125	mg/kg/day	FDA 2018; NIH 2018	Fresenius Kabi USA, LLC	lowest therapeutic dose:local anesthesia	bottle-fed infants	151	8.30	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels
Reference Dose (RfD) or Equivalent	0.00125	mg/kg/day	FDA 2018; NIH 2018	Fresenius Kabi USA, LLC	lowest therapeutic dose:local anesthesia	general population	33.8	29.0	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Screening level for pharmaceutical - general population	0.029411765	mg/L	EPA Office of Water	
Screening level for pharmaceutical - infants	0.008333333	mg/L	EPA Office of Water	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	220	mg/kg	NIH HSDB	min
LD50	317	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	4.68	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0073961	mol/kg	TEST QSAR	
Ames mutagenicity test	0.073	no units	TEST QSAR	
Developmental toxin test	0.277	no units	TEST QSAR	

Lidocaine

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	557	136	Sites	24	0.00038	0.00289	0.0318	0.438	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	75	39	Sites	52	0.00038	0.00356	0.0688	0.438	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	482	97	Sites	20	0.00038	0.00262	0.0132	0.0508	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Bradley et al. 2018 (Finished) [53]	2016	26	1	Sites	3.85	0.0237378	0.0237	0.0237	0.0237378	ug/L	
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	209	97	Sites	46	0.00042	0.00813	0.175	0.438	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	401	35	Sites	8.73	0.00058	0.00496	0.0769	0.505	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	610	132	Sites	22	0.00042	0.0069	0.154	0.505	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	8		0.0296		0.0297	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	21	Sites	55	0.0009345	0.0841	0.248	0.4088204	ug/L	
Bexfield et al. 2019 (Groundwater) [49]	2013 - 2015	1,106	2	Sites	0.18	0.0276506	0.0336	0.0384	0.0396035	ug/L	
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	19	Sites	90	0.0863121	0.321	0.586	2.6986356	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		3.11E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.35565	days	
Boiling point	OPERA QSAR	308.77	degree C	
Boiling point	TEST QSAR	323.774	degree C	
Vapor pressure	OPERA QSAR	7.96E-08	mmHg	
Vapor pressure	TEST QSAR	0.00000094	mmHg	
Solubility in water	OPERA QSAR	0.0095648	mol/L	
Solubility in water	TEST QSAR	0.00334965	mol/L	
Bioconcentration factor	OPERA QSAR	15.25	no units	
Bioconcentration factor	TEST QSAR	11.885	no units	
Henry's Law constant	OPERA QSAR	3.51E-10	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.4589	no units	

Lidocaine

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Reference Number	Full Reference
49	Bexfield, L.M., P.L. Toccalino, K. Belitz, W.T. Foreman, and E.T. Furlong. 2019. Hormones and pharmaceuticals in groundwater used as a source of drinking water across the United States. Environmental Science and Technology 53: 2950-2960.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. Environmental science & technology, 51(9), 4792-4802.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. Environmental science & technology, 52(23), 13972-13985.
77	FDA. 2018. Drugs @ FDA: FDA Approved Drug Products. U.S. Food and Drug Administration (FDA). https://www.accessdata.fda.gov/scripts/cder/daf/ .
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. Science of The Total Environment. v581-582, (909-922).
150	NIH. 2018. DailyMed Database. U.S. National Library of Medicine, National Institutes of Health (NIH). https://dailymed.nlm.nih.gov/dailymed/ .
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. Science of the Total Environment, 636, 69-79.

Linuron

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Linuron
CASRN:	330-55-2
DTXSID:	DTXSID2024163
Use:	Herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	X
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision		Final Hazard Quotient (HQ)	
Not List		0.0032	

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION					
Potency	Severity			Prevalence	Magnitude
5	non-cancer effects			1	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	50	hematological changes	general population	OPP	2019

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)		Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.1589	90th Percentile		All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X	X		

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		
Not Applicable		

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Linuron

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0077	mg/kg/day	OPP 2019	Malley 1988	hematological changes	general population	33.8	45.6	[418]	
Cancer Classification (CC)	C		OPP 2019						[418]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	3.3	mg/L	EPA HHBP	
Acute PAD	0.12	mg/kg/day	EPA HHBP	
Chronic Health-Based Guidance Value	0.001	mg/L	MN DOH	
Chronic Human Health Benchmark	0.049	mg/L	EPA HHBP	
Health-Based Screening Level	0.049	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.0077	mg/kg/day	EPA HHBP	

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	4000	mg/kg	NIH HSDB	max
LD50	500	mg/kg	NIH HSDB	min
LOAEL	261	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	3.49	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	0.79	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	63	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	10.35	percent	EPA Chemistry Dashboard	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0056494	mol/kg	TEST QSAR	
Ames mutagenicity test	0.605	no units	TEST QSAR	
Developmental toxin test	0.569	no units	TEST QSAR	

Scoring Data

Scoring Data											
Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003	293	0	Sites	0					ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	10,134	151	Sites	1.49	3.00E - 04	0.018	0.159	5.28	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	2,045	132	Sites	6.45	5.00E - 04	0.018	0.161	5.28	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	8,089	19	Sites	0.23	3.00E - 04	0.00632	0.06	0.272	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	39	506,914	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	4	10	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data		Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water			Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Finished)		2006 - 2020	3	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)		2001 - 2013	17	3	Sites	18	0.0027	0.0075	0.164	0.315	ug/L	
Ambient Water			Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Source)		2006 - 2020	41	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)		2008 - 2017	624	13	Sites	2.08	0.00218	0.00683	0.174	0.246	ug/L	
National Water Information System (USGS NWIS) (Groundwater)		2008 - 2017	1,623	3	Sites	0.18	0.003	0.071	0.0956	0.111	ug/L	
National Water Information System (USGS NWIS) (All Water)		2008 - 2017	2,247	16	Sites	0.71	0.00218	0.0113	0.111	0.246	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)		2001 - 2013	229	2	Sites	0.87	0.0042	0.00835	0.0166	0.019	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)		2001 - 2013	219	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)		2001 - 2013	12	2	Sites	17	0.0042	0.00835	0.0166	0.019	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]		1990 - 2018	6,817	178	Sites	2.61	0.0031	0.0148	0.573	5.6	ug/L	
Bradley et al. 2017 (Ambient) [52]		2012 - 2014	38	2	Sites	5.26	0.02	0.03	0.038	0.04	ug/L	
Arnold et al. 2016 (Filtered) [7]		2012 - 2013	690	8	Sites	1.16	3e-04	0.00095	0.00163	0.0017	ug/L	
Waste Water Effluent			Prevalence				Magnitude					
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes						

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
ExpoCast exposure		1.47E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMB 4 data used in the draft CCI 5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.52572	days	
Boiling point	OPERA QSAR	323.038	degree C	
Boiling point	TEST QSAR	304.222	degree C	
Vapor pressure	OPERA QSAR	0.00000285	mmHg	
Vapor pressure	TEST QSAR	0.000000679	mmHg	
Solubility in water	OPERA QSAR	0.000410555	mol/L	
Solubility in water	TEST QSAR	0.000829851	mol/L	
Bioconcentration factor	OPERA QSAR	19.518	no units	
Bioconcentration factor	TEST QSAR			
Henry's Law constant	OPERA QSAR	7.35E-10	atm·m³/mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.05317	no units	

Linuron

CCL 5 Contaminant Information Sheet

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July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
418	USEPA. 2019. Linuron: Revised Human Health Draft Risk Assessment to Support Registration Review. EPA-HQ-OPP-2010-0228-0065. DP No. D444117. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Lithium

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Lithium
CASRN:	7439-93-2
DTXSID:	DTXSID5036761
Use:	Metal, pharmaceutical. Used as Anode in electrochemical cells and batteries; as chemical intermediate in organic syntheses
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	6.3

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
3	non-cancer effects	10	9

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	10	renal, neurologic, and endocrine gland effects	general population	PPRTV	2008

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
63	90th Percentile	Finished Water	NIRS	1984-1986

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Lithium

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	2	ug/kg/day	PPRTV 2008	Baldessarini and Tarazi 2001	renal, neurologic, and endocrine gland effects	general population	33.8	11.8	[295]	
Cancer Classification (CC)	I		PPRTV 2008						[295]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Reproductive, Cardiovascular, Hepatic, Neurological, Developmental, Renal, Systemic, Immune, Metabolic	15	Ahmad, 2011; Abu-Taweel 2012	Neurological	29.94	Riadh, 2011	2007-06-01	2019-10-21	5278	46	189	5

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Subchronic Provisional RfD	0.002	mg/kg/day	EPA PPRTV	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1165	mg/kg	NIH HSDB	max
LD50	526	mg/kg	NIH HSDB	min

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity test			TEST QSAR	
Developmental toxin test			TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Lithium
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986	988	551	Sites	56	5	15	63	7929	ug/L	
Ambient Water											
		Prevalence				Magnitude					
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	5,983	5,683	Sites	95	0.15	4.51	43.9	2420	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	271	213	Sites	79	0.15	4.39	43.5	460	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	5,712	5,470	Sites	96	0.15	4.66	44.7	2420	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	1M - 10M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	7	7	Sites	100	0.003	3.3	5.2	16	ug/L	
Bradley et al. 2018 (Finished) [53]	2016	26	23	Sites	88	0.35	1.95	13.6	71.05	ug/L	
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	56		10.8		42.7	ug/L	
Community Water System Survey (CWSS) (Finished) [178]	2006	1	NA	Sites			2.7	2.7		ug/L	
Ambient Water											
		Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	21	10	Sites	48	0.002	2.8	9.7	40	ug/L	
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	1,324	1,159	Sites	88	0	4.5	43.5	70400	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	5,801	5,648	Sites	97	0.07	15.3	100	80600	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	7,115	6,797	Sites	96	0	9.46	73.4	80600	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	56		10.7		46	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	757	729	Sites	96	0.22	5.39	39.6	285	ug/L	
Waste Water Effluent											
		Prevalence				Magnitude					
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Lithium

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. Environmental science & technology, 52(23), 13972-13985.
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. Science of The Total Environment. v581-582, (909-922).
178	USEPA (US Environmental Protection Agency). (2009). 2006 Community Water System Survey. Overview, 57.
295	USEPA. 2008. Provisional Peer Reviewed Toxicity Values for Lithium (CASRN 7439-93-2). EPA/690/R-08/016F. U.S. Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment, Superfund Health Risk Technical Support Center, Cincinnati, OH.

Loratadine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Loratadine
CASRN:	79794-75-5
DTXSID:	DTXSID2023224
Use:	antihistaminic
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0057

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
8	non-cancer effects	6	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	0.3	lowest therapeutic dose: Antihistamine/relieves of symptoms due to hay fever or other upper respiratory allergies such as runny nose, itchy, watery eyes	bottle-fed infants	FDA; NIH	2018; 2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.0017	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis
Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Loratadine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	4.16667E-05	mg/kg/day	FDA 2018; NIH 2018	Bayer HealthCare LLC	lowest therapeutic dose:Antihistamine/relieves of symptoms due to hay fever or other upper respiratory allergies such as runny nose, itchy, watery eyes	bottle-fed infants	151	0.280	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels
Reference Dose (RfD) or Equivalent	4.16667E-05	mg/kg/day	FDA 2018; NIH 2018	Bayer HealthCare LLC	lowest therapeutic dose:Antihistamine/relieves of symptoms due to hay fever or other upper respiratory allergies such as runny nose, itchy, watery eyes	general population	33.8	0.980	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Maximum Recommended Daily Dose	0.167	mg/kg/day	FDA	
Screening level for pharmaceutical - general population	0.000980392	mg/L	EPA Office of Water	
Screening level for pharmaceutical - infants	0.000277778	mg/L	EPA Office of Water	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	5000	mg/kg	NIH HSDB	
Percent of active toxcast in vitro assays tested	37	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0011588	mol/kg	TEST QSAR	
Ames mutagenicity test	-0.082	no units	TEST QSAR	
Developmental toxin test	0.8	no units	TEST QSAR	

Loratadine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	557	4	Sites	0.72	0.00022	0.00059	0.0017	0.00279	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	75	3	Sites	4	0.00034	6e-04	0.00192	0.00279	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	482	1	Sites	0.21	0.00022	0.00022	0.00022	0.00022	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	205	10	Sites	4.88	0.00016	0.00154	0.0134	0.151	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	401	1	Sites	0.25	0.00097	0.00097	0.00097	0.00097	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	606	11	Sites	1.82	0.00016	0.00142	0.0134	0.151	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	6	Sites	16	0.0007989	0.00138	0.00211	0.0022605	ug/L	
Bexfield et al. 2019 (Groundwater) [49]	2013 - 2015	1,106	0	Sites	0						
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	12	Sites	57	0.0016315	0.0026	0.0153	0.0638996	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.000000259	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.35836	days	
Boiling point	OPERA QSAR	365.058	degree C	
Boiling point	TEST QSAR	474.912	degree C	
Vapor pressure	OPERA QSAR	3.83E-10	mmHg	
Vapor pressure	TEST QSAR	2.27E-10	mmHg	
Solubility in water	OPERA QSAR	0.00000725	mol/L	
Solubility in water	TEST QSAR	0.0000128	mol/L	
Bioconcentration factor	OPERA QSAR	124.017	no units	
Bioconcentration factor	TEST QSAR	28.6418	no units	
Henry's Law constant	OPERA QSAR	0.000000016	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	4.96583	no units	

Loratadine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
49	Bexfield, L.M., P.L. Toccalino, K. Belitz, W.T. Foreman, and E.T. Furlong. 2019. Hormones and pharmaceuticals in groundwater used as a source of drinking water across the United States. Environmental Science and Technology 53: 2950-2960.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. Environmental science & technology, 51(9), 4792-4802.
77	FDA. 2018. Drugs @ FDA: FDA Approved Drug Products. U.S. Food and Drug Administration (FDA). https://www.accessdata.fda.gov/scripts/cder/daf/ .
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. Science of The Total Environment. v581-582, (909-922).
150	NIH. 2018. DailyMed Database. U.S. National Library of Medicine, National Institutes of Health (NIH). https://dailymed.nlm.nih.gov/dailymed/ .
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. Science of the Total Environment, 636, 69-79.

Magnesium

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Magnesium
CASRN:	7439-95-4
DTXSID:	DTXSID0049658
Use:	Metal, used in alloys commonly with aluminum
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	5.1

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
3	non-cancer effects	10	10

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	7000	"mild diarrhea and other mild gastrointestinal complaints" -- reversible	bottle-fed infants	IOM	1997

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
35511	90th Percentile	Finished Water	NIRS	1984-1986

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Magnesium

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	5	mg/kg/day	IOM 1997	Bashir et al., 1993	mild diarrhea and other mild gastrointestinal complaints	bottle-fed infants	151	6620	[107]	NOTE: this compound is a nutrient

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity test			TEST QSAR	
Developmental toxin test			TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

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EPA - Office of Water

Magnesium
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986	988	976	Sites	99	50	9948	35511	115887	ug/L	
Ambient Water											
		Prevalence				Magnitude					
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	12,121	12,118	Sites	100	5	9630	32300	2.00E+06	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	2,620	2,620	Sites	100	41	8760	29100	2.00E+06	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	9,502	9,499	Sites	100	5	12700	40100	1800000	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	250M - 500M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	621	598	Sites	96	57	14600	32000	1400000	ug/L	
Drinking Water Monitoring Data - MA (Finished)	2006 - 2020	542	521	Sites	96	10	3500	8500	70000	ug/L	
Drinking Water Monitoring Data - WA (Finished)	2006 - 2011	206	201	Sites	98	100	8000	19720	49500	ug/L	
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	100		8810		31700	ug/L	
Community Water System Survey (CWSS) (Finished) [178]	2006	12	NA	Sites			9950	24000		ug/L	
Ambient Water											
		Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	5,422	5,288	Sites	98	3	14000	47000	7.1e+07	ug/L	
Drinking Water Monitoring Data - MA (Source)	2006 - 2020	81	81	Sites	100	400	4400	8000	55400	ug/L	
Drinking Water Monitoring Data - PA (Source)	2006 - 2011	3	3	Sites	100	2600	14800	19530	19600	ug/L	
Drinking Water Monitoring Data - WA (Source)	2006 - 2011	308	304	Sites	99	120	10850	25710	59500	ug/L	
Drinking Water Monitoring Data - WI (Source)	2012-2019	141	140	Sites	99	160	23000	43700	77300	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	100		10600		44600	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	758	757	Sites	100	13	5840	35440	133000	ug/L	
Waste Water Effluent											
		Prevalence				Magnitude					
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg- bw/day)	Notes
ExpoCast exposure			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Magnesium

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. Science of The Total Environment. v581-582, (909-922).
107	IOM. 1997. Standing Committee on the Scientific Evaluation of Dietary Reference Intakes, Food and Nutrition Board. Dietary Reference Intakes for calcium, phosphorus, magnesium, vitamin D, and fluoride. Institute of Medicine (IOM), National Academy Press, Washington, DC.
178	USEPA (US Environmental Protection Agency). (2009). 2006 Community Water System Survey. Overview, 57.

Malathion

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Malathion
CASRN:	121-75-5
DTXSID:	DTXSID4020791
Use:	Insecticide; veterinary medicine
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.0078

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	reproductive and developmental effects	9	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	10	inhibition of red blood cell acetylcholinesterase in pups	bottle-fed infants	OPP	2016

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.078	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Malathion

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.01	mg/kg/day	OPP 2016	Fulcher 2001; Barnett 2006, 2008	inhibition of red blood cell acetylcholinesterase in pups	bottle-fed infants	151	13.2	[368]	
Cancer Classification (CC)	S		OPP 2016						[368]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	0.2	mg/L	EPA DWSHA 2018	
Acute inhalation Minimal Risk Level (MRL)	0.2	mg/m ³	CDC ATSDR	
Intermediate Inhalation Minimal Risk Level (MRL)	0.02	mg/m ³	CDC ATSDR	
Intermediate Minimal Risk Level (MRL)	0.02	mg/kg/day	CDC ATSDR	
Lifetime Health Advisory	0.5	mg/L	EPA DWSHA 2018	
Maximum Allowable Concentration (MAC)	0.19	mg/L	Canadian Drinking Water Guidelines	
Cancer Classification (CC)	2A	no units	WHO IARC	
Cancer Classification (CC)	Female.Mice N	no units	HHS NTP	
Cancer Classification (CC)	Female.Mice NT	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats N	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats NT	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice N	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice NT	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats N	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats NT	no units	HHS NTP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	190	mg/kg	NIH HSDB	min
LD50	5843	mg/kg	NIH HSDB	max
LOAEL	1476	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	29	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	451	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	5	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	12.14	percent	EPA Chemistry Dashboard	
TD50	44700	mg/kg/day	NIH CPDB	max
TD50	66.6	mg/kg/day	NIH CPDB	min

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0010471	mol/kg	TEST QSAR	
Ames mutagenicity test	0.383	no units	TEST QSAR	
Developmental toxin test	0.378	no units	TEST QSAR	

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Draft Fifth Contaminant Candidate List (CCL 5)
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EPA - Office of Water

Malathion
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	11,237	416	Sites	3.7	0.00041	0.014	0.078	9.58	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	2,230	383	Sites	17	0.00041	0.014	0.078	9.58	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	9,008	33	Sites	0.37	0.00107	0.006	0.0248	0.239	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	33	1,346,697	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	10	108,619	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	3	0	Sites	0						
Drinking Water Monitoring Data - WA (Finished)	2006 - 2011	481	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	2	Sites	12	0.01	0.063	0.254	0.331	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	37	0	Sites	0						
Drinking Water Monitoring Data - WA (Source)	2006 - 2011	634	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	1,003	50	Sites	4.99	6.00E - 04	0.022	0.418	5.46	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3,060	3	Sites	0.1	0.01	0.108	0.159	0.181	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	4,062	53	Sites	1.3	6.00E - 04	0.0223	0.401	5.46	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	4	Sites	1.75	0.00999	0.0763	0.269	0.312	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	3	Sites	1.37	0.05	0.103	0.278	0.312	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	1	Sites	8.33	0.00999	0.00999	0.00999	0.00999	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	15,764	712	Sites	4.52	0.006	0.089	0.848	46	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	3	Sites	7.89	0.0166	0.0374	0.0518	0.0554	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	3	Sites	0.43	0.0011	0.0017	0.0891	0.111	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
USGS, McKenzie River, Oregon, 2012 (Ambient) [158]	2002 - 2010	133	3	Samples	2.3				0.04	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
ExpoCast exposure		0.00000153	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	25.141	days	
Boiling point	OPERA QSAR	359.971	degree C	
Boiling point	TEST QSAR	284.068	degree C	
Vapor pressure	OPERA QSAR	0.00000395	mmHg	
Vapor pressure	TEST QSAR	0.00000723	mmHg	
Solubility in water	OPERA QSAR	0.000634727	mol/L	
Solubility in water	TEST QSAR	0.000760326	mol/L	
Bioconcentration factor	OPERA QSAR	26.329	no units	
Bioconcentration factor	TEST QSAR	9.86279	no units	
Henry's Law constant	OPERA QSAR	3.85E-09	atm-m^3/mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.24648	no units	

Malathion

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
158	Reconnaissance of Land-Use Sources of Pesticides in Drinking Water, McKenzie River, Oregon. U.S. Geological Survey Scientific Investigations Report 2012–5091, 46 p. plus appendixes.
368	USEPA. 2016. Malathion: Human Health Draft Risk Assessment for Registration Review. EPA-HQ-OPP-2009-0317-0080. DP No. D414107. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Manganese

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Manganese
CASRN:	7439-96-5
DTXSID:	DTXSID2024169
Use:	Manufacturing of steel alloys, in dry-cell batteries, electrical coils, ceramics, matches, glass, dyes, fertilizers, welding rods, as oxidizing agents, and as animal food additives.
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	
Human Neurotoxics	
PubMed Neurotoxics	X
Neurodev. Disruptors	X
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	X

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.97

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	reproductive and developmental effects	10	7

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	30	various neurological endpoints in rats including behavioral and sensorimotor effects, corresponding neurostructural and neurochemical changes, persistent later-life consequences of developmental exposures after levels of manganese in the brain have returned to normal	bottle-fed infants	HC	2019

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
29.2	90th Percentile	Finished Water	UCMR4	2018 - 2019

PUBLIC NOMINATION STATUS

Public Nomination
X

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X			X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
X	Not Applicable	Not Applicable
Basis		
Manganese is a naturally occurring element and an essential nutrient of which ingestion is not known to present adverse health effects at low levels [a]. Drinking water contributes only a small portion of normal oral intake, contributing to approximately 2.8 x 10 ⁻⁴ mg/kg-day of daily manganese exposure (calculated using the median concentration of detections of NIRS data (0.012 mg/L), and assuming a daily intake of 2 L of drinking water by a 70 kg adult for a calculated exposure) [b,c]. It is unlikely that regulation of manganese in drinking water would represent a meaningful opportunity for health risk reduction in persons served by public water systems.		
[a] USEPA, 2003 [257]; [b] IOM, 2001 [106]; [c] NIRS, 2016 [151]; as cited in USEPA, 2001 [180]		

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Manganese

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mg/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.025	mg/kg/day	HC 2019	Kern et al., 2010, 2011; Beaudin et al., 2013	various neurological endpoints in rats. "In addition to demonstrating that exposure to manganese in early life can result in behavioural and sensorimotor effects, these studies provided mechanistic support by demonstrating corresponding neurostructural and neurochemical changes. Further, Kern et al. (2011) and Beaudin et al. (2013) demonstrated the ability of manganese exposure in early life to result in effects that persist into adulthood, after levels of manganese in the brain have returned to normal."	bottle-fed infants	151	33.1	[101]	
Reference Dose (RfD) or Equivalent	0.14	mg/kg/day	IRIS 1988	NRC 1989; Freeland-Graves et al. 1987; WHO 1973	"CNS effects"	general population	33.8	828	[199]	
Reference Dose (RfD) or Equivalent	0.14	mg/kg/day	OW 2004	NRC 1989; WHO 1973; Schroeder et al. 1966	"NOAEL for chronic ingestion of manganese by humans"	general population	33.8	828	[260]	
Cancer Classification (CC)	D		IRIS 1988						[199]	
Cancer Classification (CC)	D		OW 2004						[260]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mg/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Reproductive	0.01	Souza, 2019	Developmental	11	Foster, 2018	2018-05-01	2019-10-25	1413	13	91	3

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	1	mg/L	EPA DWSHA 2018	
Chronic Health-Based Guidance Value	0.1	mg/L	MN DOH	
Human Health Ambient Water Quality Criteria	0.05	mg/L	EPA Human Health Criteria for CWA	
Lifetime Health Advisory	0.3	mg/L	EPA DWSHA 2018	
Reference Concentration (RfC)	0.09	ug/m ³	CalEPA OEHHA Chemical Database	
Reference Concentration (RfC)	0.00005	mg/m ³	EPA IRIS	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity test			TEST QSAR	
Developmental toxin test			TEST QSAR	

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Manganese
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019	3,743	3,293	Sites	88	0.4	2.76	29.2	3960	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015	799	668	Sites	84	1	5.5	57	3550	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986	989	672	Sites	68	1	12	126	1341	ug/L	
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	11,988	10,113	Sites	84	0.05	18	195	59000	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	2,538	2,439	Sites	96	0.1	18.4	122	12000	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	9,451	7,674	Sites	81	0.05	17	440	59000	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)	47	31,505,117	Chemical Data Reporting (CDR) Results (EPA) (2016)	250M - 500M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	926	562	Sites	61	0.002	28	190	93300	ug/L	
Drinking Water Monitoring Data - MA (Finished)	2006 - 2020	1,665	1,305	Sites	78	0.38	59	475	159000	ug/L	
Drinking Water Monitoring Data - WA (Finished)	2006 - 2011	998	519	Sites	52	0.6	30	210	6700	ug/L	
Bradley et al. 2018 (Finished) [53]	2016	26	22	Sites	85	0.55	1.84	13.8	44.47	ug/L	
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	64		2.6		55.6	ug/L	
Community Water System Survey (CWSS) (Finished) [178]	2006	1	NA	Sites			0.003	0.003		ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	5,546	2,858	Sites	52	0.003	87	510	36000	ug/L	
Drinking Water Monitoring Data - FL (Source)	2006 - 2011	35	29	Sites	83	0.3	6.4	42	90	ug/L	
Drinking Water Monitoring Data - MA (Source)	2006 - 2020	407	362	Sites	89	0.93	182	1180	11000	ug/L	
Drinking Water Monitoring Data - PA (Source)	2006 - 2011	52	45	Sites	87	0.04	70	374	1500	ug/L	
Drinking Water Monitoring Data - WA (Source)	2006 - 2011	1,560	804	Sites	52	0.6	50	240	9150	ug/L	
Drinking Water Monitoring Data - WI (Source)	2012-2019	145	124	Sites	86	0.516	25	140	10600	ug/L	
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	3,519	3,463	Sites	98	0.04	30	231	357000	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	11,832	9,545	Sites	81	0.019	19.9	641	680000	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	15,319	12,981	Sites	85	0.019	28.8	316	680000	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	92		43		1497	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	757	653	Sites	86	0.15	8.06	175	3110	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)	14.8	ug/l	
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. <i>Environmental science & technology</i> , 52(23), 13972-13985.
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
101	Health Canada. 2019. Guideline Technical Document Manganese. Health Canada (HC), Ottawa, Ontario, Canada.
106	Institute of Medicine (IOM). 2001. Dietary Reference Intakes for Vitamin A, Vitamin K, Arsenic, Boron, Chromium, Copper, Iodine, Iron, Manganese, Molybdenum, Nickel, Silicon, Vanadium and Zinc: A Report of the Panel on Micronutrients, Subcommittees on Upper Reference Levels of Nutrients and of Interpretation and Use of Dietary Reference Intakes, and the Standing Committee on the Scientific Evaluation of Dietary Reference Intakes, Food and Nutrition Board, Institute of Medicine. Washington, DC: National Academy Press (prepublication version). Available on the Internet at:
151	NIRS. 2016. Summary of data provided in tabular form in docket; www.regulations.gov Docket ID EPA-HQ-OW-2007-1189.
178	USEPA (US Environmental Protection Agency). (2009). 2006 Community Water System Survey. Overview, 57.
180	USEPA, 2001. Regulatory Determination Support Document for Manganese. EPA 815 R-01-013.
199	USEPA. 1988. Manganese; CASRN 7439-96-5. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, DC.
257	USEPA. 2003. Health Effects Support Document for Manganese. Office of Water. EPA Report 822-R-03-003. February 2003. 164pp.
260	USEPA. 2004. Drinking Water Health Advisory for Manganese. EPA-822-R-04-003. U.S. Environmental Protection Agency, Office of Water, Health and Ecological Criteria Division, Washington, DC.

Meprobamate

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Meprobamate
CASRN:	57-53-4
DTXSID:	DTXSID3023261
Use:	anxiolytic
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0022

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	non-cancer effects	9	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	30	lowest therapeutic dose: short-term relief of the symptoms of anxiety	bottle-fed infants	FDA; NIH	2018; 2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.06641	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.005	mg/kg/day	FDA 2018; NIH 2018	Alembic Pharmaceuticals Inc.	lowest therapeutic dose: short-term relief of the symptoms of anxiety	bottle-fed infants	151	33.0	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels
Reference Dose (RfD) or Equivalent	0.005	mg/kg/day	FDA 2018; NIH 2018	Alembic Pharmaceuticals Inc.	lowest therapeutic dose: short-term relief of the symptoms of anxiety	general population	33.8	120	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Maximum Recommended Daily Dose	40	mg/kg/day	FDA	
Screening level for pharmaceutical - general population	0.117647059	mg/L	EPA Office of Water	
Screening level for pharmaceutical - infants	0.033333333	mg/L	EPA Office of Water	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1410	mg/kg	NIH HSDB	max
LD50	750	mg/kg	NIH HSDB	min
Percent of active toxcast in vitro assays tested	0.43	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0038637	mol/kg	TEST QSAR	
Ames mutagenicity test	0.522	no units	TEST QSAR	
Developmental toxin test	0.896	no units	TEST QSAR	

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Scoring Data											
Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
		Prevalence				Magnitude					
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	557	18	Sites	3.23	0.00243	0.0203	0.0664	0.164	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	75	11	Sites	15	0.00243	0.0202	0.0527	0.137	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	482	7	Sites	1.45	0.00965	0.0385	0.142	0.164	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data											
Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water			Prevalence			Magnitude					
Bradley et al. 2018 (Finished) [53]	2016	26	1	Sites	3.85	0.0183328	0.0183	0.0183	0.0183328	ug/L	
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Snyder et al. (2007) via Kumar et al. (2010) (Finished) [128]	2007	20	NA	Samples		0.0016	0.0038		0.013	ug/L	
Ambient Water			Prevalence			Magnitude					
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	210	63	Sites	30	0.00176	0.0102	0.0422	0.199	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	401	18	Sites	4.49	0.00335	0.0189	0.056	0.0658	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	611	81	Sites	13	0.00176	0.0115	0.0436	0.199	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	4		0.0142		0.01418	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	16	Sites	42	0.0085162	0.0422	0.327	0.405929	ug/L	
Bexfield et al. 2019 (Groundwater) [49]	2013 - 2015	1,106	8	Sites	0.72	0.0171232	0.0211	0.0761	0.1639527	ug/L	
Snyder et al. (2007) via Kumar et al. (2010) (Ambient) [128]	2007	20	NA	Samples		0.0014	0.0059		0.016	ug/L	
Benotti et al. (2009) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.073	ug/L	
Standley et al. (2008) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.007	ug/L	
Trenholm et al. (2006) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.01	ug/L	
Vanderford et al. (2003) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.22	ug/L	
Vanderford et al. (2006) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.594	ug/L	
Waste Water Effluent			Prevalence			Magnitude					
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	20	Sites	95	0.0341876	0.117	0.709	1.3396304	ug/L	
Trenholm et al. (2006) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						0.56	ug/L	
Vanderford et al. (2006) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						1.44	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exposure exposure		2.46E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.65279	days	
Boiling point	OPERA QSAR	255.297	degree C	
Boiling point	TEST QSAR	303.784	degree C	
Vapor pressure	OPERA QSAR	3.42E-09	mmHg	
Vapor pressure	TEST QSAR	0.000325087	mmHg	
Solubility in water	OPERA QSAR	0.0171375	mol/L	
Solubility in water	TEST QSAR	0.0240991	mol/L	
Bioconcentration factor	OPERA QSAR	1.78529	no units	
Bioconcentration factor	TEST QSAR	1.19124	no units	
Henry's Law constant	OPERA QSAR	1.04E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	0.860718	no units	

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Reference Number	Full Reference
49	Bexfield, L.M., P.L. Toccalino, K. Belitz, W.T. Foreman, and E.T. Furlong. 2019. Hormones and pharmaceuticals in groundwater used as a source of drinking water across the United States. <i>Environmental Science and Technology</i> 53: 2950-2960.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. <i>Environmental science & technology</i> , 52(23), 13972-13985.
77	FDA. 2018. Drugs @ FDA: FDA Approved Drug Products. U.S. Food and Drug Administration (FDA). https://www.accessdata.fda.gov/scripts/cder/daf/ .
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
127	Kostich, MS, et al., 2010. Predicting variability of aquatic concentrations of human pharmaceuticals. <i>Sci. Total Environ.</i> 408 (20), 4504e4510.
128	Kumar, A. and Xagorarakis, I., 2010. Human health risk assessment of pharmaceuticals in water: An uncertainty analysis for meprobamate, carbamazepine, and phenytoin. <i>Regulatory Toxicology and Pharmacology</i> , 57(2-3), pp.146-156.
150	NIH. 2018. DailyMed Database. U.S. National Library of Medicine, National Institutes of Health (NIH). https://dailymed.nlm.nih.gov/dailymed/ .
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.

Metalaxyl

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Metalaxyl
CASRN:	57837-19-1
DTXSID:	DTXSID6024175
Use:	Fungicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.000065

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	reproductive and developmental effects	9	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	700	dose-related increases in clinical signs of toxicity (e.g., post-dosing convulsions)	bottle-fed infants	OPP	2016

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.0453	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis
Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Metalaxyl

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.5	mg/kg/day	OPP 2016	Ciba-Geigy Corp. 1985	dose-related increases in clinical signs of toxicity (e.g., post-dosing convulsions)	bottle-fed infants	151	662	[369]	
Cancer Classification (CC)	NL		OPP 2016						[369]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Health-Based Screening Level	0.474	mg/L	Health-based screening levels from USGS	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	669	mg/kg	NIH HSDB	min
LD50	7120	mg/kg	NIH HSDB	max
LOAEL	30.629999	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	400	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	250	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	7.8	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	3.26	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	30.629999	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	7.8	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0090573	mol/kg	TEST QSAR	
Ames mutagenicity test	0.191	no units	TEST QSAR	
Developmental toxin test	0.606	no units	TEST QSAR	

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
		Prevalence				Magnitude					
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	5,889	367	Sites	6.23	0.00012	0.009	0.0453	3.02	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	715	277	Sites	39	0.00012	0.009	0.0426	1.48	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	5,174	90	Sites	1.74	0.00032	0.01	0.28	3.02	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	2	2,967	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	13	4	Sites	31	0.005	0.005	0.0115	0.0375	ug/L	
Bradley et al. 2018 (Finished) [53]	2016	26	2	Sites	7.69	0.0203	0.0209	0.0214	0.0215	ug/L	
Community Water System Survey (CWSS) (Finished) [178]	2006	1	NA	Sites							
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
		Prevalence				Magnitude					
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	1,407	202	Sites	14	0.00032	0.013	0.11	9.05	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3,270	61	Sites	1.87	0.00081	0.01	0.371	7.33	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	4,676	263	Sites	5.62	0.00032	0.0124	0.117	9.05	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	179	32	Sites	18	0.0042	0.005	0.0393	0.955	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	172	27	Sites	16	0.0042	0.0107	0.0589	0.955	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	7	5	Sites	71	0.005	0.005	0.0375	0.0375	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	26	0	Sites	0						
Community Water System Survey (CWSS) (Ambient) [178]	2006	1	NA	Sites			0.845	1.31		ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	8	Sites	21	0.0085	0.0437	0.116	0.1508	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	796	18	Sites	2.26	3e-04	9e-04	0.243	1.06	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Waste Water Effluent											
		Prevalence				Magnitude					
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	20	0	Sites	0						
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Expcast exposure		0.000000101	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.29311	days	
Boiling point	OPERA QSAR	299.877	degree C	
Boiling point	TEST QSAR	344.018	degree C	
Vapor pressure	OPERA QSAR	0.00000522	mmHg	
Vapor pressure	TEST QSAR	0.00000547	mmHg	
Solubility in water	OPERA QSAR	0.0163893	mol/L	
Solubility in water	TEST QSAR	0.00233884	mol/L	
Bioconcentration factor	OPERA QSAR	8.24464	no units	
Bioconcentration factor	TEST QSAR	17.1396	no units	
Henry's Law constant	OPERA QSAR	3.9E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.76605	no units	

Metalaxyl

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. <i>Environmental science & technology</i> , 52(23), 13972-13985.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
178	USEPA (US Environmental Protection Agency). (2009). 2006 Community Water System Survey. Overview, 57.
369	USEPA. 2016. Mefenoxam. Human Health Risk Assessment for Proposed Use on the Rapeseed Subgroup 20A. EPA-HQ-OPP-2015-0014-0008. DP No. D424727. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Metformin

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Metformin
CASRN:	657-24-9
DTXSID:	DTXSID2023270
Use:	antidiabetic
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0083

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	non-cancer effects	10	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	40	lowest therapeutic dose: decreases hepatic glucose production, decreases intestinal absorption of glucose, and improves insulin sensitivity by increasing peripheral glucose uptake and utilization	bottle-fed infants	FDA; NIH	2018; 2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.333	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis
Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Metformin

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.00625	mg/kg/day	FDA 2018; NIH 2018	Ascend Laboratories, LLC	lowest therapeutic dose: decreases hepatic glucose production, decreases intestinal absorption of glucose, and improves insulin sensitivity by increasing peripheral glucose uptake and utilization	bottle-fed infants	151	42.0	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels
Reference Dose (RfD) or Equivalent	0.00625	mg/kg/day	FDA 2018; NIH 2018	Ascend Laboratories, LLC	lowest therapeutic dose: decreases hepatic glucose production, decreases intestinal absorption of glucose, and improves insulin sensitivity by increasing peripheral glucose uptake and utilization	general population	33.8	150	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Maximum Recommended Daily Dose	50	mg/kg/day	FDA	
Screening level for pharmaceutical - general population	0.147058824	mg/L	EPA Office of Water	
Screening level for pharmaceutical - infants	0.041666667	mg/L	EPA Office of Water	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Percent of active toxcast in vitro assays tested	0.75	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0012106	mol/kg	TEST QSAR	
Ames mutagenicity test	0.207	no units	TEST QSAR	
Developmental toxin test			TEST QSAR	

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Metformin

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	553	70	Sites	13	0.00138	0.0275	0.333	2.64	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	75	69	Sites	92	0.00138	0.0276	0.333	2.64	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	478	1	Sites	0.21	0.00163	0.00163	0.00163	0.00163	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	205	169	Sites	82	0.0013	0.0732	0.656	13.5	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	399	11	Sites	2.76	0.00087	0.00401	0.401	0.627	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	604	180	Sites	30	0.00087	0.0721	0.633	13.5	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	25	Sites	66	0.0103849	0.41	2.05	4.3079718	ug/L	
Bexfield et al. 2019 (Groundwater) [49]	2013 - 2015	1,106	2	Sites	0.18	0.0325339	0.0356	0.0381	0.0386649	ug/L	
Benotti et al. (2007) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.092	ug/L	
Kolpin et al. (2002) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.15	ug/L	
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	19	19	Sites	100	0.0259915	1.81	28.4	35.91536	ug/L	
Benotti et al. (2007) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						47.253	ug/L	
Glassmeyer et al. (2005) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						0.698	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		1.47E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.98474	days	
Boiling point	OPERA QSAR	256.674	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	6.56E-10	mmHg	
Vapor pressure	TEST QSAR			
Solubility in water	OPERA QSAR	0.0483462	mol/L	
Solubility in water	TEST QSAR	0.530884	mol/L	
Bioconcentration factor	OPERA QSAR	1.94277	no units	
Bioconcentration factor	TEST QSAR			
Henry's Law constant	OPERA QSAR	3.46E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	0.735672	no units	

Metformin

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Reference Number	Full Reference
49	Bexfield, L.M., P.L. Toccalino, K. Belitz, W.T. Foreman, and E.T. Furlong. 2019. Hormones and pharmaceuticals in groundwater used as a source of drinking water across the United States. Environmental Science and Technology 53: 2950-2960.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. Environmental science & technology, 51(9), 4792-4802.
77	FDA. 2018. Drugs @ FDA: FDA Approved Drug Products. U.S. Food and Drug Administration (FDA). https://www.accessdata.fda.gov/scripts/cder/daf/ .
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. Science of The Total Environment. v581-582, (909-922).
127	Kostich, MS, et al., 2010. Predicting variability of aquatic concentrations of human pharmaceuticals. Sci. Total Environ. 408 (20), 4504e4510.
150	NIH. 2018. DailyMed Database. U.S. National Library of Medicine, National Institutes of Health (NIH). https://dailymed.nlm.nih.gov/dailymed/ .
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. Science of the Total Environment, 636, 69-79.

Methocarbamol

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Methocarbamol
CASRN:	532-03-6
DTXSID:	DTXSID6023286
Use:	skeletal muscle relaxant
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0025

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	non-cancer effects	9	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	100	lowest therapeutic dose:relief of discomfort associated with acute, painful musculoskeletal conditions	bottle-fed infants	FDA; NIH	2018; 2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.2468	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Methocarbamol

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.01666667	mg/kg/day	FDA 2018; NIH 2018	Granules India Ltd	lowest therapeutic dose:relief of discomfort associated with acute, painful musculoskeletal conditions	bottle-fed infants	151	110	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels
Reference Dose (RfD) or Equivalent	0.01666667	mg/kg/day	FDA 2018; NIH 2018	Granules India Ltd	lowest therapeutic dose:relief of discomfort associated with acute, painful musculoskeletal conditions	general population	33.8	390	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Maximum Recommended Daily Dose	100	mg/kg/day	FDA	
Screening level for pharmaceutical - general population	0.392156863	mg/L	EPA Office of Water	
Screening level for pharmaceutical - infants	0.111111111	mg/L	EPA Office of Water	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Percent of active toxcast in vitro assays tested	1.7	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0036141	mol/kg	TEST QSAR	
Ames mutagenicity test	0.734	no units	TEST QSAR	
Developmental toxin test	0.731	no units	TEST QSAR	

Methocarbamol
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	557	22	Sites	3.95	0.00074	0.0242	0.247	2.49	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	75	21	Sites	28	0.00074	0.026	0.259	2.49	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	482	1	Sites	0.21	0.00145	0.00145	0.00145	0.00145	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Bradley et al. 2018 (Finished) [53]	2016	26	1	Sites	3.85	0.5983694	0.598	0.598	0.5983694	ug/L	
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	207	84	Sites	41	0.00076	0.0196	0.139	0.383	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	401	6	Sites	1.5	0.00198	0.0334	0.269	0.55	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	608	90	Sites	15	0.00076	0.0196	0.139	0.55	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	8		0.0291		0.0323	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	16	Sites	42	0.0139004	0.188	0.736	2.6272938	ug/L	
Bexfield et al. 2019 (Groundwater) [49]	2013 - 2015	1,106	0	Sites	0						
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	19	Sites	90	0.0153466	0.306	0.719	7.79	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.000000165	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.48255	days	
Boiling point	OPERA QSAR	312.903	degree C	
Boiling point	TEST QSAR	362.745	degree C	
Vapor pressure	OPERA QSAR	7.2E-09	mmHg	
Vapor pressure	TEST QSAR	0.000000925	mmHg	
Solubility in water	OPERA QSAR	0.100228	mol/L	
Solubility in water	TEST QSAR	0.0132739	mol/L	
Bioconcentration factor	OPERA QSAR	1.10629	no units	
Bioconcentration factor	TEST QSAR	2.10863	no units	
Henry's Law constant	OPERA QSAR	5.9E-10	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	0.65558	no units	

Methocarbamol

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Reference Number	Full Reference
49	Bexfield, L.M., P.L. Toccalino, K. Belitz, W.T. Foreman, and E.T. Furlong. 2019. Hormones and pharmaceuticals in groundwater used as a source of drinking water across the United States. <i>Environmental Science and Technology</i> 53: 2950-2960.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. <i>Environmental science & technology</i> , 52(23), 13972-13985.
77	FDA. 2018. Drugs @ FDA: FDA Approved Drug Products. U.S. Food and Drug Administration (FDA). https://www.accessdata.fda.gov/scripts/cder/daf/ .
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
150	NIH. 2018. DailyMed Database. U.S. National Library of Medicine, National Institutes of Health (NIH). https://dailymed.nlm.nih.gov/dailymed/ .
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.

Methomyl

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Methomyl
CASRN:	16752-77-5
DTXSID:	DTXSID1022267
Use:	Insecticide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	X
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	1.5

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	reproductive and developmental effects	1	6

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	2	increases in peak red blood cell acetylcholinesterase inhibition in human	bottle-fed infants	OPP	2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
2.92	90th Percentile	Finished Water	UCM2	1993-1997

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Methomyl

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0015	mg/kg/day	OPP 2018	McFarlane 1998	increases in peak red blood cell acetylcholinesterase inhibition in human	bottle-fed infants	151	1.99	[403]	
Cancer Classification (CC)	NL		OPP 2018						[403]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	0.3	mg/L	EPA DWSHA 2018	
Lifetime Health Advisory	0.2	mg/L	EPA DWSHA 2018	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	10	mg/kg	NIH HSDB	min
LD50	45	mg/kg	NIH HSDB	max
LOAEL	10	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	56.5	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	2.5	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	38.8	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	2.28	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	12.5	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	2.5	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0002421	mol/kg	TEST QSAR	
Ames mutagenicity test	0.871	no units	TEST QSAR	
Developmental toxin test	0.501	no units	TEST QSAR	

Nationally Represented

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	43	902,435	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Nationally Representative Water Data												Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes	
<i>Finished Water</i>																							
Drinking Water Monitoring Data - CA (Finished)												2006 - 2020	169	0	Sites	0							
Drinking Water Monitoring Data - MA (Finished)												2006 - 2020	820	0	Sites	0							
Drinking Water Monitoring Data - WA (Finished)												2006 - 2011	255	0	Sites	0							
USDA Pesticide Data Program (PDP) (Finished)												2001 - 2013	17	0	Sites	0							
<i>Ambient Water</i>																							
Drinking Water Monitoring Data - CA (Source)												2006 - 2020	1,740	0	Sites	0							
Drinking Water Monitoring Data - MA (Source)												2006 - 2020	77	0	Sites	0							
Drinking Water Monitoring Data - PA (Source)												2006 - 2011	1	0	Sites	0							
Drinking Water Monitoring Data - WA (Source)												2006 - 2011	422	0	Sites	0							
Drinking Water Monitoring Data - WI (Source)												2012-2019	92	0	Sites	0							
National Water Information System (USGS NWIS) (Surface Water)												2008 - 2017	475	18	Sites	3.79	0.00024	0.00504	0.056	0.295	ug/L		
National Water Information System (USGS NWIS) (Groundwater)												2008 - 2017	1,051	3	Sites	0.29	0.009	0.011	0.0537	0.072	ug/L		
National Water Information System (USGS NWIS) (All Water)												2008 - 2017	1,526	21	Sites	1.38	0.00024	0.00797	0.0672	0.295	ug/L		
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)												2001 - 2013	229	1	Sites	0.44	0.0122	0.0122	0.0122	0.0122	ug/L		
USDA Pesticide Data Program (PDP) (Groundwater)												2001 - 2013	219	0	Sites	0							
USDA Pesticide Data Program (PDP) (Untreated)												2001 - 2013	12	1	Sites	8.33	0.0122	0.0122	0.0122	0.0122	ug/L		
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]												1990 - 2018	6,790	539	Sites	7.94	0.021	0.211	1.64	55.3	ug/L		
Bradley et al. 2017 (Ambient) [52]												2012 - 2014	38	1	Sites	2.63	0.0282	0.0282	0.0282	0.0282	ug/L		
Arnold et al. 2016 (Filtered) [7]												2012 - 2013	690	4	Sites	0.58	3e-04	0.0024	0.00778	0.01	ug/L		
<i>Waste Water Effluent</i>																							
Estimated Concentration in Water												Date	Source	Value	Units	Model	Notes						

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.54233	days	
Boiling point	OPERA QSAR	230.04	degree C	
Boiling point	TEST QSAR	204.528	degree C	
Vapor pressure	OPERA QSAR	0.0000114	mmHg	
Vapor pressure	TEST QSAR	0.000257632	mmHg	
Solubility in water	OPERA QSAR	0.237365	mol/L	
Solubility in water	TEST QSAR	0.201837	mol/L	
Bioconcentration factor	OPERA QSAR	3.54556	no units	
Bioconcentration factor	TEST QSAR	2.29615	no units	
Henry's Law constant	OPERA QSAR	2.02E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	0.58656	no units	

Methomyl

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
403	USEPA. 2018. Methomyl and Thiodicarb: Draft Human Health Risk Assessment in Support of Registration Review. EPA-HQ-OPP-2009-0432-0017. DP Nos. D420613 D439094. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Methyl mercury

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Methyl mercury
CASRN:	22967-92-6
DTXSID:	DTXSID9024198
Use:	Fungicide and seedborne diseases, as timber preservatives, and disinfectants
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	
Human Neurotoxicants	X
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	X

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.00095

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	reproductive and developmental effects	10	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.4	Developmental neuropsychological impairment	lactating women	IRIS	2001

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.00038	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis
Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Methyl mercury

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0003	mg/kg/day	ATSDR 1999; 2013	Davidson et al. 1998	Effects of prenatal and postnatal methylmercury exposure from fish consumption on neurodevelopment:	lactating women	46.9	1.28	[15] [33]	
Reference Dose (RfD) or Equivalent	0.0001	mg/kg/day	IRIS 2001	Grandjean et al., 1997; Budtz-Jørgensen et al., 1999a	Developmentalneuropsychological impairment	lactating women	46.9	0.426	[242]	
Cancer Classification (CC)	C		IRIS 2001						[242]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Systemic, Neurological	0.000913	Li, 2018	Neurological, Hepatic, Renal, Systemic	4	Abdalla, 2012	2012-03-01	2020-01-15	2245	31	125	17

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Cancer Classification (CC)	2B	no units	WHO IARC	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	58	mg/kg	NIH HSDB	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity test			TEST QSAR	
Developmental toxin test			TEST QSAR	

Methyl mercury

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	510	416	Sites	82	4.00E - 05	0.00011	0.00038	2	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	447	384	Sites	86	4.00E - 05	0.00011	0.000345	0.00406	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	63	32	Sites	51	4.00E - 05	0.00027	0.0013	2	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	552	469	Sites	85	1.00E - 05	0.00019	0.0018	0.22	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	26	18	Sites	69	5.00E - 05	0.00017	0.000536	0.0013	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	573	484	Sites	84	1.00E - 05	0.00019	0.0018	0.22	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exposure exposure			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Methyl mercury

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
15	ATSDR. 1999. TOXICOLOGICAL PROFILE FOR MERCURY. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
33	ATSDR. 2013. Addendum to the Toxicological Profile for Mercury (Alkyl and Dialkyl compounds). U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA
242	USEPA. 2001. Chemical Assessment Summary Methylmercury. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, DC.

Methyl tert-butyl ether (MTBE)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Methyl tert-butyl ether (MTBE)
CASRN:	1634-04-4
DTXSID:	DTXSID3020833
Use:	Octane booster in gasoline; manufacture of isobutene; extraction solvent
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	1.7

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
	no adverse effects	5	8

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	20	organoleptic endpoint		OW	1997

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
34.6	90th Percentile	Finished Water	UCMR1	2001-2003

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X	X	X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		
Not Applicable		

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Methyl tert-butyl ether (MTBE)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
			WHO 2005						[440]	
			OW 1997						[226]	NOTE: The MTBE Health Advisory notes that keeping levels of contamination MTBE in the range of 20 to 40 ug/L or below would protect consumer acceptance of the water resource and would also provide a large margin of exposure (safety) from toxic effects.
			HC 2006						[99]	
			ATSDR 1996						[12]	
			CALEPA 1999						[56]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Hematological, Cardiovascular	0.0055	Saeedi, 2017b	Nervous, Respiratory,	1600	Dong-mei, 2009	2005-01-01	2020-01-15	909	9	10	8

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Health-Based Guidance Value	0.7	mg/L	MN DOH	
Acute inhalation Minimal Risk Level (MRL)	2	ppm	CDC ATSDR	
Acute Minimal Risk Level (MRL)	0.4	mg/kg/day	CDC ATSDR	
Cancer Classification (CC)	3	no units	WHO IARC	
Cancer Slope Factor (CSF)	0.0018	(mg/kg/day)^-1	CalEPA OEHHA Chemical Database	
Chronic Health-Based Guidance Value	0.7	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.006	mg/L	MN DOH	
Chronic inhalation Minimal Risk Level (MRL)	0.7	ppm	CDC ATSDR	
Inhalation Unit Risk (IUR)	0.00000026	ug/m^3	CalEPA OEHHA Chemical Database	
Intermediate Inhalation Minimal Risk Level (MRL)	0.7	ppm	CDC ATSDR	
Intermediate Minimal Risk Level (MRL)	0.3	mg/kg/day	CDC ATSDR	
Public Health Goal	0.013	mg/L	CalEPA OEHHA Public Health Goals	
Reference Concentration (RfC)	3	mg/m^3	EPA IRIS	
Reference Concentration (RfC)	8000	ug/m^3	CalEPA OEHHA Chemical Database	
Short-Term/Subchronic Health-Based Guidance Value	0.7	mg/L	MN DOH	
Maximum Allowable Concentration (MAC)	None	no units	Canadian Drinking Water Guidelines	

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	4000	mg/kg	NIH HSDB	
Percent of active toxcast in vitro assays tested	2.13	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0128233	mol/kg	TEST QSAR	
Ames mutagenicity test	0.033	no units	TEST QSAR	
Developmental toxin test	0.384	no units	TEST QSAR	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
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EPA - Office of Water

Methyl tert-butyl ether (MTBE)
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003	3,871	19	Sites	0.49	5	9.2	34.6	49	ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	7,709	870	Sites	11	0.01	0.21	3.47	23000	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	263	122	Sites	46	0.01	0.24	1.81	81.3	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	7,446	748	Sites	10	0.01	0.2	6.3	23000	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)	34	1,740,624	Chemical Data Reporting (CDR) Results (EPA) (2016)	1B - 5B

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	495	13	Sites	2.63	0.024	1.8	4.4	55	ug/L	
Drinking Water Monitoring Data - MA (Finished)	2006 - 2020	926	231	Sites	25	0.5	1.3	8.1	265	ug/L	
Community Water System Survey (CWSS) (Finished) [178]	2006	1	NA	Sites			0.5	5		ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	4,763	70	Sites	1.47	0.06	6.22	36	1900	ug/L	
Drinking Water Monitoring Data - FL (Source)	2006 - 2011	5	4	Sites	80	0.14	0.52	1.6	3.7	ug/L	
Drinking Water Monitoring Data - MA (Source)	2006 - 2020	138	46	Sites	33	0.5	4.2	101	880	ug/L	
Drinking Water Monitoring Data - PA (Source)	2006 - 2011	24	14	Sites	58	0.2	6	1300	61000	ug/L	
Drinking Water Monitoring Data - WI (Source)	2012-2019	101	1	Sites	0.99	39	73.5	101	108	ug/L	
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	283	21	Sites	7.42	0.01	0.05	0.189	0.97	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	4,403	312	Sites	7.09	0.01	0.16	1.56	1080	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	4,683	333	Sites	7.11	0.01	0.15	1.38	1080	ug/L	
Community Water System Survey (CWSS) (Ambient) [178]	2006	1	NA	Sites			1.05	5.2		ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	4	Sites	11	0.01845	0.0237	0.0388	0.04319	ug/L	
Arnold et al. 2016 (Unfiltered) [7]	2012 - 2013	685	55	Sites	8.03	0.01	0.06	0.765	4.47	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.000000122	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)	< LOD	pg/ml	
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	7.21225	days	
Boiling point	OPERA QSAR	58.0708	degree C	
Boiling point	TEST QSAR	68.237	degree C	
Vapor pressure	OPERA QSAR	316.295	mmHg	
Vapor pressure	TEST QSAR	215.278	mmHg	
Solubility in water	OPERA QSAR	0.330721	mol/L	
Solubility in water	TEST QSAR	0.290402	mol/L	
Bioconcentration factor	OPERA QSAR	2.51817	no units	
Bioconcentration factor	TEST QSAR	4.0738	no units	
Henry's Law constant	OPERA QSAR	0.000937822	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.0899	no units	

Methyl tert-butyl ether (MTBE)

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
12	ATSDR. 1996. Toxicological Profile for Methyl tert-Butyl Ether. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
56	CalEPA. 1999. Public Health Goal for Methyl Tertiary Butyl Ether (MTBE) in Drinking Water. California Environmental Protection Agency (CalEPA), Office of Environmental Health Hazard Assessment, Pesticide and Environmental Toxicology Section, Sacramento, CA.
99	Health Canada. 2006. Guidelines for Canadian Drinking Water Quality: Guideline Technical Document Methyl Tertiary-Butyl Ether. Health Canada (HC), Ottawa, Ontario, Canada.
178	USEPA (US Environmental Protection Agency). (2009). 2006 Community Water System Survey. Overview, 57.
226	USEPA. 1997. Drinking Water Advisory: Consumer Acceptability Advice and Health Effects Analysis on Methyl Tertiary-Butyl Ether (MtBE). U.S. Environmental Protection Agency, Office of Water, Health and Ecological Criteria Division, Washington, DC.
440	WHO. 2005. Methyl tertiary-Butyl Ether (MTBE) in Drinking-water Background document for development of WHO Guidelines for Drinking-water Quality. World Health Organization (WHO), Geneva, Switzerland.

Metolachlor ethanesulfonic acid (ESA)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Metolachlor ethanesulfonic acid (ESA)
CASRN:	171118-09-5
DTXSID:	DTXSID1037567
Use:	Pesticide degradate
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0013

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	non-cancer effects	8	7

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	2000	increased liver weight and increased serum liver enzymes	general population	MDH	2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
2.619857	90th Percentile	Finished Water	UCMR2	2008-2010

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X	X	X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Metolachlor ethanesulfonic acid (ESA)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.07	mg/kg/day	CALEPA 2017	Altmann 1999	changes in clinical chemistry data and absolute liver weight	general population	33.8	414	[61]	
Reference Dose (RfD) or Equivalent	0.27	mg/kg/day	MDH 2018	Altmann 1999	increased liver weight and increased serum liver enzymes	general population	33.8	1600	[144]	

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Chronic Health-Based Guidance Value	0.8	mg/L	MN DOH	
Short-Term/Subchronic Health-Based Guidance Value	4	mg/L	MN DOH	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Percent of active toxcast in vitro assays tested	1.77	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0101625	mol/kg	TEST QSAR	
Ames mutagenicity test	0.62	no units	TEST QSAR	
Developmental toxin test	1.269	no units	TEST QSAR	

Technical Support Document for the
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EPA - Office of Water

Metolachlor ethanesulfonic acid (ESA)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
			Prevalence					Magnitude			
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010	1,198	19	Sites	1.59	1	1.44	2.62	3.95455	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
			Prevalence					Magnitude			
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	2,722	915	Sites	34	0.0036	0.284	1.66	35	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	422	312	Sites	74	0.0036	0.28	1.51	8.4	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	2,300	603	Sites	26	0.0048	0.315	4.92	35	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
			Prevalence					Magnitude			
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	4	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	14	Sites	82	6e-04	0.054	0.69	2.5	ug/L	
Bradley et al. 2018 (Finished) [53]	2016	26	7	Sites	27	0.02	0.027	0.212	0.23	ug/L	
Community Water System Survey (CWSS) (Finished) [178]	2006	1	NA	Sites			2.35	2.35		ug/L	
Ambient Water											
			Prevalence					Magnitude			
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	2	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	355	169	Sites	48	0.0075	0.182	0.827	2.89	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	830	290	Sites	35	0.0123	0.291	2.2	14.8	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,185	459	Sites	39	0.0075	0.208	1.25	14.8	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	193	Sites	84	0.000599	0.066	0.735	18	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	186	Sites	85	0.000599	0.0528	0.87	18	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	9	Sites	75	6e-04	0.0735	0.716	3.603	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	56	33	Sites	59	0.05	0.128	0.272	0.502	ug/L	
Community Water System Survey (CWSS) (Ambient) [178]	2006	1	NA	Sites			1.55	6.01		ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	22	Sites	58	0.02	0.125	0.416	1	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	106	Sites	18	0.0048	0.338	3.48	31.1	ug/L	
Waste Water Effluent											
			Prevalence					Magnitude			
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg- bw/day)	Notes
Expcast exposure		0.000000125	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.64024	days	
Boiling point	OPERA QSAR	314.443	degree C	
Boiling point	TEST QSAR	404.135	degree C	
Vapor pressure	OPERA QSAR	5.03E-08	mmHg	
Vapor pressure	TEST QSAR			
Solubility in water	OPERA QSAR	0.0102496	mol/L	
Solubility in water	TEST QSAR	0.00190108	mol/L	
Bioconcentration factor	OPERA QSAR	9.61626	no units	
Bioconcentration factor	TEST QSAR	9.95405	no units	
Henry's Law constant	OPERA QSAR	4.27E-10	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.49063	no units	

Metolachlor ethanesulfonic acid (ESA)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. <i>Environmental science & technology</i> , 52(23), 13972-13985.
61	CalEPA. 2017. Public Health Concentration: Metolachlor and Metolachlor Degradates Ethanesulfonic Acid and Oxanilic Acid in Groundwater. California Environmental Protection Agency (CalEPA), Office of Environmental Health Hazard Assessment, Pesticide and Environmental Toxicology Branch, Sacramento, CA.
144	MDH. 2018. Toxicological Summary for: Metolachlor ESA. Health Based Guidance for Water. Minnesota Department of Health (MDH), Environmental Health Division, Health Risk Assessment Unit, St Paul, MN.
178	USEPA (US Environmental Protection Agency). (2009). 2006 Community Water System Survey. Overview, 57.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Metolachlor oxanilic acid (OA)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Metolachlor oxanilic acid (OA)
CASRN:	152019-73-3
DTXSID:	DTXSID6037568
Use:	Pesticide degradate
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0017

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	non-cancer effects	1	8

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	2000	changes in blood chemistry parameters without identified specific target organs	general population	MDH	2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
3.4468	90th Percentile	Finished Water	UCMR2	2008-2010

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X	X	X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Metolachlor oxanilic acid (OA)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.17	mg/kg/day	CALEPA 2017	Lees 2004	changes in clinic chemistry data	general population	33.8	1010	[61]	
Reference Dose (RfD) or Equivalent	0.27	mg/kg/day	MDH 2018	Syngenta 2004	changes in blood chemistry parameters without identified specific target organs	general population	33.8	1600	[145]	

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Health-Based Guidance Value	3	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.8	mg/L	MN DOH	
Short-Term/Subchronic Health-Based Guidance Value	3	mg/L	MN DOH	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Percent of active toxcast in vitro assays tested	0.72	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0094624	mol/kg	TEST QSAR	
Ames mutagenicity test	0.353	no units	TEST QSAR	
Developmental toxin test	0.732	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Metolachlor oxanilic acid (OA)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010	1,198	1	Sites	0.08	2.502	3.08	3.45	3.539	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
		Prevalence				Magnitude					
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	2,723	500	Sites	18	0.01	0.245	1.02	19	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	423	234	Sites	55	0.01	0.244	0.942	12	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	2,300	266	Sites	12	0.02	0.28	1.97	19	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	4	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	13	Sites	76	0.003	0.036	0.315	4.42	ug/L	
Bradley et al. 2018 (Finished) [53]	2016	26	4	Sites	15	0.03	0.155	0.332	0.38	ug/L	
Community Water System Survey (CWSS) (Finished) [178]	2006	1	NA	Sites			1.77	1.77		ug/L	
Ambient Water											
		Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	2	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	355	110	Sites	31	0.012	0.17	0.508	2.5	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	830	160	Sites	19	0.02	0.19	1.5	19.6	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,185	270	Sites	23	0.012	0.178	0.738	19.6	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	181	Sites	79	0.003	0.04	0.29	4.36	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	174	Sites	79	0.003	0.0213	0.214	4.36	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	9	Sites	75	0.003	0.0565	0.311	1.5	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	56	22	Sites	39	0.05	0.062	0.0924	0.113	ug/L	
Community Water System Survey (CWSS) (Ambient) [178]	2006	1	NA	Sites			1.08	5.14		ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	16	Sites	42	0.02	0.04	0.205	0.66	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	30	Sites	5.14	0.051	0.314	1.84	17.6	ug/L	
Waste Water Effluent											
		Prevalence				Magnitude					
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Expocast exposure		0.000000119	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.35407	days	
Boiling point	OPERA QSAR	319.319	degree C	
Boiling point	TEST QSAR	356.287	degree C	
Vapor pressure	OPERA QSAR	0.000000191	mmHg	
Vapor pressure	TEST QSAR	0.000000653	mmHg	
Solubility in water	OPERA QSAR	0.00424338	mol/L	
Solubility in water	TEST QSAR	0.00225944	mol/L	
Bioconcentration factor	OPERA QSAR	2.91419	no units	
Bioconcentration factor	TEST QSAR	1.57398	no units	
Henry's Law constant	OPERA QSAR	8.32E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.6119	no units	

Metolachlor oxanilic acid (OA)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. <i>Environmental science & technology</i> , 52(23), 13972-13985.
61	CalEPA. 2017. Public Health Concentration: Metolachlor and Metolachlor Degradates Ethanesulfonic Acid and Oxanilic Acid in Groundwater. California Environmental Protection Agency (CalEPA), Office of Environmental Health Hazard Assessment, Pesticide and Environmental Toxicology Branch, Sacramento, CA.
145	MDH. 2018. Toxicological Summary for: Metolachlor OXA. Health Based Guidance for Water. Minnesota Department of Health (MDH), Environmental Health Division, Health Risk Assessment Unit, St Paul, MN.
178	USEPA (US Environmental Protection Agency). (2009). 2006 Community Water System Survey. Overview, 57.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Metoprolol

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Metoprolol
CASRN:	51384-51-1
DTXSID:	DTXSID2023309
Use:	beta-1 blocking agent that is commonly used to treat ANGINA PECTORIS; HYPERTENSION; and CARDIAC ARRHYTHMIAS
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.18

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	non-cancer effects	8	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	0.7	lowest therapeutic dose: treatment of hypertension	bottle-fed infants	FDA; NIH	2018; 2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.126	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Metoprolol

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.000104167	mg/kg/day	FDA 2018; NIH 2018	Ethex Corporation	lowest therapeutic dose: treatment of hypertension	bottle-fed infants	151	0.690	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels
Reference Dose (RfD) or Equivalent	0.000104167	mg/kg/day	FDA 2018; NIH 2018	Ethex Corporation	lowest therapeutic dose: treatment of hypertension	general population	33.8	2.50	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References Identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
							2020-01-28	3342			

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Maximum Recommended Daily Dose	6.67	mg/kg/day	FDA	
Screening level for pharmaceutical - general population	0.00245098	mg/L	EPA Office of Water	
Screening level for pharmaceutical - infants	0.000694444	mg/L	EPA Office of Water	

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1158	mg/kg	NIH HSDB	min
LD50	3090	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	2.99	percent	EPA Chemistry Dashboard	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0121339	mol/kg	TEST QSAR	
Ames mutagenicity test	0.04	no units	TEST QSAR	
Developmental toxin test	0.497	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
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EPA - Office of Water

Metoprolol
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data											
Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	557	13	Sites	2.33	0.00147	0.0156	0.126	0.416	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	75	12	Sites	16	0.00147	0.0169	0.128	0.416	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	482	1	Sites	0.21	0.00196	0.00196	0.00196	0.00196	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data											
Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	12		0.0085		0.0184	ug/L	
Padhye et al. 2013 (Finished) [155]	2009 - 2010	8	1	Samples	12	0	0		1e-07 +/- 0	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	205	55	Sites	27	0.00146	0.00776	0.171	0.521	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	401	3	Sites	0.75	0.0668	0.123	0.164	0.182	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	606	58	Sites	9.57	0.00146	0.0083	0.176	0.521	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	32		0.0114		0.0378	ug/L	
Batt et al. 2016 (Ambient) [46]	2008 - 2009	182	73	Sites	40	0.0043	0.0175	0.0751	0.2177	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	16	Sites	42	0.0020983	0.0637	0.116	0.3671431	ug/L	
Bexfield et al. 2019 (Groundwater) [49]	2013 - 2015	1,106	0	Sites	0						
Padhye et al. 2013 (Ambient) [155]	2009 - 2010	8	8	Samples	100	1e-07 +/- 0	1e-07		3e-07 +/- 1e-07	ug/L	
Batt et al. (2008) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.012	ug/L	
Fono et al. (2006) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.571	ug/L	
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	21	Sites	100	0.0201093	0.173	0.654	6.989373	ug/L	
Kostich et al. 2014 (Wastewater) [126]	not reported	50	49	Sites	98	0.1077	0.398	0.723	1.1692	ug/L	
Batt et al. (2008) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						0.65	ug/L	
Conkle et al. (2008) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						0.211	ug/L	
Fono et al. (2006) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						2.269	ug/L	
Hugget et al. (2003) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						1.2	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exposure assessment			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.35452	days	
Boiling point	OPERA QSAR	311.409	degree C	
Boiling point	TEST QSAR	361.85	degree C	
Vapor pressure	OPERA QSAR	0.000000498	mmHg	
Vapor pressure	TEST QSAR	0.0000013	mmHg	
Solubility in water	OPERA QSAR	0.0459364	mol/L	
Solubility in water	TEST QSAR	0.0223357	mol/L	
Bioconcentration factor	OPERA QSAR	17.2182	no units	
Bioconcentration factor	TEST QSAR	32.8852	no units	
Henry's Law constant	OPERA QSAR	0.000000126	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.93639	no units	

Metoprolol

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
46	Batt, A. L., Kincaid, T. M., Kostich, M. S., Lazorchak, J. M., & Olsen, A. R. (2016). Evaluating the extent of pharmaceuticals in surface waters of the United States using a National-scale Rivers and Streams Assessment survey. <i>Environmental toxicology and chemistry</i> , 35(4), 874-881.
49	Bexfield, L.M., P.L. Toccalino, K. Belitz, W.T. Foreman, and E.T. Furlong. 2019. Hormones and pharmaceuticals in groundwater used as a source of drinking water across the United States. <i>Environmental Science and Technology</i> 53: 2950-2960.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
77	FDA. 2018. Drugs @ FDA: FDA Approved Drug Products. U.S. Food and Drug Administration (FDA). https://www.accessdata.fda.gov/scripts/cder/daf/ .
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
126	Kostich MS, et al. 2014 Concentrations of prioritized pharmaceuticals in effluents from 50 large wastewater treatment plants in the US and implications for risk estimation. <i>Environ Pollut</i> . 2014 Jan;184:354-9. doi: 10.1016/j.envpol.2013.09.013. Epub 2013 Oct 3. PMID: 24095705.
127	Kostich, MS, et al., 2010. Predicting variability of aquatic concentrations of human pharmaceuticals. <i>Sci. Total Environ</i> . 408 (20), 4504e4510.
150	NIH. 2018. DailyMed Database. U.S. National Library of Medicine, National Institutes of Health (NIH). https://dailymed.nlm.nih.gov/dailymed/ .
155	Padhye, L.P., Yao, H., Kung'u, F.T., and Huang, C.H. Year-long evaluation on the occurrence and fate of pharmaceuticals, personal care products, and endocrine disrupting chemicals in an urban drinking water treatment plant. 2014. <i>Water Research</i> 51 (2014) 266-276.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.

Metribuzin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Metribuzin
CASRN:	21087-64-9
DTXSID:	DTXSID6024204
Use:	Herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.013

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	non-cancer effects	1	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	8	increased thyroid and liver weights, thyroid follicular cell hyperplasia	general population	OPP	2017

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.1	90th Percentile	Finished Water	UCM2	1993-1997

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X			

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
X	Not Applicable	Not Applicable
Basis		

Metribuzin may cause adverse health effects at high doses, as evidences has shown from animal studies, but its occurrence in public water systems and the numbers of people potentially exposed through drinking water are low [a,b,c,d,e]. Therefore, metribuzin may not occur in drinking water at frequencies that are of public health concern or that regulation represents a meaningful opportunity for health risk reduction in persons served by public water systems [a,b,c,d,e].

[a] USEPA, 1998 [184]; [b] Kolpin, Barbash, & Gilliom, 1998 [124]; [c] USEPA, 2001 [239]; [d] USEPA, 2001 [247]; [e] USEPA, 2003 [186]; as cited in USEPA, 2001 [181]

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Metribuzin

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0013	mg/kg/day	OPP 2017	Christenson & Wahle, 1993	increased thyroid and liver weights, thyroid follicular cell hyperplasia, decreased body weight and body weight gains	general population	33.8	7.69	[386]	
Cancer Classification (CC)	D		OPP 2017						[386]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	5	mg/L	EPA DWSHA 2018	
Acute Health-Based Guidance Value	0.01	mg/L	MN DOH	
Acute Health-Based Guidance Value	0.03	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.01	mg/L	MN DOH	
Lifetime Health Advisory	0.07	mg/L	EPA DWSHA 2018	
Maximum Allowable Concentration (MAC)	0.08	mg/L	Canadian Drinking Water Guidelines	
Short-Term/Subchronic Health-Based Guidance Value	0.01	mg/L	MN DOH	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	2200	mg/kg	NIH HSDB	max
LD50	250	mg/kg	NIH HSDB	min
LOAEL	200	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	7.5	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	1.5	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	70	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	3.22	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	3	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	1.25	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0042658	mol/kg	TEST QSAR	
Ames mutagenicity test	0.63	no units	TEST QSAR	
Developmental toxin test	0.056	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Metribuzin
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997	13,512	1	Sites	0.01	0.1	0.1	0.1	0.1	ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
		Prevalence				Magnitude					
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	11,379	606	Sites	5.33	0.001	0.02	0.17	15.6	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	2,318	466	Sites	20	0.001	0.0205	0.17	15.6	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	9,062	140	Sites	1.54	0.002	0.013	0.204	3.69	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	48	5,804,692	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	8	15,725	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	182	0	Sites	0						
Drinking Water Monitoring Data - MA (Finished)	2006 - 2020	822	1	Sites	0.12	0.1	0.1	0.1	0.1	ug/L	
Drinking Water Monitoring Data - WA (Finished)	2006 - 2011	822	1	Sites	0.12	0.05	0.085	0.223	0.28	ug/L	
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	15	3	Sites	20	0.0107	0.257	1.63	3.76	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
		Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	2,171	0	Sites	0						
Drinking Water Monitoring Data - MA (Source)	2006 - 2020	78	0	Sites	0						
Drinking Water Monitoring Data - WA (Source)	2006 - 2011	997	0	Sites	0						
Drinking Water Monitoring Data - WI (Source)	2012-2019	92	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	965	151	Sites	16	0.0018	0.0319	0.146	6.7	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3,126	43	Sites	1.38	0.002	0.0105	0.0286	0.319	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	4,090	194	Sites	4.74	0.0018	0.028	0.139	6.7	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	226	3	Sites	1.33	0.0107	0.106	2.4	29.742	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	218	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	9	3	Sites	33	0.0107	0.106	2.4	29.742	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	1,320	27	Sites	2.05	0.006	0.012	0.0394	0.182	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	3	Sites	7.89	0.0159	0.0184	0.436	0.541	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	4	Sites	0.58	0.0038	0.292	0.628	0.651	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Waste Water Effluent											
		Prevalence				Magnitude					
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Expocast exposure		0.000000012	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.7541	days	
Boiling point	OPERA QSAR	299.501	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.000000949	mmHg	
Vapor pressure	TEST QSAR			
Solubility in water	OPERA QSAR	0.00612378	mol/L	
Solubility in water	TEST QSAR	0.00851138	mol/L	
Bioconcentration factor	OPERA QSAR	2.56621	no units	
Bioconcentration factor	TEST QSAR			
Henry's Law constant	OPERA QSAR	2.17E-09	atm-m^3/mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.70267	no units	

Metribuzin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
124	Kolpin, D.W., J.E. Barbash, and R.J. Gilliom. 1998. Occurrence of Pesticides in Shallow Groundwater of the United States: Initial Results from the National Water Quality Assessment Program. <i>Env. Sci. Tech.</i> 32:558-566.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
181	USEPA, 2001. Regulatory Determination Support Document for Metribuzin. EPA 815 R-01-010.
184	USEPA. 1998. R.E.D. Facts: Metribuzin. EPA Report 738-F-96-006. 7 pp. Available on the Internet at: http://www.epa.gov/oppsrrd1/REDS/ Last modified: 8/29/2000.
186	USEPA. 2003. Health Effects Support Document for Metribuzin. Office of Water. EPA Report 822-R-03-004. February 2003. 84 pp.
239	USEPA. 2001. Analysis of National Occurrence of the 1998 Contaminant Candidate List Regulatory Determination Priority Contaminants in Public Water Systems. Office of Water. EPA report 815-D-01-002. 77 pp.
247	USEPA. 2001. Occurrence of Unregulated Contaminants in Public Water Systems: An Initial Assessment. Office of Water. EPA report 815-P-00-001. Office of Water. 50 pp.
386	USEPA. 2017. Metribuzin: Draft Risk Assessment for Registration Review. EPA-HQ-OPP-2012-0487-0022. DP No. D432005. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Molybdenum

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Molybdenum
CASRN:	7439-98-7
DTXSID:	DTXSID1024207
Use:	Use data for molybdenum trioxide: As steel alloy; chemical reagent; naturally-occurring
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.25

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	non-cancer effects	10	7

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	30	increased uric acid levels	general population	IRIS	1992

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
7.5	90th Percentile	Finished Water	UCMR3	2013-2015

PUBLIC NOMINATION STATUS

Public Nomination
X

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
		X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Molybdenum

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.07	mg/L	WHO 2011	Chappell et al. 1979	altered urinary levels of molybdenum and copper, altered serum levels of uric acid and ceruloplasmin	general population	33.8	414	[442]	
Reference Dose (RfD) or Equivalent	0.005	mg/kg/day	IRIS 1992	Koval'skiy et al., 1961	increased uric acid levels	general population	33.8	29.6	[215]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Endocrine, Immune, Neurological	5	Murray 2019	Reproductive, Renal,	40	Murray 2019	2016-04-01	2020-02-13	1086	2	34	1

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	0.08	mg/L	EPA DWSHA 2018	
Chronic inhalation Minimal Risk Level (MRL)	0.0004	mg/m³	CDC ATSDR	
Lifetime Health Advisory	0.04	mg/L	EPA DWSHA 2018	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity test			TEST QSAR	
Developmental toxin test			TEST QSAR	

July 2021

Scoring Data

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	10M - 50M

Non-Storing Data											
Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water			Prevalence				Magnitude				
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	81	57	Sites	70	0.011	2.58	7.1	55	ug/L	
Bradley et al. 2018 (Finished) [53]	2016	26	21	Sites	81	0.09	0.65	2.1	10.58	ug/L	
Community Water System Survey (CWSS) (Finished) [178]	2006	2	NA	Sites			16	31		ug/L	
Ambient Water			Prevalence				Magnitude				
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	173	127	Sites	73	0.11	3.27	10	230	ug/L	
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	1,379	1,188	Sites	86	0.01	0.602	4.09	1137	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	6,146	5,571	Sites	91	0.01	1.76	11	28000	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	7,514	6,751	Sites	90	0.01	1.02	7.1	28000	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	757	658	Sites	87	0.014	0.544	7	110	ug/L	
Waste Water Effluent			Prevalence				Magnitude				
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)	107	µg/l	

UCMB 4 data used in the draft CCI 5 is a partial dataset and will be complete in Dec. 2020.

Molybdenum

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. Environmental science & technology, 52(23), 13972-13985.
178	USEPA (US Environmental Protection Agency). (2009). 2006 Community Water System Survey. Overview, 57.
215	USEPA. 1992. Chemical Assessment Summary, Molybdenum. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, D.C.
442	WHO. 2011. Molybdenum in Drinking-water. Background document for development of WHO Guidelines for Drinking-water Quality. World Health Organization (WHO), Geneva, Switzerland.

Morphine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Morphine
CASRN:	57-27-2
DTXSID:	DTXSID9023336
Use:	narcotic analgesic
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.091

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	non-cancer effects	1	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	0.8	lowest therapeutic dose:severe pain management	bottle-fed infants	FDA; NIH	2018; 2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.07293	90th Percentile	All Ambient Water	NWIS	2008-2017

PUBLIC NOMINATION STATUS

Public Nomination
X

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Morphine

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.000125	mg/kg/day	FDA 2018; NIH 2018	Actavis Pharma, Inc.	lowest therapeutic dose:severe pain management	bottle-fed infants	151	0.830	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug
Reference Dose (RfD) or Equivalent	0.000125	mg/kg/day	FDA 2018; NIH 2018	Actavis Pharma, Inc.	lowest therapeutic dose:severe pain management	general population	33.8	2.90	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Maximum Recommended Daily Dose	1.67	mg/kg/day	FDA	
Screening level for pharmaceutical - general population	0.002941176	mg/L	EPA Office of Water	
Screening level for pharmaceutical - infants	0.000833333	mg/L	EPA Office of Water	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	335	mg/kg	NIH HSDB	min
LD50	745	mg/kg	NIH HSDB	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0007345	mol/kg	TEST QSAR	
Ames mutagenicity test	0.366	no units	TEST QSAR	
Developmental toxin test	0.915	no units	TEST QSAR	

Morphine

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water				Prevalence				Magnitude			
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water				Prevalence				Magnitude			
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	557	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	75	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	482	0	Sites	0						

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water				Prevalence				Magnitude			
Furlong et al 2017 (Finished) [83]	2007 - 2012	NA	NA	Sites	0					ug/L	
Ambient Water				Prevalence				Magnitude			
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	205	6	Sites	2.93	0.00224	0.0189	0.0729	0.185	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	401	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	606	6	Sites	0.99	0.00224	0.0189	0.0729	0.185	ug/L	
Furlong et al 2017 (Ambient) [83]	2007 - 2012	NA	NA	Sites	0					ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	7	Sites	18	0.0057436	0.0152	0.0868	0.1145373	ug/L	
Bexfield et al. 2019 (Groundwater) [49]	2013 - 2015	1,106	0	Sites	0						
Waste Water Effluent				Prevalence				Magnitude			
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	13	Sites	62	0.0086904	0.0583	0.547	0.5896521	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Expocast exposure			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	25.9487	days	
Boiling point	OPERA QSAR	385.353	degree C	
Boiling point	TEST QSAR	430.461	degree C	
Vapor pressure	OPERA QSAR	2.04E-09	mmHg	
Vapor pressure	TEST QSAR	2.4E-09	mmHg	
Solubility in water	OPERA QSAR	0.000940938	mol/L	
Solubility in water	TEST QSAR	0.00465586	mol/L	
Bioconcentration factor	OPERA QSAR	52.5833	no units	
Bioconcentration factor	TEST QSAR	71.2853	no units	
Henry's Law constant	OPERA QSAR	6.9E-11	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.06081	no units	

Morphine

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Reference Number	Full Reference
49	Bexfield, L.M., P.L. Toccalino, K. Belitz, W.T. Foreman, and E.T. Furlong. 2019. Hormones and pharmaceuticals in groundwater used as a source of drinking water across the United States. Environmental Science and Technology 53: 2950-2960.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. Environmental science & technology, 51(9), 4792-4802.
77	FDA. 2018. Drugs @ FDA: FDA Approved Drug Products. U.S. Food and Drug Administration (FDA). https://www.accessdata.fda.gov/scripts/cder/daf/ .
83	Furlong, E.T., Batt, A.L., Glassmeyer, S.T., Noriega, M.C., Kolpin, D.W., Mash, H., Schenck, K.M. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States: Pharmaceuticals. Science of The Total Environment. 579 (1629-1642).
150	NIH. 2018. DailyMed Database. U.S. National Library of Medicine, National Institutes of Health (NIH). https://dailymed.nlm.nih.gov/dailymed/ .
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. Science of the Total Environment, 636, 69-79.

Morphine-3-Glucuronide

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Morphine-3-Glucuronide
CASRN:	20290-09-9
DTXSID:	DTXSID80174157
Use:	Central Nervous System Stimulants
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date

PUBLIC NOMINATION STATUS

Public Nomination
X

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis
Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Morphine-3-Glucuronide

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity test			TEST QSAR	
Developmental toxin test			TEST QSAR	

Morphine-3-Glucuronide

CCL 5 Contaminant Information Sheet

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Ambient Water											
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exposure exposure			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR			
Boiling point	OPERA QSAR			
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR			
Vapor pressure	TEST QSAR			
Solubility in water	OPERA QSAR			
Solubility in water	TEST QSAR			
Bioconcentration factor	OPERA QSAR			
Bioconcentration factor	TEST QSAR			
Henry's Law constant	OPERA QSAR			
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR			

Morphine-3-Glucuronide

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference

Myclobutanil

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Myclobutanil
CASRN:	88671-89-0
DTXSID:	DTXSID8024315
Use:	Fungicide used on fruit
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	X
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision

Not List

Final Hazard Quotient (HQ)

0.0004

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	reproductive and developmental effects	9	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	100	decreased testicular weights and increased testicular atrophy	general population	OPP	2019

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.04	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		
Not Applicable		

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Myclobutanil

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.025	mg/kg/day	OPP 2019	Wolfe 1993; Shellenberger et al. 1986	decreased testicular weights and increased testicular atrophy	general population	33.8	148	[421]	
Cancer Classification (CC)	E		OPP 2019						[421]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	20	mg/L	EPA HHBP	
Acute PAD	0.6	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.16	mg/L	EPA HHBP	
Health-Based Screening Level	0.16	mg/L	Health-based screening levels from	
Population-Adjusted Dose (PAD)	0.025	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1600	mg/kg	NIH HSDB	min
LD50	2290	mg/kg	NIH HSDB	max
LOAEL	393.5	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	9.8400002	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	2.5	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	93.77	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	13.57	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	150	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic LOAEL	5	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	0.25	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	50	mg/kg/day	EPA Toxicity Reference Database	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0057677	mol/kg	TEST QSAR	
Ames mutagenicity test	0.709	no units	TEST QSAR	
Developmental toxin test	0.554	no units	TEST QSAR	

OCCURRENCE DATA

Scoring Data

Scoring Data											
Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
		Prevalence				Magnitude					
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	4,941	170	Sites	3.44	0.00033	0.011	0.04	0.668	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	581	150	Sites	26	0.00033	0.011	0.04	0.668	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	4,360	20	Sites	0.46	0.00468	0.012	0.0346	0.266	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	40	103,368	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	6	0.98	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Storing Data											
Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water			Prevalence				Magnitude				
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	2	Sites	12	0.0027	0.0188	0.0188	0.0188	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water			Prevalence				Magnitude				
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	903	106	Sites	12	0.00092	0.013	0.309	24	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	2,510	10	Sites	0.4	0.008	0.0127	0.0822	0.146	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	3,412	116	Sites	3.4	0.00092	0.013	0.282	24	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	6	Sites	2.62	0.0027	0.0188	0.083	0.083	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	2	Sites	0.91	0.004828	0.0439	0.0752	0.083	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	4	Sites	33	0.0027	0.0188	0.083	0.083	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	24	0	Sites	0						
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	2	Sites	5.26	0.0497	0.161	0.251	0.273	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	3	Sites	0.43	0.0061	0.0098	0.0116	0.012	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Waste Water Effluent			Prevalence				Magnitude				
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
ExpoCast exposure		8.75E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.35213	days	
Boiling point	OPERA QSAR	337.658	degree C	
Boiling point	TEST QSAR	396.923	degree C	
Vapor pressure	OPERA QSAR	0.00000101	mmHg	
Vapor pressure	TEST QSAR	0.000000126	mmHg	
Solubility in water	OPERA QSAR	0.000735975	mol/L	
Solubility in water	TEST QSAR	0.0000383	mol/L	
Bioconcentration factor	OPERA QSAR	33.7291	no units	
Bioconcentration factor	TEST QSAR	103.514	no units	
Henry's Law constant	OPERA QSAR	0.000000439	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.98801	no units	

Myclobutanil

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
421	USEPA. 2019. Myclobutanil: Human Health Risk Assessment for Registration Review. EPA-HQ-OPP-2015-0053-0018. DP No. D448816. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

N,N-Diethyl-m-toluamide (DEET)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	N,N-Diethyl-m-toluamide (DEET)
CASRN:	134-62-3
DTXSID:	DTXSID2021995
Use:	Broad-spectrum insect repellent
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
		10	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.22	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

N,N-Diethyl-m-toluamide (DEET)
CCL 5 Contaminant Information Sheet
HEALTH EFFECTS DATA

EPA-OGWDW and OST

July 2021

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	1	mg/kg/day	ATSDR 2017	EPA. 1989. [EPA memorandum 007645 from Whang Phang, Subject: Review of a two-generation reproduction on DEET, dated 13 December 1989]	reduced body weight in F1 and F2 male and female pups on lactation day 21	lactating women	46.9	4260	[35]	
			OPP 2014						[331]	NOTE: There is no HRL for DEET because there are no toxicity values provided in the OPP assessment. The document states "no dietary or occupational exposures are anticipated, residential and aggregate were not risks of concern due to the lack of hazard." An ATSDR Toxicological Profile exists for this compound. See entry in "other qualifying information"

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Health-Based Guidance Value	0.2	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.2	mg/L	MN DOH	
Short-Term/Subchronic Health-Based Guidance Value	0.2	mg/L	MN DOH	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1584	mg/kg	NIH HSDB	min
LD50	1950	mg/kg	NIH HSDB	max
LOAEL	1000	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	25	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	100	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	500	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxicant in vitro assays tested	1.51	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	304	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	61	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0091411	mol/kg	TEST QSAR	
Ames mutagenicity test	-0.042	no units	TEST QSAR	
Developmental toxin test	0.57	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

N,N-Diethyl-m-tolamide (DEET)
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	538	114	Sites	21	0.01	0.06	0.22	2.2	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	60	43	Sites	72	0.01	0.07	0.24	2.2	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	478	71	Sites	15	0.01	0.02	0.094	0.29	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Padhye et al. 2013 (Finished) [155]	2009 - 2010	8	8	Samples	100	5e-07 +/- 1e-07	1.19e-05		2.4e-05 +/- 8.2e-06	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	1	Sites	100	0.1	0.1	0.1	0.1	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	710	522	Sites	74	0.01	0.05	0.22	5.07	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	683	244	Sites	36	0.01	0.03	0.358	7.9	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,393	766	Sites	55	0.01	0.05	0.23	7.9	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	26	12	Sites	46	0.0106	0.146	0.473	0.912	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	4		0.098		0.098	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	22	Sites	58	0.0035	0.0311	0.0899	0.119	ug/L	
Padhye et al. 2013 (Ambient) [155]	2009 - 2010	8	8	Samples	100	2.33e-05 +/- 3e-06	0.0001224		0.0002557 +/- 6.25e-05	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	2	Sites	100						
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	17	Sites	81	0.085	0.195	0.449	1	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.00000017	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)	< LOD	ug/l	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.35701	days	
Boiling point	OPERA QSAR	287.874	degree C	
Boiling point	TEST QSAR	307.376	degree C	
Vapor pressure	OPERA QSAR	0.0019251	mmHg	
Vapor pressure	TEST QSAR	0.00031989	mmHg	
Solubility in water	OPERA QSAR	0.00200679	mol/L	
Solubility in water	TEST QSAR	0.0209894	mol/L	
Bioconcentration factor	OPERA QSAR	3.31548	no units	
Bioconcentration factor	TEST QSAR	10.3276	no units	
Henry's Law constant	OPERA QSAR	0.000000145	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.25645	no units	

N,N-Diethyl-m-toluamide (DEET)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
35	ATSDR. 2017. Toxicological Profile for DEET (N,N-Diethyl-Meta-Toluamide). U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
155	Padhye, L.P., Yao, H., Kung'u, F.T., and Huang, C.H. Year-long evaluation on the occurrence and fate of pharmaceuticals, personal care products, and endocrine disrupting chemicals in an urban drinking water treatment plant. 2014. <i>Water Research</i> 51 (2014) 266-276.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
331	USEPA. 2014. DEET (N,N-diethyl-meta-toluamide). Revised Human Health Risk Assessment in Support of Registration Review. EPA-HQ-OPP-2012-0162-0003. DP No. D413872. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Naled

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Naled
CASRN:	300-76-5
DTXSID:	DTXSID1024209
Use:	Insecticide; veterinary medicine
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	X
Human Neurotoxics	X
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.02

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	non-cancer effects	3	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	10	brain cholinesterase inhibition	general population	OPP	2009

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.1972	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Naled

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.002	mg/kg/day	OPP 2006	Batham et al. 1984	brain cholinesterase inhibition	general population	33.8	11.8	[266]	
Cancer Classification (CC)	E		OPP 2006						[266]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.07	mg/L	EPA HHBP	
Acute PAD	0.01	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.01	mg/L	EPA HHBP	
Health-Based Screening Level	0.01	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.002	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	430	mg/kg	NIH HSDB	max
LD50	92	mg/kg	NIH HSDB	min
LOAEL	2	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	40	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	0.2	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	10	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	24.11	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0002851	mol/kg	TEST QSAR	
Ames mutagenicity test	0.559	no units	TEST QSAR	
Developmental toxin test			TEST QSAR	

Naled

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	1,698	4	Sites	0.24	0.004	0.0221	0.197	0.367	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	322	3	Sites	0.93	0.004	0.0173	0.0253	0.0274	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	1,376	1	Sites	0.07	0.367	0.367	0.367	0.367	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	6	293,220	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	1	10	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	1	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	3	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	299	2	Sites	0.67	0.0578	0.0595	0.0605	0.0612	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	528	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	827	2	Sites	0.24	0.0578	0.0595	0.0605	0.0612	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	2,547	0	Sites	0						
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exposure		0.00000122	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.13863	days	
Boiling point	OPERA QSAR	275.202	degree C	
Boiling point	TEST QSAR	291.332	degree C	
Vapor pressure	OPERA QSAR	0.000367639	mmHg	
Vapor pressure	TEST QSAR	0.0069024	mmHg	
Solubility in water	OPERA QSAR	0.00699769	mol/L	
Solubility in water	TEST QSAR	0.00360579	mol/L	
Bioconcentration factor	OPERA QSAR	3.99441	no units	
Bioconcentration factor	TEST QSAR	5.90201	no units	
Henry's Law constant	OPERA QSAR	0.00000793	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.56699	no units	

Naled

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
266	USEPA. 2006. Finalization of Interim Reregistration Eligibility Decisions (IREDs) and Interim Tolerance Reassessment and Risk Management Decisions (TREDs) for the Organophosphate Pesticides, and Completion of the Tolerance Reassessment and Reregistration Eligibility Process for the Organophosphate Pesticides. Interim Reregistration Eligibility Decision for Naled. EPA-HQ-OPP-2002-0307-0002. EPA 738-R-02-008. U.S. Environmental Protection Agency, Office of Prevention, Pesticides and Toxic Substances, Washington, D.C.
301	USEPA. 2009. Naled. Human Health Assessment Scoping Document in Support of Registration Review. EPA-HQ-OPP-2009-0053-0005. DP No. D356244. Office of Prevention, Pesticides and Toxic Substances, United States Environmental Protection Agency, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Naphthalene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Naphthalene
CASRN:	91-20-3
DTXSID:	DTXSID8020913
Use:	Former pesticide; chemical intermediate; moth repellent
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.012

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	non-cancer effects	7	6

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	600	decreases in body weights and body weight gains, renal effects	general population	OPP	2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
7.4	90th Percentile	Finished Water	UCM1	1988-1992

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X			

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
X	Not Applicable	Not Applicable

Basis

Naphthalene regulation does not represent a meaningful opportunity for health risk reduction in persons served by public water systems. While there is evidence that naphthalene may cause adverse health effects in humans at high doses, specifically hemolytic anemia [a,b], it is unlikely that it will occur in drinking water at frequencies or concentrations that are of public health concern. The UCM Round 2 survey data estimates only 0.002% of the population served by PWS are exposed to concentrations greater than ½ the HRL and no exposures at concentrations greater than an HRL of 140 µg/L [c].

[a] Gidron & Leurer, 1956 [84]; [b] ATSDR, 1995 [3]; [c] USEPA, 1999 [232]; as cited in USEPA, 2001 [182]

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Naphthalene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.1	mg/kg/day	OPP 2018	NTP 1980	decreases in body weights and renal effects	general population	33.8	592	[405]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	0.5	mg/L	EPA DWSHA 2018	
Acute Health-Based Guidance Value	0.07	mg/L	MN DOH	
Acute Health-Based Guidance Value	0.07	mg/L	MN DOH	
Acute Minimal Risk Level (MRL)	0.6	mg/kg/day	CDC ATSDR	
Benchmark	0.017	mg/L	CalEPA OEHHA Chemical Database	
Cancer Slope Factor (CSF)	0.12	(mg/kg/day)^-1	CalEPA OEHHA Chemical Database	
Chronic Health-Based Guidance Value	0.07	mg/L	MN DOH	
Chronic Inhalation Minimal Risk Level (MRL)	0.0007	ppm	CDC ATSDR	
Inhalation Unit Risk (IUR)	0.000034	ug/m^3	CalEPA OEHHA Chemical Database	
Intermediate Minimal Risk Level (MRL)	0.6	mg/kg/day	CDC ATSDR	
Lifetime Health Advisory	0.1	mg/L	EPA DWSHA 2018	
Reference Concentration (RfC)	0.003	mg/m^3	EPA IRIS	
Reference Concentration (RfC)	9	ug/m^3	CalEPA OEHHA Chemical Database	
Short-Term/Subchronic Health-Based Guidance Value	0.07	mg/L	MN DOH	
Cancer Classification (CC)	2B	no units	WHO IARC	
Cancer Classification (CC)	Female.Mice NT	no units	HHS NTP	
Cancer Classification (CC)	Female.Mice SE	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats NT	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats P	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice NE	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice NT	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats NT	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats P	no units	HHS NTP	

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	2600	mg/kg	NIH HSDB	max
LD50	490	mg/kg	NIH HSDB	min
LOAEL	50	mg/kg/day	EPA Toxicity Reference Database	
Percent of active toxcast in vitro assays tested	2.54	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0109648	mol/kg	TEST QSAR	
Ames mutagenicity test	-0.01	no units	TEST QSAR	
Developmental toxin test	0.32	no units	TEST QSAR	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Naphthalene

CCL 5 Contaminant Information Sheet

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
			Prevalence					Magnitude			
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997	22,923	173	Sites	0.75	0.07	0.73	3.08	90	ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992	13,452	159	Sites	1.18	0.03	1	7.4	906	ug/L	
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
			Prevalence					Magnitude			
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	7,850	68	Sites	0.87	0.008	0.2	1.02	70	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	310	30	Sites	9.68	0.008	0.1	0.3	1.12	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	7,540	38	Sites	0.5	0.048	0.42	5.69	70	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)	49	2,359,983	Chemical Data Reporting (CDR) Results (EPA) (2016)	100M - 250M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
			Prevalence					Magnitude			
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	366	3	Sites	0.82	0.003	0.0105	0.93	7	ug/L	
Drinking Water Monitoring Data - MA (Finished)	2006 - 2020	887	14	Sites	1.58	0.5	1.3	2.03	3.1	ug/L	
Drinking Water Monitoring Data - WA (Finished)	2006 - 2011	1,188	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
			Prevalence					Magnitude			
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	3,888	21	Sites	0.54	0.001	0.565	3.21	5.8	ug/L	
Drinking Water Monitoring Data - MA (Source)	2006 - 2020	131	5	Sites	3.82	0.5	1.2	2.58	4.5	ug/L	
Drinking Water Monitoring Data - PA (Source)	2006 - 2011	15	1	Sites	6.67	1.08	1.16	1.23	1.25	ug/L	
Drinking Water Monitoring Data - WA (Source)	2006 - 2011	1,665	2	Sites	0.12	0.66	34.4	35.8	36	ug/L	
Drinking Water Monitoring Data - WI (Source)	2012-2019	101	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	978	159	Sites	16	0.008	0.02	0.07	6	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	4,211	87	Sites	2.07	0.007	0.096	43.4	16000	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	5,186	246	Sites	4.74	0.007	0.0205	0.282	16000	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	3	Sites	7.89	0.0162	0.025	0.0277	0.0284	ug/L	
Arnold et al. 2016 (Unfiltered) [7]	2012 - 2013	685	1	Sites	0.15	0.78	0.78	0.78	0.78	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Waste Water Effluent											
			Prevalence					Magnitude			
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	2	Sites	9.52	0.021	0.025	0.0282	0.029	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg- bw/day)	Notes
Expocast exposure		0.0000737	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	5.12244	days	
Boiling point	OPERA QSAR	221.854	degree C	
Boiling point	TEST QSAR	233.31	degree C	
Vapor pressure	OPERA QSAR	0.0632206	mmHg	
Vapor pressure	TEST QSAR	0.057544	mmHg	
Solubility in water	OPERA QSAR	0.000165649	mol/L	
Solubility in water	TEST QSAR	0.00030903	mol/L	
Bioconcentration factor	OPERA QSAR	89.6573	no units	
Bioconcentration factor	TEST QSAR	244.67	no units	
Henry's Law constant	OPERA QSAR	0.000415844	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.32388	no units	

Naphthalene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
3	Agency for Toxic Substances and Disease Registry (ATSDR). 1995. Toxicological Profile for Naphthalene (Update). Atlanta: Agency for Toxic Substances and Disease Registry. 200pp.
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. Environmental science & technology, 51(9), 4792-4802.
84	Gidron, E. and J. Leurer. 1956. Naphthalene Poisoning. Lancet. 4:228-230 (as cited in ATSDR, 1995).
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. Science of the Total Environment, 636, 69-79.
182	USEPA, 2001. Regulatory Determination Support Document for Naphthalene. EPA 815 R-01-008.
232	USEPA. 1999. A Review of Contaminant Occurrence in Public Water Systems. Office of Water. EPA Report 816-R-99-006. 78 pp.
405	USEPA. 2018. Naphthalene: Human Health Risk Assessment in Support of Registration Review. EPA-HQ-OPP-2016-0113-0018. DP No. D440842. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.

Nicotine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Nicotine
CASRN:	54-11-5
DTXSID:	DTXSID1020930
Use:	Restricted use pesticide; component in cigarettes
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	X
PubMed Neurotoxicants	
Neurodev. Disruptors	X
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	X

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.78

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
8	non-cancer effects	10	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	0.2	lowest therapeutic dose: smoking cessation/reduces withdrawal symptoms, including nicotine craving associated with quitting smoking	bottle-fed infants	FDA; NIH	2018; 2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.1566	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Nicotine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.000025	mg/kg/day	FDA 2018; NIH 2018	Wal-Mart Stores Inc	lowest therapeutic dose:smoking cessation/reduces withdrawal symptoms, including nicotine craving associated with quitting smoking	bottle-fed infants	151	0.170	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels
Reference Dose (RfD) or Equivalent	0.000025	mg/kg/day	FDA 2018; NIH 2018	Wal-Mart Stores Inc	lowest therapeutic dose:smoking cessation/reduces withdrawal symptoms, including nicotine craving associated with quitting smoking	general population	33.8	0.590	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Screening level for pharmaceutical - general population	0.000588235	mg/L	EPA Office of Water	
Screening level for pharmaceutical - infants	0.000166667	mg/L	EPA Office of Water	

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	188	mg/kg	NIH HSDB	max
LD50	24	mg/kg	NIH HSDB	min
Percent of active toxcast in vitro assays tested	2.39	percent	EPA Chemistry Dashboard	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0053088	mol/kg	TEST QSAR	
Ames mutagenicity test	0.047	no units	TEST QSAR	
Developmental toxin test	0.645	no units	TEST QSAR	

Nicotine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. <i>Environmental science & technology</i> , 52(23), 13972-13985.
77	FDA. 2018. Drugs @ FDA: FDA Approved Drug Products. U.S. Food and Drug Administration (FDA). https://www.accessdata.fda.gov/scripts/cder/daf/ .
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
150	NIH. 2018. DailyMed Database. U.S. National Library of Medicine, National Institutes of Health (NIH). https://dailymed.nlm.nih.gov/dailymed/ .
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
433	Uslu, M., Jasim, S., Arvai, A., Bewtra, J. and Biswas, N., 2013. A Survey of Occurrence and Risk Assessment of Pharmaceutical Substances in the Great Lakes Basin. <i>Ozone: Science & Engineering</i> , 35(4), pp.249-262.

Nonylphenol

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Nonylphenol
CASRN:	25154-52-3
DTXSID:	DTXSID3021857
Use:	In the preparation of lubricating oil additives, resins, plasticizers, surface active agents; antioxidants for plastics and rubber
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	X
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.15

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	non-cancer effects	9	7

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	30	renal mineralization	general population	MDH	2015

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
4.4	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
			X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Nonylphenol

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0049	mg/kg/day	MDH 2015	NTP, 1997/Chapin, 1999	Renal Mineralization	general population	33.8	29.0	[136]	

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Metabolic, Systemic	0.00002	Yu, 2018	Endocrine	456	Masutomi, 2004		2020-01-28	2685	64	16	50

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Health-Based Guidance Value	0.1	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.02	mg/L	MN DOH	
Short-Term/Subchronic Health-Based Guidance Value	0.04	mg/L	MN DOH	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1600	mg/kg	NIH HSDB	min
LD50	1620	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	26.88	percent	EPA Chemistry Dashboard	min
Percent of active toxcast in	38.23	percent	EPA Chemistry Dashboard	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0116681	mol/kg	TEST QSAR	
Ames mutagenicity test	-0.104	no units	TEST QSAR	
Developmental toxin test	0.533	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Nonylphenol

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	567	45	Sites	7.94	0.3	1.85	4.4	13	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	88	43	Sites	49	0.3	1.85	4.4	13	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	479	2	Sites	0.42	1.5	2.35	2.86	3.2	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)	24	42,754	Chemical Data Reporting (CDR) Results (EPA) (2016)	100M - 250M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Padhye et al. 2013 (Finished) [155]	2009 - 2010	8	8	Samples	100	1.24e-05 +/- 5.3e-06	1.95e-05		6.06e-05 +/- 1.92e-05	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	10	Sites	26	0.105	0.278	0.448	0.461	ug/L	
Padhye et al. 2013 (Ambient) [155]	2009 - 2010	8	8	Samples	100	5.34e-05 +/- 5.8e-06	8.32e-05		0.0001856 +/- 2e-05	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	17	Sites	81	1.1	1.1	1.1	1.1	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exposure exposure		0.000000872	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.94705	days	
Boiling point	OPERA QSAR	269.167	degree C	
Boiling point	TEST QSAR	316.679	degree C	
Vapor pressure	OPERA QSAR	0.00114475	mmHg	
Vapor pressure	TEST QSAR	0.000034	mmHg	
Solubility in water	OPERA QSAR	0.0000344	mol/L	
Solubility in water	TEST QSAR	0.00000575	mol/L	
Bioconcentration factor	OPERA QSAR	431.548	no units	
Bioconcentration factor	TEST QSAR	96.8278	no units	
Henry's Law constant	OPERA QSAR	0.0000106	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	5.68641	no units	

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Reference Number	Full Reference
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
136	MDH. 2015. Toxicological Summary for p-Nonylphenol, branched isomers. Minnesota Department of Health (MDH), Environmental Health Division, Health Risk Assessment Unit, St Paul, MN.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
155	Padhye, L.P., Yao, H., Kung'u, F.T., and Huang, C.H. Year-long evaluation on the occurrence and fate of pharmaceuticals, personal care products, and endocrine disrupting chemicals in an urban drinking water treatment plant. 2014. <i>Water Research</i> 51 (2014) 266-276.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.

Norflurazon

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Norflurazon
CASRN:	27314-13-2
DTXSID:	DTXSID8024234
Use:	Herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.049

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	non-cancer effects	9	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	9	increased incidence of thyroid colloid/vacuoles and epithelial desquamation, increased liver weight, ALP, and cholesterol in males	general population	OPP	2017

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.44	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Norflurazon

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0015	mg/kg/day	OPP 2017	Klotzsche et al. 1973	increased incidence of thyroid colloid/vacuoles and epithelial desquamation, increased liver weight, ALP, and cholesterol in males	general population	33.8	8.88	[387]	
Cancer Classification (CC)	C		OPP 2017						[387]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.8	mg/L	EPA HHBP	
Acute PAD	0.03	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.096	mg/L	EPA HHBP	
Health-Based Screening Level	0.096	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.015	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	8000	mg/kg	NIH HSDB	
LOAEL	102.5	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	4.77	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	1.58	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	81.7	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxicant in vitro assays tested	7.86	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0101391	mol/kg	TEST QSAR	
Ames mutagenicity test	0.227	no units	TEST QSAR	
Developmental toxin test	0.941	no units	TEST QSAR	

Storing Data											
Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	7,803	217	Sites	2.78	0.00025	0.021	0.44	26.5	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	1,222	107	Sites	8.76	0.00025	0.02	0.36	7.3	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	6,581	110	Sites	1.67	0.00029	0.042	1.06	26.5	ug/L	

Non-Scoring Data												
Non-Nationally Representative Water Data		Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water			Prevalence				Magnitude					
Drinking Water Monitoring Data - WA (Finished)		2006 - 2011	1	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)		2001 - 2013	17	2	Sites	12	0.0313	0.0313	0.0928	0.096	ug/L	
Ambient Water			Prevalence				Magnitude					
Drinking Water Monitoring Data - WA (Source)		2006 - 2011	4	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)		2008 - 2017	475	21	Sites	4.42	0.00035	0.00798	0.155	0.53	ug/L	
National Water Information System (USGS NWIS) (Groundwater)		2008 - 2017	1,056	19	Sites	1.8	3.00E - 04	0.03	0.828	1.49	ug/L	
National Water Information System (USGS NWIS) (All Water)		2008 - 2017	1,531	40	Sites	2.61	3.00E - 04	0.02	0.53	1.49	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)		2001 - 2013	229	9	Sites	3.93	0.007992	0.0313	0.0992	0.352	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)		2001 - 2013	219	6	Sites	2.74	0.007992	0.0248	0.222	0.352	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)		2001 - 2013	12	3	Sites	25	0.0313	0.0313	0.09	0.132	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]		1990 - 2018	1,090	125	Sites	11	0.05	0.13	0.424	1.49	ug/L	
Bradley et al. 2017 (Ambient) [52]		2012 - 2014	38	2	Sites	5.26	0.0137	0.0206	0.026	0.0274	ug/L	
Arnold et al. 2016 (Filtered) [7]		2012 - 2013	690	12	Sites	1.74	3e-04	0.00195	0.045	0.0563	ug/L	
Waste Water Effluent			Prevalence				Magnitude					
Estimated Concentration in Water		Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
ExpoCast exposure		0.000000108	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.54354	days	
Boiling point	OPERA QSAR	329.74	degree C	
Boiling point	TEST QSAR	355.301	degree C	
Vapor pressure	OPERA QSAR	0.00016561	mmHg	
Vapor pressure	TEST QSAR	0.000000708	mmHg	
Solubility in water	OPERA QSAR	0.000311995	mol/L	
Solubility in water	TEST QSAR	0.0000906	mol/L	
Bioconcentration factor	OPERA QSAR	22.9102	no units	
Bioconcentration factor	TEST QSAR			
Henry's Law constant	OPERA QSAR	1.18E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.43139	no units	

Norflurazon

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
387	USEPA. 2017. Norflurazon: Draft Human Health Risk Assessment in Support of Registration Review. EPA-HQ-OPP-2012-0565-0025. DP No. D432685. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

o-Toluidine

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	o-Toluidine
CASRN:	95-53-4
DTXSID:	DTXSID1026164
Use:	intermediate in the manufacture of dyes, rubber, pharmaceuticals and pesticides
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.031

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	carcinogen with linear MOA	8	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	2	subcutaneous fibromas and fibrosarcomas	general population	PPRTV	2012

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.06164	90th Percentile	Finished Water	UCMR4	2018-2019

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
		X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

o-Toluidine

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Cancer Slope Factor (CSF)	0.016	(mg/kg/day)^-1	PPRTV 2012	Weisburger et al. 1978	subcutaneous fibromas and fibrosarcomas in males	general population	33.8	1.85	[328]	
Cancer Classification (CC)	L		PPRTV 2012						[328]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Systemic	226.6	Toyoda, 2019	Renal	226.6	Toyoda, 2019	2011-12-01	2020-04-06	73	1	5	1

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Cancer Classification (CC)	1	no units	WHO IARC	
Cancer Slope Factor (CSF)	0.18	(mg/kg/day)^-1	CalEPA OEHHA Chemical Database	
Inhalation Unit Risk (IUR)	0.000051	ug/m^3	CalEPA OEHHA Chemical Database	
Subchronic Provisional RfD	0.02	mg/kg/day	EPA PPRTV	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	300	mg/kg	NIH HSDB	min
LD50	940	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	1.47	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0067298	mol/kg	TEST QSAR	
Ames mutagenicity test	0.335	no units	TEST QSAR	
Developmental toxin test	0.559	no units	TEST QSAR	

o-Toluidine

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EPA-OGWDW and OST

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019	3,678	67	Sites	1.82	0.007	0.012	0.0616	0.38	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)	10	6,328	Chemical Data Reporting (CDR) Results (EPA) (2016)	50M - 100M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	21	0	Sites	0						
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	15	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	36	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.00000421	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.81183	days	
Boiling point	OPERA QSAR	212.346	degree C	
Boiling point	TEST QSAR	206.895	degree C	
Vapor pressure	OPERA QSAR	0.177328	mmHg	
Vapor pressure	TEST QSAR	0.134586	mmHg	
Solubility in water	OPERA QSAR	0.182954	mol/L	
Solubility in water	TEST QSAR	0.0475335	mol/L	
Bioconcentration factor	OPERA QSAR	4.90019	no units	
Bioconcentration factor	TEST QSAR	6.54636	no units	
Henry's Law constant	OPERA QSAR	0.0000019	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.4043	no units	

o-Toluidine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
328	USEPA. 2012. Provisional Peer-Reviewed Toxicity Values for o-Toluidine. U.S. Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment, Superfund Health Risk Technical Support Center, Cincinnati, OH.

Oxadiazon

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Oxadiazon
CASRN:	19666-30-9
DTXSID:	DTXSID3024239
Use:	Herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	120

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	carcinogen with linear MOA	1	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.4	increase in liver adenomas and/or carcinomas combined in males	general population	OPP	2014

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
46.3		EDWC SW Chronic	OPP	2020

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Oxadiazon

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Cancer Slope Factor (CSF)	0.0711	(mg/kg/day) ⁻¹	OPP 2014	Shirasu 1987	increase in liver adenomas and/or carcinomas combined in males	general population	33.8	0.416	[333]	NOTE: a non-cancer toxicity value was not provided in this assessment because there are no food or feed uses of oxadiazon
Cancer Classification (CC)	L		OPP 2014						[333]	NOTE: a non-cancer toxicity value was not provided in this assessment because there are no food or feed uses of oxadiazon

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	3500	mg/kg	NIH HSDB	min
LD50	5000	mg/kg	NIH HSDB	max
LOAEL	180	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	3.5	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	0.44	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	60	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	21.59	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	100	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic LOAEL	25	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	25	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0017989	mol/kg	TEST QSAR	
Ames mutagenicity test	0.434	no units	TEST QSAR	
Developmental toxin test	0.874	no units	TEST QSAR	

July 2021

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.7926	days	
Boiling point	OPERA QSAR	343.796	degree C	
Boiling point	TEST QSAR	356.765	degree C	
Vapor pressure	OPERA QSAR	0.000000128	mmHg	
Vapor pressure	TEST QSAR	8.81E-08	mmHg	
Solubility in water	OPERA QSAR	0.00000508	mol/L	
Solubility in water	TEST QSAR	0.00000867	mol/L	
Bioconcentration factor	OPERA QSAR	1204.35	no units	
Bioconcentration factor	TEST QSAR	94.189	no units	
Henry's Law constant	OPERA QSAR	7.72E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	4.67306	no units	

Oxadiazon

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
333	USEPA. 2014. Oxadiazon. Human Health Assessment Scoping Document in Support of Registration Review. EPA-HQ-OPP-2014-0782-0004. DP No. D420616. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Oxyfluorfen

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Oxyfluorfen
CASRN:	42874-03-3
DTXSID:	DTXSID7024241
Use:	Pesticide; herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.6

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	carcinogen with linear MOA	2	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.4	hepatocellular adenomas and carcinomas	general population	OPP	2019

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.2415	90th Percentile	Finished Water	UCMR4	2018-2019

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
		X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Oxyfluorfen

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.04	mg/kg/day	OPP 2019	Goldenthal and Wazeter 1977	multiple signs of liver toxicity	general population	33.8	237	[422]	
Cancer Slope Factor (CSF)	0.0732	(mg/kg/day)^-1	OPP 2019	Goldenthal & Wazeter 1977	hepatocellular adenomas and carcinomas	general population	33.8	0.404	[422]	
Cancer Classification (CC)	C		OPP 2019						[422]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Cancer Slope Factor (CSF)	0.0732	(mg/kg/day)^-1	EPA HHBP	
Chronic Human Health Benchmark	0.2	mg/L	EPA HHBP	
Chronic Human Health Benchmark	0.000437	mg/L	EPA HHBP	
Health-Based Screening Level	0.2	mg/L	Health-based screening levels from USGS	
Health-Based Screening Level	0.000437	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.03	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LOAEL	18.5	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	183	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	3.1	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	36.4	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	13.39	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	51.400002	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	585	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	150.5	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	18	mg/kg/day	EPA Toxicity Reference Database	min

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0087498	mol/kg	TEST QSAR	
Ames mutagenicity test	0.253	no units	TEST QSAR	
Developmental toxin test	0.864	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Oxyfluorfen
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019	3,649	6	Sites	0.16	0.053	0.0717	0.242	0.38	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	4,284	24	Sites	0.56	0.001	0.011	0.045	0.852	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	406	22	Sites	5.42	0.001	0.011	0.0442	0.605	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	3,878	2	Sites	0.05	0.002	0.427	0.682	0.852	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	29	969,226	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	5	3,643	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	13	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	759	28	Sites	3.69	0.001	0.0447	0.188	4.27	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	1,453	1	Sites	0.07	0.008	0.008	0.008	0.008	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	2,211	29	Sites	1.31	0.001	0.0426	0.183	4.27	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	8	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	2	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	6	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	1,939	208	Sites	11	0.0038	0.0995	0.481	9.23	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	6	Sites	16	0.00147	0.00482	0.0487	0.0864	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.00000013	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.54009	days	
Boiling point	OPERA QSAR	358.749	degree C	
Boiling point	TEST QSAR	366.917	degree C	
Vapor pressure	OPERA QSAR	0.000000254	mmHg	
Vapor pressure	TEST QSAR	0.000000226	mmHg	
Solubility in water	OPERA QSAR	0.000000308	mol/L	
Solubility in water	TEST QSAR	0.000000334	mol/L	
Bioconcentration factor	OPERA QSAR	12909	no units	
Bioconcentration factor	TEST QSAR	320.627	no units	
Henry's Law constant	OPERA QSAR	0.00000347	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	4.70955	no units	

Oxyfluorfen

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
422	USEPA. 2019. Oxyfluorfen: Draft Human Health Risk Assessment for Registration Review. EPA-HQ-OPP-2014-0778-0025. DP No. D445742. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

p,p'-DDE

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	p,p'-DDE
CASRN:	72-55-9
DTXSID:	DTXSID9020374
Use:	Product of degradation of DDT
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	X
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	33

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	carcinogen with linear MOA	1	7

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.09	hepatocellular carcinomas, hepatomas; increased incidence of liver tumors including carcinomas in two strains of mice and in hamsters and of thyroid tumors in female rats by diet	general population	IRIS	1988

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
3	90th Percentile	Finished Water	UCMR1	2001 - 2003

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X	X		

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	X	Not Applicable
Basis		
DDE appears to occur infrequently at levels of concern in PWSs. DDE was detected in only one of the PWSs monitored under the UCMR 1 at a level greater than the MRL (0.8 ug/L) [a]. The MRL is greater than the HRL of 0.2 ug/L but represents a concentration that is within the 10-4 to the 10-6 cancer risk range targeted by EPA [b]. In addition, ambient water data from the USGS indicate that the maximum concentrations detected in surface and ground water were less than the HRL [c,d].		
[a] USEPA, 2008 [297]; [b] USEPA, 2000 [238]; [c] Martin, Crawford, & Larson, 2003 [134]; [d] Kolpin & Martin, 2003 [123]; as cited in USEPA, 2008 [296]		

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

p,p'-DDE

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	1	mg/kg/day	PPRTV 2017	Yamasaki et al., 2009	increased relative liver weight in adult male offspring exposed during gestation and via lactation	bottle-fed infants	151	1320	[391]	
Cancer Slope Factor (CSF)	0.34	(mg/kg/day)^-1	IRIS 1988	Rossi et al. 1983; NCI 1978; Tomatis et al. 1974	"hepatocellular carcinomas, hepatomas"; "increased incidence of liver tumors including carcinomas in two strains of mice and in hamsters and of thyroid tumors in female rats by diet."	general population	33.8	0.0870	[200]	NOTE: the 2017 PPRTV assessment declines to derive a cancer slope factor for DDE because a carcinogenicity assessment is available on IRIS
Cancer Classification (CC)	B2		IRIS 1988						[200]	NOTE: the 2017 PPRTV assessment declines to derive a cancer slope factor for DDE because a carcinogenicity assessment is

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
			Metabolic, Systemic	0.834	Myrmet,2016	2016-09-01	2019-10-22	563	10	112	1

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Cancer Slope Factor (CSF)	0.34	(mg/kg/day)^-1	CalEPA OEHHA Chemical Database	
Chronic Health-Based Guidance Value	0.0001	mg/L	MN DOH	
Human Health Ambient Water Quality Criteria	0.000000018	mg/L	EPA Human Health Criteria for CWA	
Inhalation Unit Risk (IUR)	0.000097	ug/m^3	CalEPA OEHHA Chemical Database	
Subchronic Provisional RfD	0.0003	mg/kg/day	EPA PPRTV	
Cancer Classification (CC)	Female.Mice P	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats N	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice P	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats N	no units	HHS NTP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	700	mg/kg	NIH HSDB	min
LD50	880	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	28.17	percent	EPA Chemistry Dashboard	
TD50	119	mg/kg/day	NIH CPDB	max
TD50	7.48	mg/kg/day	NIH CPDB	min

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.001219	mol/kg	TEST QSAR	
Ames mutagenicity test	-0.248	no units	TEST QSAR	
Developmental toxin test	0.419	no units	TEST QSAR	

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p,p'-DDE
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OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003	3,874	1	Sites	0.03	3	3	3	3	ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	8,246	458	Sites	5.55	0	0.002	0.01	0.062	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	1,836	251	Sites	14	0	0.003	0.011	0.062	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	6,411	207	Sites	3.23	0	0.001	0.003	0.008	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	47	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	13	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	294	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	464	21	Sites	4.53	4.00E - 04	0.00466	0.0162	0.068	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	886	12	Sites	1.35	0.001	0.003	0.0446	0.08	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,350	33	Sites	2.44	4.00E - 04	0.0046	0.0261	0.08	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	8	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	2	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	6	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	600	47	Sites	7.83	0.003	0.01	0.0428	0.57	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	5	Sites	13	0.000848	0.0032	0.0159	0.0238	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		9.84E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)	1170	ng/g	
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	13.4608	days	
Boiling point	OPERA QSAR	338.523	degree C	
Boiling point	TEST QSAR	360.317	degree C	
Vapor pressure	OPERA QSAR	0.00000416	mmHg	
Vapor pressure	TEST QSAR	0.00000353	mmHg	
Solubility in water	OPERA QSAR	0.000000159	mol/L	
Solubility in water	TEST QSAR	0.000000262	mol/L	
Bioconcentration factor	OPERA QSAR	12264.3	no units	
Bioconcentration factor	TEST QSAR	17298.2	no units	
Henry's Law constant	OPERA QSAR	0.0000268	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	6.45816	no units	

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Reference Number	Full Reference
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
123	Kolpin, D.W. and J.D. Martin. 2003. Pesticides in Ground Water: Summary Statistics; Preliminary Results from Cycle I of the National Water Quality Assessment Program (NAWQA), 1992-2001. Available on the Internet at: http://ca.water.usgs.gov/pnsp/pestgw/Pest-GW_2001_Text.html .
134	Martin, J.D., C.G. Crawford, and S.J. Larson. 2003. Pesticides in Streams: Summary Statistics; Preliminary Results from Cycle I of the National Water Quality Assessment Program (NAWQA), 1992-2001. Available on the Internet at: http://ca.water.usgs.gov/pnsp/pestsw/Pest-SW_2001_Text.html .
200	USEPA. 1988. p,p'-Dichlorodiphenyldichloroethylene (DDE); CASRN 72-55-9. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, DC.
238	USEPA. 2000. Unregulated Contaminant Monitoring Regulation Analytical Methods and Quality Control Manual. EPA 815-R-00-006.
296	USEPA. 2008. Regulatory Determinations Support Document for Selected Contaminants from the Second Drinking Water Contaminant Candidate List (CCL 2). EPA Report 815-R-08-012. June 2008.
297	USEPA. 2008. The Analysis of Occurrence Data from the First Unregulated Contaminant Monitoring Regulation (UCMR 1) in Support of Regulatory Determinations for the Second Drinking Water Contaminant Candidate List. EPA 815-R-08-013. June.
391	USEPA. 2017. Provisional Peer-Reviewed Toxicity Values for p,p'-Dichlorodiphenyldichloroethylene (p,p'-DDE) (CASRN 72-55-9). EPA/690/R-17/007. U.S. Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment, Superfund Health Risk Technical Support Center, Cincinnati, OH.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

p-Cresol

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	p-Cresol
CASRN:	106-44-5
DTXSID:	DTXSID7021869
Use:	Chemical intermediate making synthetic resins; in disinfectants and fumigants; as industrial solvent.
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	X
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0018

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	reproductive and developmental effects	9	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	100	neurotoxicity and mortality in pregnant rabbits	women of childbearing age	PPRTV	2010

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.181	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

p-Cresol

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.02	mg/kg/day	PPRTV 2010	BRRC (1988a)	neurotoxicity and mortality in pregnant rabbits	women of childbearing age	35.4	113	[315]	NOTE: Though the critical effects in this study are not reproductive or developmental effects, they were observed in a study of pregnant rabbits. The assessment notes that no chronic studies were available to calculate a chronic duration RfD. Given the data gaps in non-pregnant adult animals, we make the conservative assumption that the effects observed in the 2-gen study are pregnancy related. For this reason we use the exposure factors for women of

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
						2009-09-01	2019-12-17	433	0	9	

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Chronic Health-Based Guidance Value	0.003	mg/L	MN DOH	
Subchronic Provisional RfD	0.02	mg/kg/day	EPA PPRTV	

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1800	mg/kg	NIH HSDB	max
LD50	207	mg/kg	NIH HSDB	min
Percent of active toxcast in vitro assays tested	1.59	percent	EPA Chemistry Dashboard	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0048306	mol/kg	TEST QSAR	
Ames mutagenicity test	0.06	no units	TEST QSAR	
Developmental toxin test	0.214	no units	TEST QSAR	

p-Cresol
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
		Prevalence				Magnitude					
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	566	45	Sites	7.95	0.01	0.03	0.181	73	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	88	37	Sites	42	0.01	0.04	0.177	73	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	478	8	Sites	1.67	0.01	0.02	0.078	0.19	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)	8	421,441	Chemical Data Reporting (CDR) Results (EPA) (2016)	50M - 100M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
		Prevalence				Magnitude					
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	722	305	Sites	42	0.01	0.03	0.186	91.1	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	771	52	Sites	6.74	0.01	0.05	0.47	11.6	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,493	357	Sites	24	0.01	0.03	0.19	91.1	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	21	Sites	55	0.0086	0.0219	0.0391	0.135	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	2	Sites	100						
Waste Water Effluent											
		Prevalence				Magnitude					
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	13	Sites	62	0.046	0.3	1.1	1.2	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.00000396	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	5.33885	days	
Boiling point	OPERA QSAR	200.232	degree C	
Boiling point	TEST QSAR	185.666	degree C	
Vapor pressure	OPERA QSAR	0.0992564	mmHg	
Vapor pressure	TEST QSAR	0.21677	mmHg	
Solubility in water	OPERA QSAR	0.168658	mol/L	
Solubility in water	TEST QSAR	0.141579	mol/L	
Bioconcentration factor	OPERA QSAR	15.2284	no units	
Bioconcentration factor	TEST QSAR	9.39723	no units	
Henry's Law constant	OPERA QSAR	0.000000807	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.94663	no units	

p-Cresol

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
315	USEPA. 2010. Provisional Peer-Reviewed Toxicity Values for 4-Methylphenol (p-Cresol) (CASRN 106-44-5). EPA/690/R-10/019F. U.S. Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment, Superfund Health Risk Technical Support Center, Cincinnati, OH.

Pendimethalin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Pendimethalin
CASRN:	40487-42-1
DTXSID:	DTXSID7024245
Use:	Selective herbicide for control of broadleaf weeds and grassy weed species
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.000044

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	reproductive and developmental effects	9	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	2000	hormonal and histopathological changes in the thyroid	women of childbearing age	OPP	2019

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.088	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Pendimethalin

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.3	mg/kg/day	OPP 2019	Fischer 1991 and 1993; Devito and Braverman 1993	hormonal and histopathological changes in the thyroid	women of childbearing age	35.4	1690	[423]	
Cancer Classification (CC)	C		OPP 2019						[423]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	7	mg/L	EPA HHBP	
Acute PAD	1	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	2	mg/L	EPA HHBP	
Drinking Water Guideline Value	0.02	mg/L	WHO Drinking Water Quality Guidelines	
Health-Based Screening Level	2	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.3	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1050	mg/kg	NIH HSDB	min
LD50	5000	mg/kg	NIH HSDB	max
LOAEL	51	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	622.09998	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	46	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	78.3	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	15.43	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	250	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	25	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0067453	mol/kg	TEST QSAR	
Ames mutagenicity test	0.117	no units	TEST QSAR	
Developmental toxin test	0.948	no units	TEST QSAR	

Technical Support Document for the
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EPA - Office of Water

Pendimethalin
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data											
Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
			Prevalence					Magnitude			
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
			Prevalence					Magnitude			
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	11,234	412	Sites	3.67	2.00E - 04	0.019	0.088	42	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	2,224	387	Sites	17	2.00E - 04	0.019	0.0871	42	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	9,010	25	Sites	0.28	7.00E - 04	0.0185	0.107	0.824	ug/L	
Pesticide Application Data				Toxic Release Data				Chemical Production Data			
Number of States	Amount Applied (lbs/year)	Date		Number of States	Amount Released (lbs/year)			Chemical Data Reporting (CDR) Results (EPA) (2016)	Production Volume (lbs/year)		
Estimated Annual Agricultural Pesticide Use (USGS)	48	17,968,965	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	11	5,858					

Non-Scoring Data											
Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
			Prevalence					Magnitude			
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	1	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	15	2	Sites	13	0.007492	0.008	0.0664	0.076	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
			Prevalence					Magnitude			
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	2	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	1,006	109	Sites	11	0.001	0.024	0.118	2.46	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3,066	2	Sites	0.07	0.011	0.0175	0.0384	0.048	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	4,071	111	Sites	2.73	0.001	0.024	0.115	2.46	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	225	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	218	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	8	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	4,405	416	Sites	9.44	0.005	0.191	1.28	8.35	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	13	Sites	34	0.000319	0.0039	0.0301	0.578	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	4	Sites	0.58	7e-04	0.00145	0.00437	0.0056	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Waste Water Effluent											
			Prevalence					Magnitude			
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Expocast exposure		1.66E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.53725	days	
Boiling point	OPERA QSAR	330.972	degree C	
Boiling point	TEST QSAR	363.278	degree C	
Vapor pressure	OPERA QSAR	0.0000268	mmHg	
Vapor pressure	TEST QSAR	0.000000621	mmHg	
Solubility in water	OPERA QSAR	0.00000164	mol/L	
Solubility in water	TEST QSAR	0.00000984	mol/L	
Bioconcentration factor	OPERA QSAR	979.509	no units	
Bioconcentration factor	TEST QSAR	59.5662	no units	
Henry's Law constant	OPERA QSAR	0.00000168	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	5.0582	no units	

Pendimethalin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
423	USEPA. 2019. Pendimethalin - Human Health Risk Assessment to Support the Proposed New Uses on Leaf Petiole Vegetable Subgroup 22B, Monarda and Rosemary. EPA-HQ-OPP-2018-0619-0008. DP No. D448588. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Permethrin

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Permethrin
CASRN:	52645-53-1
DTXSID:	DTXSID8022292
Use:	Insecticide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	X
Compounds with neurodev effects, Mundy et al 2015	X

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.052

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	carcinogen with linear MOA	4	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	3	lung adenomas and/or carcinomas in female mice	general population	OPP	2017

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.1558	90th Percentile	Finished Water	UCMR4	2018-2019

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
		X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Permethrin
CCL 5 Contaminant Information Sheet
HEALTH EFFECTS DATA

EPA-OGWDW and OST

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Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.147	mg/kg/day	OPP 2017	Wolansky et al., 2006	reduced motor activity	bottle-fed infants	151	195	[388]	
Cancer Slope Factor (CSF)	0.009567	(mg/kg/day)^-1	OPP 2017	Ellison, 1979; Barton, 2000	lung adenomas and/or carcinomas in female mice	general population	33.8	3.09	[388]	
Cancer Classification (CC)	L		OPP 2017						[388]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	1.7	mg/L	EPA HHBP	
Acute Minimal Risk Level (MRL)	0.3	mg/kg/day	CDC ATSDR	
Acute PAD	0.25	mg/kg/day	EPA HHBP	
Cancer Classification (CC)	3	no units	WHO IARC	
Cancer Slope Factor (CSF)	0.009567	(mg/kg/day)^-1	EPA HHBP	
Chronic Human Health Benchmark	1.6	mg/L	EPA HHBP	
Chronic Human Health Benchmark	0.003344	mg/L	EPA HHBP	
Health-Based Screening Level	1.6	mg/L	Health-based screening levels from USGS	
Health-Based Screening Level	0.003344	mg/L	Health-based screening levels from USGS	
Intermediate Minimal Risk Level (MRL)	0.2	mg/kg/day	CDC ATSDR	
Population-Adjusted Dose (PAD)	0.25	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	250	mg/kg	NIH HSDB	min
LD50	6000	mg/kg	NIH HSDB	max
LOAEL	1200	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	91.5	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	5	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	600	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	8.43	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0018578	mol/kg	TEST QSAR	
Ames mutagenicity test	0.272	no units	TEST QSAR	
Developmental toxin test	0.816	no units	TEST QSAR	

Permethrin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019	3,649	10	Sites	0.27	0.04	0.054	0.156	0.212	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	14	2	Sites	14	0.0077	0.00885	0.00954	0.01	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	14	2	Sites	14	0.0077	0.00885	0.00954	0.01	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	45	604,727	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	9	20,106	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	3	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	9	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	140	5	Sites	3.57	0.0044	0.0053	0.0108	0.0146	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	143	5	Sites	3.5	0.0044	0.0053	0.0108	0.0146	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	6,049	452	Sites	7.47	0.000608	0.0169	0.113	180.9	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.000002	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.34923	days	
Boiling point	OPERA QSAR	401.477	degree C	
Boiling point	TEST QSAR	412.391	degree C	
Vapor pressure	OPERA QSAR	3.02E-08	mmHg	
Vapor pressure	TEST QSAR	0.00000001	mmHg	
Solubility in water	OPERA QSAR	0.000000627	mol/L	
Solubility in water	TEST QSAR	5.13E-08	mol/L	
Bioconcentration factor	OPERA QSAR	469.919	no units	
Bioconcentration factor	TEST QSAR	727.78	no units	
Henry's Law constant	OPERA QSAR	4.13E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	6.4075	no units	

Permethrin

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EPA-OGWDW and OST

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Reference Number	Full Reference
388	USEPA. 2017. Permethrin: Human Health Draft Risk Assessment for Registration Review. EPA-HQ-OPP-2011-0039-0088. DP No. 414137. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Phenanthrene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Phenanthrene
CASRN:	85-01-8
DTXSID:	DTXSID6024254
Use:	Dyestuffs, explosives, synthesis of drugs, biochemical research, manufacturing phenanthrenequinone.
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
		9	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.048	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Phenanthrene

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Cancer Classification (CC)	D		IRIS 1990						[208]	
Cancer Classification (CC)	D		OW 1991						[212]	
Cancer Classification (CC)	I		PPRTV 2009						[303]	
			ATSDR 1995						[10]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
						2008-03-08	2020-03-16	2319	0	16	

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Cancer Classification (CC)	3	no units	WHO IARC	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	700	mg/kg	NIH HSDB	
Percent of active toxcast in vitro assays tested	5.92	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0089331	mol/kg	TEST QSAR	
Ames mutagenicity test	0.629	no units	TEST QSAR	
Developmental toxin test	0.651	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
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EPA - Office of Water

Phenanthrene

CCL 5 Contaminant Information Sheet

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
		Prevalence				Magnitude					
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	593	39	Sites	6.58	0.003	0.014	0.048	0.13	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	101	29	Sites	29	0.003	0.0145	0.05	0.13	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	492	10	Sites	2.03	0.008	0.013	0.017	0.044	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)	27	287,091	Chemical Data Reporting (CDR) Results (EPA) (2016)	500K - 1M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	28	1	Sites	3.57	0.001	0.002	0.002	0.002	ug/L	
Drinking Water Monitoring Data - WA (Finished)	2006 - 2011	481	0	Sites	0						
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
		Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	233	2	Sites	0.86	0.1	0.3	0.356	0.37	ug/L	
Drinking Water Monitoring Data - WA (Source)	2006 - 2011	634	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	866	258	Sites	30	0.003	0.02	0.255	26.3	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	1,099	98	Sites	8.92	0.002	0.017	0.0818	140	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,965	356	Sites	18	0.002	0.02	0.24	140	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	6	Sites	16	0.0074	0.0176	0.0239	0.0241	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Waste Water Effluent											
		Prevalence				Magnitude					
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	2	Sites	9.52	0.0086	0.0087	0.00878	0.0088	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg- bw/day)	Notes
ExpoCast exposure		0.00000121	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	63.7756	days	
Boiling point	OPERA QSAR	340.536	degree C	
Boiling point	TEST QSAR	340.522	degree C	
Vapor pressure	OPERA QSAR	0.0000303	mmHg	
Vapor pressure	TEST QSAR	0.000049	mmHg	
Solubility in water	OPERA QSAR	0.00000116	mol/L	
Solubility in water	TEST QSAR	0.00000355	mol/L	
Bioconcentration factor	OPERA QSAR	2227.32	no units	
Bioconcentration factor	TEST QSAR	633.87	no units	
Henry's Law constant	OPERA QSAR	0.0000518	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	4.52256	no units	

Phenanthrene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
10	ATSDR. 1995. Toxicological Profile for Polycyclic Aromatic Hydrocarbons. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
208	USEPA. 1990. Chemical Assessment Summary, Phenanthrene. U.S. Environmental Protection Agency, National Center for Environmental Protection, Integrated Risk Information System (IRIS), Washington, D.C.
212	USEPA. 1991. Drinking Water Criteria Document for Polycyclic Aromatic Hydrocarbons (PAHs). U.S. Environmental Protection Agency, Office of Health and Environmental Assessment, Environmental Criteria and Assessment Office, Cincinnati, OH.
303	USEPA. 2009. Provisional Peer-Reviewed Toxicity Values for Phenanthrene. U.S. Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment, Superfund Health Risk Technical Support Center, Cincinnati, OH.

Phenol

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Phenol
CASRN:	108-95-2
DTXSID:	DTXSID5021124
Use:	Pesticide; chemical intermediate
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	X
Human Neurotoxics	X
PubMed Neurotoxics	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.00029

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
3	reproductive and developmental effects	10	6

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	3000	reductions in mean fetal body weight per litter	women of childbearing age	OPP	2019

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.864	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

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Draft Fifth Contaminant Candidate List (CCL 5)
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Phenol

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.6	mg/kg/day	OPP 2019	Jones-Price and Ledoux 1983	reductions in mean fetal body weight per litter	women of childbearing age	35.4	3390	[426]	
Cancer Classification (CC)	I		OPP 2019						[426]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	6	mg/L	EPA DWSHA 2018	
Acute Minimal Risk Level (MRL)	1	mg/kg/day	CDC ATSDR	
Cancer Classification (CC)	3	no units	WHO IARC	
Chronic Health-Based Guidance Value	4	mg/L	MN DOH	
Human Health Ambient Water Quality Criteria	4	mg/L	EPA Human Health Criteria for CWA	
Lifetime Health Advisory	2	mg/L	EPA DWSHA 2018	
Reference Concentration (RfC)	200	ug/m ³	CalEPA OEHHA Chemical Database	
Cancer Classification (CC)	Female.Mice N	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats N	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice N	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats N	no units	HHS NTP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	100	mg/kg	NIH HSDB	min
LD50	530	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	0.44	percent	EPA Chemistry Dashboard	
TD50	133	mg/kg/day	NIH CPDB	min
TD50	18500	mg/kg/day	NIH CPDB	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0046132	mol/kg	TEST QSAR	
Ames mutagenicity test	0.246	no units	TEST QSAR	
Developmental toxin test	0.58	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
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EPA - Office of Water

Phenol
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	462	98	Sites	21	0.08	0.34	0.864	12	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	93	43	Sites	46	0.09	0.29	0.652	12	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	369	55	Sites	15	0.08	0.41	1.16	2.5	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)	44	5,965,893	Chemical Data Reporting (CDR) Results (EPA) (2016)	1B - 5B

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	7	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	34	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	833	183	Sites	22	0.02	0.14	0.888	54.3	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	1,018	85	Sites	8.35	0.03	0.15	1.06	35.7	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,851	268	Sites	14	0.02	0.14	1.04	54.3	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	4	Sites	11	0.0548	0.0674	0.13	0.151	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	2	Sites	100	0.1	0.45	0.73	0.8	ug/L	
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	11	Sites	52	1	1.6	3.55	5.4	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.0000876	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.58026	days	
Boiling point	OPERA QSAR	187.496	degree C	
Boiling point	TEST QSAR	176.783	degree C	
Vapor pressure	OPERA QSAR	0.256635	mmHg	
Vapor pressure	TEST QSAR	0.151356	mmHg	
Solubility in water	OPERA QSAR	0.647838	mol/L	
Solubility in water	TEST QSAR	0.294442	mol/L	
Bioconcentration factor	OPERA QSAR	16.2785	no units	
Bioconcentration factor	TEST QSAR	7.60326	no units	
Henry's Law constant	OPERA QSAR	0.000000495	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.57532	no units	

Phenol

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
426	USEPA. 2019. Registration Review Draft Risk Assessment for Phenol and Salts. EPA-HQ-OPP-2012-0810-0007. DP No. 453361. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.

Phenol, 4-(1,1,3,3-tetramethylbutyl)-
CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Phenol, 4-(1,1,3,3-tetramethylbutyl)-
CASRN:	140-66-9
DTXSID:	DTXSID9022360
Use:	Used in nonionic surfactants, plasticizers, antioxidants, fuel oil stabilizer, intermediate for resins, fungicides, bactericides, dyestuffs, adhesives, rubber chemicals
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	X
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0014

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	reproductive and developmental effects	9	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	70	decreased uterine weight, decreased pup body weight, increased time to preputial separation, decreased adult body weight	bottle-fed infants	MDH	2015

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.099	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Phenol, 4-(1,1,3,3-tetramethylbutyl)-
CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.051	mg/kg/day	MDH 2015	Tyl et al. 1999	decreased uterine weight, decreased pup body weight, increased time to preputial separation, decreased adult body weight	bottle-fed infants	151	67.6	[137]	

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Reproductive	0.0000275	Blake, 2004	Systemic	450	Bian, 2006		2020-04-07	538	17	6	12

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Health-Based Guidance Value	0.1	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.1	mg/L	MN DOH	
Short-Term/Subchronic Health-Based Guidance Value	0.1	mg/L	MN DOH	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	2000	mg/kg	NIH HSDB	min
LD50	3210	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	40.93	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0070146	mol/kg	TEST QSAR	
Ames mutagenicity test	0.049	no units	TEST QSAR	
Developmental toxin test	0.75	no units	TEST QSAR	

Phenol, 4-(1,1,3,3-tetramethylbutyl)-
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	567	38	Sites	6.7	0.01	0.04	0.099	0.59	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	88	22	Sites	25	0.01	0.02	0.12	0.19	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	479	16	Sites	3.34	0.02	0.05	0.09	0.59	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	50M - 100M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	717	61	Sites	8.51	0.01	0.1	0.1	1	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	689	29	Sites	4.21	0.01	0.25	1.32	42.6	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,406	90	Sites	6.4	0.01	0.1	0.2	42.6	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	8	Sites	21	0.0204	0.0374	0.286	0.355	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	14	Sites	67	0.1	0.19	0.223	0.23	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.0000755	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)	0.2	ug/l	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.08153	days	
Boiling point	OPERA QSAR	263.357	degree C	
Boiling point	TEST QSAR	293.064	degree C	
Vapor pressure	OPERA QSAR	0.00142088	mmHg	
Vapor pressure	TEST QSAR	0.00156315	mmHg	
Solubility in water	OPERA QSAR	0.000088	mol/L	
Solubility in water	TEST QSAR	0.000132434	mol/L	
Bioconcentration factor	OPERA QSAR	344.461	no units	
Bioconcentration factor	TEST QSAR	139.637	no units	
Henry's Law constant	OPERA QSAR	0.00000786	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	4.86646	no units	

Phenol, 4-(1,1,3,3-tetramethylbutyl)-

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
137	MDH. 2015. Toxicological Summary for: 4-tert-Octylphenol. Minnesota Department of Health (MDH), Environmental Health Division, Health Risk Assessment Unit, St Paul, MN.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.

Phorate

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Phorate
CASRN:	298-02-2
DTXSID:	DTXSID4032459
Use:	Insecticide used on corn, sugar beets, cotton, brassicas, and coffee
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	X
Human Neurotoxics	X
PubMed Neurotoxics	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.42

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	reproductive and developmental effects	3	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.2	red blood cell and brain cholinesterase inhibition	bottle-fed infants	OPP	2006

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.0848	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Phorate

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.00017	mg/kg/day	OPP 2006	Shellenberger and Tegeris, 1987	red blood cell and brain cholinesterase inhibition	bottle-fed infants	151	0.225	[273]	NOTE: this compound is a organophosphate pesticide. EPA has created a cumulative risk assessment regarding the common mechanisms of organophosphate compounds.
Cancer Classification (CC)	E		OPP 2006						[273]	NOTE: this compound is a organophosphate pesticide. EPA has created a cumulative risk assessment regarding the common mechanisms of organophosphate compounds.

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.005	mg/L	EPA HHBP	
Acute PAD	0.0008	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.0011	mg/L	EPA HHBP	
Health-Based Screening Level	0.0011	mg/L	Health-based screening levels from USGS	
Maximum Allowable Concentration (MAC)	0.002	mg/L	Canadian Drinking Water Guidelines	
Population-Adjusted Dose (PAD)	0.00017	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1.1	mg/kg	NIH HSDB	min
LD50	3.7	mg/kg	NIH HSDB	max
LOAEL	0.8	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	0.05	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	0.01	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	0.4	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in	5.26	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	7.83E-06	mol/kg	TEST QSAR	
Ames mutagenicity test	-0.017	no units	TEST QSAR	
Developmental toxin test	-0.176	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Phorate
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	11,241	24	Sites	0.21	0.002	0.012	0.0848	0.6	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	2,230	21	Sites	0.94	0.002	0.0125	0.082	0.6	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	9,012	3	Sites	0.03	0.00317	0.006	0.147	0.208	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	19	945,534	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	1	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	1	Sites	5.88	0.078	0.078	0.078	0.078	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	4	0	Sites	0						
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	1	Sites	0.44	0.062	0.062	0.062	0.062	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	1	Sites	8.33	0.062	0.062	0.062	0.062	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	11,178	13	Sites	0.12	0.016	0.075	0.129	0.22	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	1	Sites	0.14	0.0032	0.0032	0.0032	0.0032	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		1.23E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	139.463	days	
Boiling point	OPERA QSAR	285.229	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.000319476	mmHg	
Vapor pressure	TEST QSAR	0.000179473	mmHg	
Solubility in water	OPERA QSAR	0.000199114	mol/L	
Solubility in water	TEST QSAR	0.000233346	mol/L	
Bioconcentration factor	OPERA QSAR	71.5592	no units	
Bioconcentration factor	TEST QSAR	55.5904	no units	
Henry's Law constant	OPERA QSAR	0.00000156	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.43867	no units	

Phorate

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
273	USEPA. 2006. Reregistration Eligibility Decision for Phorate. EPA-HQ-OPP-2008-0174-0003. U.S. Environmental Protection Agency, Office of Prevention, Pesticides and Toxic Substances, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Phosmet

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Phosmet
CASRN:	732-11-6
DTXSID:	DTXSID5024261
Use:	
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.23

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	reproductive and developmental effects	2	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.2	pup red blood cell acetylcholinesterase inhibition	bottle-fed infants	OPP	2016

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.045	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Phosmet

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.00016	mg/kg/day	OPP 2016	Barnett 2009	pup red blood cell acetylcholinesterase inhibition	bottle-fed infants	151	0.212	[371]	
Cancer Classification (CC)	S		OPP 2016						[371]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.08	mg/L	EPA HHBP	
Acute PAD	0.012	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.003	mg/L	EPA HHBP	
Health-Based Screening Level	0.003	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.0006	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	160	mg/kg	NIH HSDB	max
LD50	26	mg/kg	NIH HSDB	min
Percent of active toxcast in vitro assays tested	6.25	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0001349	mol/kg	TEST QSAR	
Ames mutagenicity test	0.722	no units	TEST QSAR	
Developmental toxin test	0.568	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

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July 2021

EPA - Office of Water

Phosmet
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	3,376	4	Sites	0.12	0.006	0.0125	0.045	0.063	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	380	3	Sites	0.79	0.006	0.018	0.0495	0.063	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	2,996	1	Sites	0.03	0.007	0.007	0.007	0.007	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	40	844,617	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	15	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	569	2	Sites	0.35	0.017	0.0945	0.141	0.172	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	1,971	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	2,539	2	Sites	0.08	0.017	0.0945	0.141	0.172	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	119	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	111	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	8	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	9,749	7	Sites	0.07	0.0535	0.375	0.978	1.5	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	106	0	Sites	0						
Southeast Stream Quality Assessment (SESQA) (Ambient) [102]	2014	1	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		9.34E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	125.261	days	
Boiling point	OPERA QSAR	403.932	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.000000516	mmHg	
Vapor pressure	TEST QSAR	0.000000668	mmHg	
Solubility in water	OPERA QSAR	0.0000549	mol/L	
Solubility in water	TEST QSAR	0.0000598	mol/L	
Bioconcentration factor	OPERA QSAR	2.48955	no units	
Bioconcentration factor	TEST QSAR	9.18333	no units	
Henry's Law constant	OPERA QSAR	3.84E-10	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.89029	no units	

Phosmet

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
102	https://webapps.usgs.gov/rsqa/#!/region/SESQA
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
371	USEPA. 2016. Phosmet. Draft Human Health Risk Assessment to Support Registration Review. EPA-HQ-OPP-2009-0316-0022. DP No. D420736. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Phosphorus

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Phosphorus
CASRN:	7723-14-0
DTXSID:	DTXSID1024382
Use:	Former pesticide; chemical intermediate; as ammunition
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	X
PubMed Neurotoxics	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0013

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
	no adverse effects	10	10

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	300000	no adverse effects	pregnant women	IOM	1997

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
381	90th Percentile	Finished Water	NIRS	1984-1986

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Phosphorus
CCL 5 Contaminant Information Sheet
HEALTH EFFECTS DATA

EPA-OGWDW and OST

July 2021

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
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Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	4000	mg/day	IOM 1997		There is no evidence that individuals consuming this intake may experience adverse effects.	lactating women	2720	294000	[107]	NOTE: IOM identifies Upper Tolerable Intake values for many populations. The lowest UTI was for pregnant women, which is the group used for this CCL Screening Level - this value is reported as mg/day as opposed to mg/kg/day. For this reason, the DWI for pregnant women in units of ml/day is used as opposed to the intake in mg/kg/day.
Reference Dose (RfD) or Equivalent	3500	mg/day	IOM 1997		There is no evidence that individuals consuming this intake may experience adverse effects.	pregnant women	2642	265000	[107]	NOTE: IOM identifies Upper Tolerable Intake values for many populations. The lowest UTI was for pregnant women, which is the group used for this CCL Screening Level - this value is reported as mg/day as opposed to mg/kg/day. For this reason, the DWI for pregnant women in units of ml/day is used as opposed to the intake in mg/kg/day.
Reference Dose (RfD) or Equivalent	4000	mg/day	IOM 1997		metastatic calcification, skeletal porosity, interference with calcium absorption	general population	2413	332000	[107]	NOTE: IOM identifies Upper Tolerable Intake values for many populations. The lowest UTI was for pregnant women, which is the group used for this CCL Screening Level - this value is reported as mg/day as opposed to mg/kg/day. For this reason, the DWI for pregnant women in units of ml/day is used as opposed to the intake in mg/kg/day.

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
The full citation for the critical study is provided in the corresponding health assessment.
PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	3.03	mg/kg	NIH HSDB	min
LD50	4.85	mg/kg	NIH HSDB	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity test			TEST QSAR	
Developmental toxin test			TEST QSAR	

Phosphorus
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986	987	392	Sites	40	42	104	381	5546	ug/L	
Ambient Water											
		Prevalence				Magnitude					
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	3,889	185	Sites	4.76	3	92	680	10100	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	1,278	165	Sites	13	3	92	681	10100	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	2,613	20	Sites	0.77	10	70	523	1400	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	250M - 500M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	68		200		700	ug/L	
Community Water System Survey (CWSS) (Finished) [178]	2006	1	NA	Sites			380	380		ug/L	
Ambient Water											
		Prevalence				Magnitude					
Drinking Water Monitoring Data - WI (Source)	2012-2019	1	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	2,063	466	Sites	23	1	61	399	15900	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	1,357	345	Sites	25	1	101	631	380000	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	3,413	811	Sites	24	1	61	408	380000	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	88		70		220	ug/L	
Waste Water Effluent											
		Prevalence				Magnitude					
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR			
Boiling point	OPERA QSAR			
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR			
Vapor pressure	TEST QSAR			
Solubility in water	OPERA QSAR			
Solubility in water	TEST QSAR			
Bioconcentration factor	OPERA QSAR			
Bioconcentration factor	TEST QSAR			
Henry's Law constant	OPERA QSAR			
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR			

Phosphorus

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Reference Number	Full Reference
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. Science of The Total Environment. v581-582, (909-922).
107	IOM. 1997. Standing Committee on the Scientific Evaluation of Dietary Reference Intakes, Food and Nutrition Board. Dietary Reference Intakes for calcium, phosphorus, magnesium, vitamin D, and fluoride. Institute of Medicine (IOM), National Academy Press, Washington, DC.
178	USEPA (US Environmental Protection Agency). (2009). 2006 Community Water System Survey. Overview, 57.

Phostebupirim

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Phostebupirim
CASRN:	96182-53-5
DTXSID:	DTXSID1032482
Use:	Insecticide used on corn
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	X
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.21

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
8	reproductive and developmental effects	8	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.03	plasma, red blood cell, and brain cholinesterase inhibition	bottle-fed infants	OPP	2009

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.006258	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Phostebupirim

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.00002	mg/kg/day	OPP 2009	Porter et al. 1991	plasma, red blood cell, and brain cholinesterase inhibition	bottle-fed infants	151	0.0265	[306]	
Cancer Classification (CC)	E		OPP 2009						[306]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.001	mg/L	EPA HHBP	
Acute PAD	0.00017	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.0001	mg/L	EPA HHBP	
Health-Based Screening Level	0.0001	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.00002	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1.3	mg/kg	NIH HSDB	min
LD50	14	mg/kg	NIH HSDB	max
LOAEL	0.125	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	38.779999	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	0.0175	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	5.32	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	18.87	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	1	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	3.5999999	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	0.3	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	1	mg/kg/day	EPA Toxicity Reference Database	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.000278	mol/kg	TEST QSAR	
Ames mutagenicity test	-0.032	no units	TEST QSAR	
Developmental toxin test	0.634	no units	TEST QSAR	

Phostebupirim

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	1,994	48	Sites	2.41	7.00E - 05	0.00144	0.00626	0.232	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	338	46	Sites	14	7.00E - 05	0.00143	0.00581	0.191	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	1,656	2	Sites	0.12	0.00029	0.222	0.229	0.232	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	19	296,550	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	15	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	359	15	Sites	4.18	0.00032	0.00141	0.241	0.266	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	528	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	887	15	Sites	1.69	0.00032	0.00141	0.241	0.266	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	225	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	218	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	8	0	Sites	0						
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	1	Sites	0.17	3e-04	3e-04	3e-04	3e-04	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.000000109	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.75549	days	
Boiling point	OPERA QSAR	343.127	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.0000536	mmHg	
Vapor pressure	TEST QSAR	0.0000449	mmHg	
Solubility in water	OPERA QSAR	0.0000241	mol/L	
Solubility in water	TEST QSAR	0.0000417	mol/L	
Bioconcentration factor	OPERA QSAR	33.1025	no units	
Bioconcentration factor	TEST QSAR	174.582	no units	
Henry's Law constant	OPERA QSAR	0.000000466	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.53897	no units	

Phostebupirim

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
306	USEPA. 2009. Tebupirimphos (Phostebupirim) in/on Corn, field, pop, sweet. Health Effects Division (HED) Risk Assessment. EPA-HQ-OPP-2008-0940-0010. DP No. D368530. U.S. Environmental Protection Agency, Office of Prevention, Pesticides and Toxic Substances, Washington, D.C.

Piperonyl butoxide

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Piperonyl butoxide
CASRN:	51-03-6
DTXSID:	DTXSID1021166
Use:	Synergist for the pyrethrins and related insecticides
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.000022

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	non-cancer effects	9	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	900	decrease in body weight gain, and increases in alkaline phosphatase activity, liver weight and hepatocellular hypertrophy	general population	OPP	2017

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.0202	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis
Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

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Piperonyl butoxide
CCL 5 Contaminant Information Sheet
HEALTH EFFECTS DATA

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Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.16	mg/kg/day	OPP 2017	Goldenthal 1993a and b	decrease in body weight gain, and increases in alkaline phosphatase activity, liver weight and hepatocellular hypertrophy, decreased body weight	general population	33.8	947	[389]	
Cancer Classification (CC)	C		OPP 2017						[389]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	42	mg/L	EPA HHBP	
Acute PAD	6.3	mg/kg/day	EPA HHBP	
Cancer Classification (CC)	3	no units	WHO IARC	
Chronic Human Health Benchmark	0.992	mg/L	EPA HHBP	
Health-Based Screening Level	0.992	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.155	mg/kg/day	EPA HHBP	
Cancer Classification (CC)	Female.Mice N	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats N	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice N	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats N	no units	HHS NTP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	11500	mg/kg	NIH HSDB	max
LD50	2600	mg/kg	NIH HSDB	min
LOAEL	15.5	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	500	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	2.9	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	200	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in	13.43	percent	EPA Chemistry Dashboard	
TD50	1180	mg/kg/day	NIH CPDB	min
TD50	7820	mg/kg/day	NIH CPDB	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0074131	mol/kg	TEST QSAR	
Ames mutagenicity test	0.08	no units	TEST QSAR	
Developmental toxin test	0.43	no units	TEST QSAR	

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Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

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EPA - Office of Water

Piperonyl butoxide
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	1,891	115	Sites	6.08	1.00E - 04	0.0054	0.0202	0.369	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	324	107	Sites	33	1.00E - 04	0.00545	0.0202	0.369	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	1,567	8	Sites	0.51	0.0015	0.0023	0.0635	0.239	ug/L	
Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data			Number of States	Amount Released (lbs/year)	Chemical Production Data		Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	3	9,087	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			8	27	Chemical Data Reporting (CDR) Results (EPA) (2016)		500K - 1M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	11	1	Sites	9.09	0.095	0.095	0.095	0.095	ug/L	
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	555	90	Sites	16	0.00022	0.0058	0.064	0.47	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	731	7	Sites	0.96	0.00021	0.00172	0.0222	0.0934	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,286	97	Sites	7.54	0.00021	0.0053	0.0642	0.47	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	6	1	Sites	17	0.062	0.062	0.062	0.062	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	2	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	4	1	Sites	25	0.062	0.062	0.062	0.062	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	267	78	Sites	29	0.000676	0.0184	1.18	11.2	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	12	Sites	32	0.0084	0.064	0.118	0.2049	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	5	Sites	0.86	0.0021	0.0024	0.014	0.0196	ug/L	
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	17	Sites	81	0.0015966	0.0254	0.094	0.0989808	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		2.25E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.73603	days	
Boiling point	OPERA QSAR	324.392	degree C	
Boiling point	TEST QSAR	393.28	degree C	
Vapor pressure	OPERA QSAR	8.18E-08	mmHg	
Vapor pressure	TEST QSAR	0.000000708	mmHg	
Solubility in water	OPERA QSAR	0.0000389	mol/L	
Solubility in water	TEST QSAR	0.0000724	mol/L	
Bioconcentration factor	OPERA QSAR	126.704	no units	
Bioconcentration factor	TEST QSAR	18.55	no units	
Henry's Law constant	OPERA QSAR	0.00000225	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	4.39613	no units	

Piperonyl butoxide

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
389	USEPA. 2017. Piperonyl Butoxide (PBO). Draft Human Health Risk Assessment Registration Review and for Proposed New Use on Edible Fungi Crop Group 21. EPA-HQ-OPP-2010-0498-0021. DP Nos. D434163 D439507. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Potassium

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Potassium
CASRN:	7440-09-7
DTXSID:	DTXSID9049748
Use:	Metal, laboratory reagent
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
		10	10

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
5939	90th Percentile	Finished Water	NIRS	1984-1986

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Potassium

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
			HC 2008						[93]	NOTE: assessment states "no RfD derived because potassium intake from drinking water is well below the level at which adverse health effects may occur." Additional information from the 2019 IOM report for potassium and sodium: Short-term potassium supplementation of approximately 2,500 mg/d (64 mmol/d) on the background of a usual diet appears to be safe for generally healthy individuals. This level of potassium intake would likely be below the UL for individuals without kidney disease, diabetes, heart failure, adrenal insufficiency, or individuals using ACE-Is, ARBs, or other medications that may raise blood potassium concentrations to levels that could lead to adverse effects. There is evidence that very high doses of supplemental potassium ingestion can lead to adverse events, and in extreme cases has led to death, even in the absence of kidney disease or other factors that alter potassium excretion. However, without a specific indicator of a toxicological effect of high potassium intake, a potassium UL cannot be established."

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	4700	mg/day	IOM 2005		arrhythmias and hyperkalemia in individuals with impaired potassium excretion, detrimental for individuals with impaired kidney function	general population	2413	390000	[109]	
			IOM 2019						[112]	

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity test			TEST QSAR	
Developmental toxin test			TEST QSAR	

July 2021

Scoring Data

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Storing Data												
Non-Nationally Representative Water Data		Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water			Prevalence				Magnitude					
Glassmeyer et al 2017 (Finished) [86]		2007 - 2012	25	NA	Sites	100		3070		6870	ug/L	
Community Water System Survey (CWSS) (Finished) [178]		2006	10	NA	Sites			2510	4100		ug/L	
Ambient Water			Prevalence				Magnitude					
Glassmeyer et al 2017 (Ambient) [86]		2007 - 2012	25	NA	Sites	100		2720		6930	ug/L	
Arnold et al. 2016 (Filtered) [7]		2012 - 2013	758	757	Sites	100	80	2300	8618	61200	ug/L	
Waste Water Effluent			Prevalence				Magnitude					
Estimated Concentration in Water		Date	Source	Value	Units	Model	Notes					

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

UCMB 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Potassium

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. Science of The Total Environment. v581-582, (909-922).
93	HC. 2008. Guidance on Potassium from Water Softeners. Health Canada (HC), Water, Air and Climate Change Bureau, Healthy Environments and Consumer Safety Branch, Ottawa, Ontario, Canada.
109	IOM. 2005. Dietary Reference Intakes for Water, Potassium, Sodium, Chloride, and Sulfate. Institute of Medicine (IOM), National Academies of Science, Washington, D.C.
112	IOM. 2019. Dietary Reference Intakes for Sodium and Potassium (2019). Institute of Medicine (IOM), National Academies of Science, Washington, D.C.
178	USEPA (US Environmental Protection Agency). (2009). 2006 Community Water System Survey. Overview, 57.

Profenofos

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Profenofos
CASRN:	41198-08-7
DTXSID:	DTXSID3032464
Use:	Pesticide, insecticide, acaricide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	2.6

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	reproductive and developmental effects	1	6

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.2	inhibition of brain acetylcholinesterase	bottle-fed infants	OPP	2015

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.5144	90th Percentile	Finished Water	UCMR4	2018-2019

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
		X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Profenofos

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.00012	mg/kg/day	OPP 2015	Burdock et al. 1981	inhibition of brain acetylcholinesterase	bottle-fed infants	151	0.159	[351]	
Cancer Classification (CC)	E		OPP 2015						[351]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.03	mg/L	EPA HHBP	
Acute PAD	0.005	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.0003	mg/L	EPA HHBP	
Health-Based Screening Level	0.0003	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.00005	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1.9	mg/kg	NIH HSDB	min
LD50	700	mg/kg	NIH HSDB	max
LOAEL	1	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	120	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	0.03	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	30	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	15.19	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	0.05	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	0.005	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0004498	mol/kg	TEST QSAR	
Ames mutagenicity test	0.137	no units	TEST QSAR	
Developmental toxin test	0.615	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Profenofos
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019	3,649	2	Sites	0.05	0.464	0.492	0.514	0.52	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	1,953	7	Sites	0.36	0.00019	0.00128	0.144	0.21	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	338	5	Sites	1.48	0.00019	0.00128	0.0522	0.128	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	1,615	2	Sites	0.12	0.00072	0.105	0.168	0.21	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	1	58	2012	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	13	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	303	2	Sites	0.66	0.209	0.214	0.217	0.219	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	528	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	831	2	Sites	0.24	0.209	0.214	0.217	0.219	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	8	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	2	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	6	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	809	0	Sites	0						
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	1	Sites	0.17	7e-04	7e-04	7e-04	7e-04	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.000000144	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.35324	days	
Boiling point	OPERA QSAR	364.071	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.00000174	mmHg	
Vapor pressure	TEST QSAR	0.00000244	mmHg	
Solubility in water	OPERA QSAR	0.0000653	mol/L	
Solubility in water	TEST QSAR	0.0000518	mol/L	
Bioconcentration factor	OPERA QSAR	1513.33	no units	
Bioconcentration factor	TEST QSAR	55.0808	no units	
Henry's Law constant	OPERA QSAR	0.0000089	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	4.76488	no units	

Profenofos

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
351	USEPA. 2015. Profenofos: Human Health Draft Risk Assessment (DRA) for Registration Review. EPA-HQ-OPP-2008-0345-0024. DP No. D414150. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Prometon

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Prometon
CASRN:	1610-18-0
DTXSID:	DTXSID6022341
Use:	Herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.00015

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	non-cancer effects	1	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	300	emesis and decreased body weight	general population	OPP	2017

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.046	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X	X		

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Prometon

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.05	mg/kg/day	OPP 2017	Breckenridge and Green 1986; Tisdell 1992; Salamon 1987	emesis and decreased body weight	general population	33.8	296	[390]	
Cancer Classification (CC)	NL		OPP 2017						[390]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	0.2	mg/L	EPA DWSHA 2018	
Chronic Health-Based Guidance Value	0.1	mg/L	MN DOH	
Lifetime Health Advisory	0.4	mg/L	EPA DWSHA 2018	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	2980	mg/kg	NIH HSDB	max
LD50	503	mg/kg	NIH HSDB	min
LOAEL	23.299999	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	737	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	1.18	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	120	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	4.59	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0026915	mol/kg	TEST QSAR	
Ames mutagenicity test	0.106	no units	TEST QSAR	
Developmental toxin test	0.947	no units	TEST QSAR	

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OCCURRENCE DATA

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003	295	0	Sites	0					ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	11,365	2,286	Sites	20	0	0.01	0.046	40	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	2,297	1,377	Sites	60	0	0.01	0.044	25.1	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	9,069	909	Sites	10	0.00033	0.011	0.078	40	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	1	0.22	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	49	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	11	Sites	65	0.00028	0.0025	0.009	0.092	ug/L	
Bradley et al. 2018 (Finished) [53]	2016	26	1	Sites	3.85	0.0084	0.0084	0.0084	0.0084	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	1	Sites	100	0.01	0.01	0.01	0.01	ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	450	4	Sites	0.89	0.1	0.11	0.12	0.12	ug/L	
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	1,613	594	Sites	37	0.00015	0.009	0.05	6.51	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3,729	320	Sites	8.58	0.00059	0.01	0.05	0.495	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	5,341	914	Sites	17	0.00015	0.009	0.05	6.51	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	82	Sites	36	0.00028	0.0025	0.013	0.891	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	74	Sites	34	0.00028	0.0011	0.0056	0.054	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	8	Sites	67	0.00028	0.0025	0.013	0.891	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	4,469	98	Sites	2.19	0.006	0.0873	0.276	1.6	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	18	Sites	47	0.0049	0.00695	0.0295	0.133	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	64	Sites	9.28	4e-04	0.0036	0.0126	0.0438	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	2	Sites	100	0.01	0.01	0.015	0.02	ug/L	
USGS, McKenzie River, Oregon, 2012 (Ambient) [158]	2002 - 2010	133	19	Samples	14				0.06	ug/L	
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	0	Sites	0						
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exposure exposure		7.95E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.81769	days	
Boiling point	OPERA QSAR	336.341	degree C	
Boiling point	TEST QSAR	329.884	degree C	
Vapor pressure	OPERA QSAR	0.00000249	mmHg	
Vapor pressure	TEST QSAR	0.000000752	mmHg	
Solubility in water	OPERA QSAR	0.00205423	mol/L	
Solubility in water	TEST QSAR	0.00400867	mol/L	
Bioconcentration factor	OPERA QSAR	3.05344	no units	
Bioconcentration factor	TEST QSAR	7.8886	no units	
Henry's Law constant	OPERA QSAR	1.75E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.05368	no units	

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. <i>Environmental science & technology</i> , 52(23), 13972-13985.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
158	Reconnaissance of Land-Use Sources of Pesticides in Drinking Water, McKenzie River, Oregon. U.S. Geological Survey Scientific Investigations Report 2012–5091, 46 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
390	USEPA. 2017. Prometon. Chronic Dietary (Drinking Water Only) Exposure and Risk Assessment for the Registration Review Draft Risk Assessment. EPA-HQ-OPP-2013-0068-0015. DP No. D443014. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Prometryn

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Prometryn
CASRN:	7287-19-6
DTXSID:	DTXSID4024272
Use:	Herbicide for most annual grasses, broadleaf weeds in cotton and celery
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.00025

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	non-cancer effects	9	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	200	renal and hepatic degenerative changes, bone marrow atrophy	general population	OPP	2013

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.051	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Prometryn

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.04	mg/kg/day	OPP 2013	Woodard et al. 1965	renal and hepatic degenerative changes, bone marrow atrophy	general population	33.8	237	[329]	
Cancer Classification (CC)	E		OPP 2013						[329]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	3.3	mg/L	EPA HHBP	
Acute PAD	0.12	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.3	mg/L	EPA HHBP	
Health-Based Screening Level	0.3	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.04	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1265	mg/kg	NIH HSDB	min
LD50	5233	mg/kg	NIH HSDB	max
LOAEL	37.5	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	72	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	0.7	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	37.25	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	7.17	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0075858	mol/kg	TEST QSAR	
Ames mutagenicity test	0.177	no units	TEST QSAR	
Developmental toxin test	0.57	no units	TEST QSAR	

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OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	5,273	139	Sites	2.64	0.00017	0.007	0.051	3.73	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	712	106	Sites	15	0.00017	0.007	0.053	3.73	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	4,561	33	Sites	0.72	0.00048	0.006	0.0279	0.277	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	20	1,458,440	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	2	860	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	99	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	5	Sites	29	0.00028	0.025	0.0866	0.231	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	1,207	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	880	53	Sites	6.02	0.00017	0.009	0.119	0.658	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	2,579	15	Sites	0.58	0.00015	0.006	0.0108	0.037	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	3,458	68	Sites	1.97	0.00015	0.008	0.0993	0.658	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	8	Sites	3.49	0.00028	0.00028	0.00552	0.118	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	8	Sites	67	0.00028	0.00028	0.00552	0.118	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	3,433	92	Sites	2.68	0.0031	0.122	0.756	20	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	2	Sites	5.26	0.0032	0.0159	0.0261	0.0286	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.000000069	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.74373	days	
Boiling point	OPERA QSAR	338.854	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.00000143	mmHg	
Vapor pressure	TEST QSAR	0.000000959	mmHg	
Solubility in water	OPERA QSAR	0.000138089	mol/L	
Solubility in water	TEST QSAR	0.000322849	mol/L	
Bioconcentration factor	OPERA QSAR	12.3056	no units	
Bioconcentration factor	TEST QSAR	9.35406	no units	
Henry's Law constant	OPERA QSAR	2.33E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.60968	no units	

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CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
329	USEPA. 2013. Prometryn. Human-Health Assessment Scoping Document in Support of Registration Review. EPA-HQ-OPP-2013-0032-0006. DP No. D407422. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Pronamide

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Pronamide
CASRN:	23950-58-5
DTXSID:	DTXSID2020420
Use:	Selective herbicide used on annual and perennial grasses
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	X
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.00026

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	reproductive and developmental effects	7	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	200	decreases in body weight, weight gain, and food consumption; increased liver weight and lesions in liver, thyroid, and ovaries	women of childbearing age	OPP	2015

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.052	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Pronamide

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.04	mg/kg/day	OPP 2015	Andrus and Hukkanen 2011	decreases in body weight, weight gain, and food consumption; increased liver weight; lesions in liver, thyroid, and ovaries	women of childbearing age	35.4	226	[352]	
Cancer Classification (CC)	NL		OPP 2015						[352]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	0.8	mg/L	EPA DWSHA 2018	
Acute Human Health Benchmark	0.3	mg/L	EPA HHBP	
Acute PAD	0.04	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.3	mg/L	EPA HHBP	
Health-Based Screening Level	0.3	mg/L	Health-based screening levels from USGS	
Lifetime Health Advisory	0.001	mg/L	EPA DWSHA 2018	
Population-Adjusted Dose (PAD)	0.04	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	5600	mg/kg	NIH HSDB	min
LD50	8350	mg/kg	NIH HSDB	max
LOAEL	123.2	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	20	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	17.5	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	5	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	8.08	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	60	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	15	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0070632	mol/kg	TEST QSAR	
Ames mutagenicity test	0.667	no units	TEST QSAR	
Developmental toxin test	0.574	no units	TEST QSAR	

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EPA - Office of Water

Pronamide
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
		Prevalence				Magnitude					
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	11,233	143	Sites	1.27	0.00021	0.009	0.052	1.35	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	2,224	133	Sites	5.98	0.00021	0.009	0.0512	1.35	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	9,009	10	Sites	0.11	0.0012	0.00695	0.23	0.82	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	3	137,018	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	4	0.35	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	13	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
		Prevalence				Magnitude					
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	1,020	22	Sites	2.16	7.00E - 04	0.0104	0.24	5.75	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3,065	2	Sites	0.07	0.0075	0.0146	0.0188	0.0216	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	4,084	24	Sites	0.59	7.00E - 04	0.0104	0.234	5.75	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	8	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	2	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	6	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	641	49	Sites	7.64	0.005	0.017	0.0448	0.25	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	1	Sites	2.63	0.1134	0.113	0.113	0.1134	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
USGS, McKenzie River, Oregon, 2012 (Ambient) [158]	2002 - 2010	133	1	Samples	0.8				0.014	ug/L	
Waste Water Effluent											
		Prevalence				Magnitude					
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		1.59E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.30719	days	
Boiling point	OPERA QSAR	312.471	degree C	
Boiling point	TEST QSAR	339.245	degree C	
Vapor pressure	OPERA QSAR	0.000000538	mmHg	
Vapor pressure	TEST QSAR	0.00000364	mmHg	
Solubility in water	OPERA QSAR	0.0000887	mol/L	
Solubility in water	TEST QSAR	0.000169044	mol/L	
Bioconcentration factor	OPERA QSAR	56.9152	no units	
Bioconcentration factor	TEST QSAR			
Henry's Law constant	OPERA QSAR	1.53E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.32595	no units	

Pronamide

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
158	Reconnaissance of Land-Use Sources of Pesticides in Drinking Water, McKenzie River, Oregon. U.S. Geological Survey Scientific Investigations Report 2012–5091, 46 p. plus appendixes.
352	USEPA. 2015. Pronamide. Human Health Risk Assessment for Registration Review and to Support New Section 3 Use on Leaf Lettuce (Revised). EPA-HQ-OPP-2009-0326-0017. DP Nos. D422207 D410291. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Propachlor

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Propachlor
CASRN:	1918-16-7
DTXSID:	DTXSID4024274
Use:	selective herbicide used for preemergence weed control of annual grasses and broadleaf weeds
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	1.3

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	carcinogen with linear MOA	1	5

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.9	ovarian tumors	general population	OPP	1998

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
1.18	90th Percentile	Finished Water	UCM2	1993-1997

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Propachlor

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.054	mg/kg/day	OPP 1998	Naylor and Thake 1996	stomach lesions in males and liver lesions in both sexes	general population	33.8	320	[231]	
Cancer Slope Factor (CSF)	0.032	(mg/kg/day)^-1	OPP 1998	Hamada 1987	ovarian tumors	general population	33.8	0.925	[231]	
Cancer Classification (CC)	L		OPP 1998						[231]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	0.5	mg/L	EPA DWSHA 2018	
Chronic Health-Based Guidance Value	0.09	mg/L	MN DOH	
Lifetime Health Advisory	0.001	mg/L	EPA DWSHA 2018	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1800	mg/kg	NIH HSDB	max
LD50	290	mg/kg	NIH HSDB	min
LOAEL	125.3	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	25	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	5	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	65.5	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	37.97	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0016181	mol/kg	TEST QSAR	
Ames mutagenicity test	0.347	no units	TEST QSAR	
Developmental toxin test	0.777	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
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EPA - Office of Water

Propachlor
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data											
Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water			Prevalence			Magnitude					
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997	12,050	6	Sites	0.05	0.1	0.11	1.18	2.5	ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water			Prevalence			Magnitude					
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	8,480	98	Sites	1.16	0.001	0.008	0.0912	2.99	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	1,867	92	Sites	4.93	0.001	0.0085	0.0918	2.99	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	6,614	6	Sites	0.09	0.002	0.0055	0.033	0.057	ug/L	
Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data		Number of States	Amount Released (lbs/year)	Chemical Production Data		Production Volume (lbs/year)	
Estimated Annual Agricultural Pesticide Use (USGS)	4	120,862	2005	Toxic Release Inventory (TRI) Program (EPA) (2016)		2	15	Chemical Data Reporting (CDR) Results (EPA) (2016)			

Non-Scoring Data											
Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	180	0	Sites	0						
Drinking Water Monitoring Data - MA (Finished)	2006 - 2020	822	1	Sites	0.12	0.093	0.093	0.093	0.093	ug/L	
Drinking Water Monitoring Data - WA (Finished)	2006 - 2011	822	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	3	Sites	18	0.00107	0.00107	0.145	0.287	ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	2,047	0	Sites	0						
Drinking Water Monitoring Data - MA (Source)	2006 - 2020	78	0	Sites	0						
Drinking Water Monitoring Data - WA (Source)	2006 - 2011	997	0	Sites	0						
Drinking Water Monitoring Data - WI (Source)	2012-2019	92	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	313	2	Sites	0.64	0.002	0.041	0.0644	0.08	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	812	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,125	2	Sites	0.18	0.002	0.041	0.0644	0.08	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	2	Sites	0.87	0.00107	0.00298	0.00452	0.0049	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	2	Sites	17	0.00107	0.00298	0.00452	0.0049	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	707	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Expcast exposure		6.56E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.36055	days	
Boiling point	OPERA QSAR	292.103	degree C	
Boiling point	TEST QSAR	300.836	degree C	
Vapor pressure	OPERA QSAR	0.000341887	mmHg	
Vapor pressure	TEST QSAR	0.000100925	mmHg	
Solubility in water	OPERA QSAR	0.00447549	mol/L	
Solubility in water	TEST QSAR	0.00156675	mol/L	
Bioconcentration factor	OPERA QSAR	32.0372	no units	
Bioconcentration factor	TEST QSAR	20.797	no units	
Henry's Law constant	OPERA QSAR	0.000000124	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.28865	no units	

Propachlor

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Reference Number	Full Reference
231	USEPA. 1998. Reregistration Eligibility Decision (RED) Propachlor. EPA 738-R-015. U.S. Environmental Protection Agency, Office of Prevention, Pesticides and Toxic Substances, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Propanil

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Propanil
CASRN:	709-98-8
DTXSID:	DTXSID8022111
Use:	Post emergent herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	1.4

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	reproductive and developmental effects	7	8

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	50	increased methemoglobin; increased spleen weight in females; and enlarged seminal vesicles/prostates in males	general population	OPP	2006

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
72		EEC SW 30-Year	OPP	2006

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Propanil

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.009	mg/kg/day	OPP 2006	Bellringer 1994	increased methemoglobin; increased spleen weight in females; and enlarged seminal vesicles/prostates in males	general population	33.8	53.3	[264]	
Cancer Classification (CC)	S		OPP 2006						[264]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Chronic Human Health Benchmark	0.06	mg/L	EPA HHBP	
Health-Based Screening Level	0.06	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.009	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1384	mg/kg	NIH HSDB	max
LD50	360	mg/kg	NIH HSDB	min
LOAEL	100	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	5	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	15	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	20	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	12.91	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	49	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	9.6	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.003767	mol/kg	TEST QSAR	
Ames mutagenicity test	-0.006	no units	TEST QSAR	
Developmental toxin test	0.688	no units	TEST QSAR	

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Propanil
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	7	6,860,055	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	4	79,889	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	1	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	16	6	Sites	38	0.0112	0.042	0.116	0.17	ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	1	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	936	23	Sites	2.46	0.00188	0.0354	0.574	6.5	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	2,045	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	2,980	23	Sites	0.77	0.00188	0.0354	0.574	6.5	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	228	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	11	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	1,424	201	Sites	14	0.004	0.591	5.68	57.6	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	1	Sites	2.63	3.0096	3.01	3.01	3.0096	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	0	Sites	0						
Southeast Stream Quality Assessment (SESQA) (Ambient) [102]	2014	77	1	Sites	1.3	0.0020539	0.00205	0.00205	0.0020539	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					
Estimated Environmental Concentration (EEC) in Surface Water, 30-Year Mean	2006	OPP	72	ug/L	Exposure Analysis Modeling System (EXAMS)	The modeled surface water 30-year mean estimated environmental concentration provided by the EPA OPP health assessment was selected as the occurrence value for propanil. This value coincides with the chronic health effects data and was considered the most appropriate for estimates of chronic drinking water exposures.					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		6.68E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.50968	days	
Boiling point	OPERA QSAR	341.956	degree C	
Boiling point	TEST QSAR	325.947	degree C	
Vapor pressure	OPERA QSAR	0.00000055	mmHg	
Vapor pressure	TEST QSAR	0.00000265	mmHg	
Solubility in water	OPERA QSAR	0.000730631	mol/L	
Solubility in water	TEST QSAR	0.000447713	mol/L	
Bioconcentration factor	OPERA QSAR	53.3998	no units	
Bioconcentration factor	TEST QSAR	16.9824	no units	
Henry's Law constant	OPERA QSAR	1.79E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.219	no units	

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
102	https://webapps.usgs.gov/rsqa/#!/region/SESQA
264	USEPA. 2006. Amendment to the Reregistration Eligibility Decision (RED) for Propanil (March 2006) and the Propanil RED (September 2003). EPA-HQ-OPP-2003-0348. U.S. Environmental Protection Agency, Office of Prevention, Pesticides and Toxic Substances, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Propargite

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Propargite
CASRN:	2312-35-8
DTXSID:	DTXSID4024276
Use:	Insecticide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	2.8

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	carcinogen with linear MOA	6	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.2	jejunal tumors	general population	OPP	2019

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.5508	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Propargite

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.04	mg/kg/day	OPP 2019	Trutter 1991; Goldenthal 1993	decreased pup weight in all generations	bottle-fed infants	151	53.0	[424]	
Cancer Slope Factor (CSF)	0.192	(mg/kg/day)^-1	OPP 2019	Goldenthal 1993	jejunal tumors	general population	33.8	0.154	[424]	
Cancer Classification (CC)	B2		OPP 2019						[424]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Health-Based Screening Level	0.3	mg/L	Health-based screening levels from USGS	
Health-Based Screening Level	0.000167	mg/L	Health-based screening levels from USGS	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1480	mg/kg	NIH HSDB	min
LD50	2947	mg/kg	NIH HSDB	max
LOAEL	105	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	6	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	2	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	25	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	32.06	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.011885	mol/kg	TEST QSAR	
Ames mutagenicity test			TEST QSAR	
Developmental toxin test	0.793	no units	TEST QSAR	

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OCCURRENCE DATA

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	10,698	73	Sites	0.68	6.00E - 04	0.044	0.551	20	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	2,055	70	Sites	3.41	6.00E - 04	0.044	0.56	20	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	8,643	3	Sites	0.03	0.008	0.009	0.174	0.245	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	18	8,790,953	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	2	165	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	13	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	891	7	Sites	0.79	0.00169	0.106	0.199	0.212	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	2,018	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	2,908	7	Sites	0.24	0.00169	0.106	0.199	0.212	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	8	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	2	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	6	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	1,146	65	Sites	5.67	0.0084	0.086	1.45	20	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.000000139	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	5.67573	days	
Boiling point	OPERA QSAR	362.004	degree C	
Boiling point	TEST QSAR	325.241	degree C	
Vapor pressure	OPERA QSAR	0.000000359	mmHg	
Vapor pressure	TEST QSAR	0.00000018	mmHg	
Solubility in water	OPERA QSAR	0.00000239	mol/L	
Solubility in water	TEST QSAR	0.00000271	mol/L	
Bioconcentration factor	OPERA QSAR	10.8905	no units	
Bioconcentration factor	TEST QSAR			
Henry's Law constant	OPERA QSAR	0.00000979	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	4.882	no units	

Propargite

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
424	USEPA. 2019. Propargite: Draft Human Health Risk Assessment in Support of Registration Review. EPA-HQ-OPP-2014-0131-0051. DP No. D449759. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Propazine

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Propazine
CASRN:	139-40-2
DTXSID:	DTXSID3021196
Use:	Selective post-emergence herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.0005

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	reproductive and developmental effects	10	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	100	attenuation of LH surge	women of childbearing age	OPP	2015

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.05	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Propazine

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0242	mg/kg/day	OPP 2015	national health and environmental effects research laboratory; Morales and	attenuation of LH surge	women of childbearing age	35.4	137	[353]	
Cancer Classification (CC)	NL		OPP 2015						[353]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Lifetime Health Advisory	0.01	mg/L	EPA DWSHA 2018	
Maximum Allowable Daily Level	100	ug/day	CalEPA OEHHA Chemical Database	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1200	mg/kg	NIH HSDB	min
LD50	15380	mg/kg	NIH HSDB	max
LOAEL	450	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	50	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	150	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	5	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxicant in vitro assays tested	3.67	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.006368	mol/kg	TEST QSAR	
Ames mutagenicity test	0.045	no units	TEST QSAR	
Developmental toxin test	0.695	no units	TEST QSAR	

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OCCURRENCE DATA

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	2,165	260	Sites	12	2.00E - 04	0.0051	0.05	1.79	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	462	209	Sites	45	2.00E - 04	0.00514	0.05	1.79	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	1,703	51	Sites	2.99	0.00025	0.00246	0.265	1.69	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	7	637,396	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	4	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	10	7	Sites	70	7e-04	0.0028	0.013	0.032	ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	19	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	426	115	Sites	27	0.00021	0.007	0.05	0.39	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	817	44	Sites	5.39	0.00026	0.01	0.03	0.0894	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,243	159	Sites	13	0.00021	0.00716	0.05	0.39	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	227	14	Sites	6.17	7e-04	0.0055	0.013	0.071	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	7	Sites	3.2	7e-04	0.00105	0.0111	0.023	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	10	7	Sites	70	7e-04	0.0055	0.013	0.071	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	68	2	Sites	2.94	1.1	1.55	1.91	2	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	3	Sites	7.89	0.03	0.036	0.04	0.041	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	9	Sites	1.54	5e-04	0.001	0.00266	0.0029	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		7.85E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.96717	days	
Boiling point	OPERA QSAR	338.333	degree C	
Boiling point	TEST QSAR	318.777	degree C	
Vapor pressure	OPERA QSAR	0.000000183	mmHg	
Vapor pressure	TEST QSAR	0.000000593	mmHg	
Solubility in water	OPERA QSAR	0.000053	mol/L	
Solubility in water	TEST QSAR	0.000355631	mol/L	
Bioconcentration factor	OPERA QSAR	13.2841	no units	
Bioconcentration factor	TEST QSAR	13.3352	no units	
Henry's Law constant	OPERA QSAR	1.24E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.08299	no units	

Propazine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
353	USEPA. 2015. Propazine. Acute and Chronic Dietary (Food Only) Exposure Assessments for Registration Review. EPA-HQ-OPP-2013-0250-0070. DP D428624. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Propiconazole

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Propiconazole
CASRN:	60207-90-1
DTXSID:	DTXSID8024280
Use:	Fungicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.000065

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	non-cancer effects	9	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	600	Liver toxicity; increased liver weight in males, and increase in liver lesions (masses/raised areas/swellings/nodular areas)	general population	OPP	2019

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.039	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis
Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Propiconazole

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.1	mg/kg/day	OPP 2019	Ciba Geigy Corporation 1982	Liver toxicity; increased liver weight in males, and increase in liver lesions (masses/raised areas/ swellings/nodular areas)	general population	33.8	592	[425]	
Cancer Classification (CC)	C		OPP 2019						[425]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	2	mg/L	EPA HHBP	
Acute PAD	0.3	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.6	mg/L	EPA HHBP	
Health-Based Screening Level	0.6	mg/L	Health-based screening levels from USGS	
Health-Based Screening Level	0.6	mg/L	Health-based screening levels from USGS	
Health-Based Screening Level	0.6	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.1	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1490	mg/kg	NIH HSDB	min
LD50	1517	mg/kg	NIH HSDB	max
LOAEL	300	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	8.3999996	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	1.9	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	100	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	19.93	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	6.25	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	77.589996	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	1.25	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	16.82	mg/kg/day	EPA Toxicity Reference Database	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0040551	mol/kg	TEST QSAR	
Ames mutagenicity test	0.333	no units	TEST QSAR	
Developmental toxin test	0.484	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Propiconazole
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	3,055	101	Sites	3.31	0.001	0.009	0.039	1.23	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	190	95	Sites	50	0.001	0.009	0.039	1.23	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	2,865	6	Sites	0.21	0.003	0.0075	0.018	0.024	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	48	2,454,476	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	11	40,199	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	5	Sites	29	0.0057	0.0057	0.012	0.029	ug/L	
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	11	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	11	0	Sites	0						
Bradley et al. 2018 (Finished) [53]	2016	26	2	Sites	7.69	0.0141	0.0154	0.0165	0.0168	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	832	187	Sites	22	0.00041	0.0116	0.103	3.72	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	1,796	11	Sites	0.61	0.003	0.0065	0.0331	0.075	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	2,627	198	Sites	7.54	0.00041	0.0112	0.1	3.72	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	10	Sites	4.37	0.005661	0.01	0.027	0.1916	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	5	Sites	2.28	0.005661	0.0057	0.134	0.1916	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	5	Sites	42	0.0057	0.01	0.0195	0.07	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	134	13	Sites	9.7	0.02	0.0298	0.0452	0.051	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	8	Sites	21	0.0029	0.0127	0.0662	0.13	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	6	Sites	16	0.0202	0.0644	0.271	0.4045	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	8	Sites	21	0.005	0.0174	0.115	0.217	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	902	6	Sites	0.67	0.0023	0.00845	0.0225	0.031	ug/L	
USGS, McKenzie River, Oregon, 2012 (Ambient) [158]	2002 - 2010	42	3	Samples	7.1				0.051	ug/L	
USGS, McKenzie River, Oregon, 2012 (Ambient) [158]	2002 - 2010	42	3	Samples	7.1				0.08	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exposure exposure		1.63E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.35915	days	
Boiling point	OPERA QSAR	350.158	degree C	
Boiling point	TEST QSAR	366.386	degree C	
Vapor pressure	OPERA QSAR	0.000000409	mmHg	
Vapor pressure	TEST QSAR	7.08E-08	mmHg	
Solubility in water	OPERA QSAR	0.000222763	mol/L	
Solubility in water	TEST QSAR	0.000192309	mol/L	
Bioconcentration factor	OPERA QSAR	45.858	no units	
Bioconcentration factor	TEST QSAR	102.094	no units	
Henry's Law constant	OPERA QSAR	0.00000378	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.54562	no units	

Propiconazole

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. <i>Environmental science & technology</i> , 52(23), 13972-13985.
158	Reconnaissance of Land-Use Sources of Pesticides in Drinking Water, McKenzie River, Oregon. U.S. Geological Survey Scientific Investigations Report 2012–5091, 46 p. plus appendixes.
425	USEPA. 2019. Propiconazole Human Health Risk Assessment for the New Use of Propiconazole on Avocado, along with Conversion to Brassica, leafy greens, subgroup 4-16B, except watercress, Leaf petiole vegetable subgroup 22B, Celtuce, Florence fennel, Swiss chard, and the expansion to Vegetable, root, except sugar beet, subgroup 1B. EPA-HQ-OPP-2018-0127-0007. DP No. D446376. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Propoxur

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Propoxur
CASRN:	114-26-1
DTXSID:	DTXSID7021948
Use:	Insecticide used on cane, cocoa, fruit grapes, maize, rice, sugar, vegetables, cotton, lucerne, and ornamentals, etc
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	X
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.02

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	reproductive and developmental effects	1	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.5	red blood cell acetylcholinesterase inhibition in pups	bottle-fed infants	OPP	2015

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.01	90th Percentile	All Ambient Water	NWIS	2008-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Propoxur

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.00038	mg/kg/day	OPP 2015	Toot 2012a and b	red blood cell acetylcholinesterase inhibition in pups	bottle-fed infants	151	0.503	[354]	
Cancer Slope Factor (CSF)	0.00352	(mg/kg/day)^-1	OPP 2015	Suberg and Loeser 1984	urinary bladder papillomas and carcinomas, borderline significant increased incidence of uterine carcinomas	general population	33.8	8.41	[354]	
Cancer Classification (CC)	B2		OPP 2015						[354]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	0.04	mg/L	EPA DWSHA 2018	
Lifetime Health Advisory	0.003	mg/L	EPA DWSHA 2018	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	23.5	mg/kg	NIH HSDB	min
LD50	800	mg/kg	NIH HSDB	max
LOAEL	472.39999	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	9	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	150.4	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	3	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	2.68	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0009886	mol/kg	TEST QSAR	
Ames mutagenicity test	0.614	no units	TEST QSAR	
Developmental toxin test	0.684	no units	TEST QSAR	

Nationally Representative Water Data

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)		0		Toxic Release Inventory (TRI) Program (EPA) (2016)	1	0.57	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Nationally Representative Water Data

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exnocast exposure		7.16E-08	

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.65857	days	
Boiling point	OPERA QSAR	284.046	degree C	
Boiling point	TEST QSAR	285.351	degree C	
Vapor pressure	OPERA QSAR	0.00000821	mmHg	
Vapor pressure	TEST QSAR	0.0000306	mmHg	
Solubility in water	OPERA QSAR	0.00570894	mol/L	
Solubility in water	TEST QSAR	0.00252348	mol/L	
Bioconcentration factor	OPERA QSAR	6.97685	no units	
Bioconcentration factor	TEST QSAR	4.9545	no units	
Henry's Law constant	OPERA QSAR	1.38E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.70194	no units	

A-711

Propoxur

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
102	https://webapps.usgs.gov/rsqa/#!/region/SESQA
158	Reconnaissance of Land-Use Sources of Pesticides in Drinking Water, McKenzie River, Oregon. U.S. Geological Survey Scientific Investigations Report 2012–5091, 46 p. plus appendixes.
354	USEPA. 2015. Propoxur: Human Health Draft Risk Assessment for Registration Review. EPA-HQ-OPP-2009-0806-0023. DP No. D414135. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Prosulfuron

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Prosulfuron
CASRN:	94125-34-5
DTXSID:	DTXSID9034868
Use:	Post-emergent herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.00011

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	non-cancer effects	6	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	300	decreased feed efficiency, hematological findings and hepatotoxicity	general population	OPP	2015

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.03224	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Prosulfuron

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.053	mg/kg/day	OPP 2015	Chow and Richter 1992	decreased feed efficiency, hematological findings and hepatotoxicity	general population	33.8	314	[355]	
Cancer Classification (CC)	NL		OPP 2015						[355]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.7	mg/L	EPA HHBP	
Acute PAD	0.1	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.34	mg/L	EPA HHBP	
Health-Based Screening Level	0.34	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.053	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	546	mg/kg	NIH HSDB	
LOAEL	18.6	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	508	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	1.95	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	200	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	2.29	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	31	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	69.300003	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	2.88	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	6.5	mg/kg/day	EPA Toxicity Reference Database	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0170608	mol/kg	TEST QSAR	
Ames mutagenicity test			TEST QSAR	
Developmental toxin test	1.087	no units	TEST QSAR	

Prosulfuron
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	1,760	16	Sites	0.91	7.00E - 04	0.00635	0.0322	0.274	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	322	13	Sites	4.04	7.00E - 04	0.0062	0.0222	0.173	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	1,438	3	Sites	0.21	0.0018	0.0065	0.194	0.274	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	29	25,349	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	8	1	Sites	12	0.0025	0.0025	0.0025	0.0025	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	306	4	Sites	1.31	0.0055	0.114	0.192	0.197	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	528	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	834	4	Sites	0.48	0.0055	0.114	0.192	0.197	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	121	1	Sites	0.83	0.0025	0.0025	0.0025	0.0025	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	113	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	8	1	Sites	12	0.0025	0.0025	0.0025	0.0025	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg- bw/day)	Notes
ExpoCast exposure		0.000000157	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)	< LOD	ug/l	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.63586	days	
Boiling point	OPERA QSAR	264.577	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	3.93E-11	mmHg	
Vapor pressure	TEST QSAR	5.45E-11	mmHg	
Solubility in water	OPERA QSAR	0.0000576	mol/L	
Solubility in water	TEST QSAR	0.000104472	mol/L	
Bioconcentration factor	OPERA QSAR	2.58961	no units	
Bioconcentration factor	TEST QSAR	1.15345	no units	
Henry's Law constant	OPERA QSAR	2.63E-11	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.02925	no units	

Prosulfuron

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
355	USEPA. 2015. Prosulfuron. Draft Human Health Risk Assessment in Support of Registration Review. EPA-HQ-OPP-2011-1010-0019. DP No. D426092. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.

Pymetrozine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Pymetrozine
CASRN:	123312-89-0
DTXSID:	DTXSID2032637
Use:	Pesticide used to control aphids and whiteflies in vegetables, ornamentals, cotton, field crops, deciduous and citrus fruit; control of plant hoppers in rice
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0069

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	carcinogen with linear MOA	3	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	2	liver benign hepatoma and hepatocarcinoma	general population	OPP	2017

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.01384	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis
Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Pymetrozine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.008	mg/kg/day	OPP 2017	Pinto 2003	morphometric changes in brains of pups	bottle-fed infants	151	10.6	[392]	
Cancer Slope Factor (CSF)	0.0119	(mg/kg/day) ⁻¹	OPP 2017	Gerspach 1995	liver benign hepatoma and hepatocarcinoma	general population	33.8	2.49	[392]	
Cancer Classification (CC)	L		OPP 2017						[392]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.05	mg/L	EPA HHBP	
Acute PAD	0.008	mg/kg/day	EPA HHBP	
Cancer Slope Factor (CSF)	0.0119	(mg/kg/day) ⁻¹	EPA HHBP	
Chronic Human Health Benchmark	0.05	mg/L	EPA HHBP	
Chronic Human Health Benchmark	0.00269	mg/L	EPA HHBP	
Health-Based Screening Level	0.05	mg/L	Health-based screening levels from USGS	
Health-Based Screening Level	0.00269	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.008	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	5693	mg/kg	NIH HSDB	min
LD50	5955	mg/kg	NIH HSDB	max
LOAEL	3.76	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	300	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	0.454	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	100	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	1.26	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	14	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	360	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	3.12	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	34.5	mg/kg/day	EPA Toxicity Reference Database	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0028445	mol/kg	TEST QSAR	
Ames mutagenicity test	0.37	no units	TEST QSAR	
Developmental toxin test	0.66	no units	TEST QSAR	

Pymetrozine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	844	2	Sites	0.24	0.0032	0.00985	0.0138	0.0165	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	276	1	Sites	0.36	0.0032	0.0032	0.0032	0.0032	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	568	1	Sites	0.18	0.0165	0.0165	0.0165	0.0165	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	21	21,675	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	88	0	Sites	0						
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	28	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	116	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	3	0	Sites	0						
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	1	Sites	0.17	0.0165	0.0165	0.0165	0.0165	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		1.15E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.35411	days	
Boiling point	OPERA QSAR	258.726	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.0000821	mmHg	
Vapor pressure	TEST QSAR	0.00000504	mmHg	
Solubility in water	OPERA QSAR	0.00388089	mol/L	
Solubility in water	TEST QSAR	0.00295801	mol/L	
Bioconcentration factor	OPERA QSAR	2.35119	no units	
Bioconcentration factor	TEST QSAR			
Henry's Law constant	OPERA QSAR	0.000000712	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.0895	no units	

Pymetrozine

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
392	USEPA. 2017. Pymetrozine. Draft Human Health Risk Assessment for Registration Review. EPA-HQ-OPP-2013-0368-0017. DP No. D439601. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Pyraclostrobin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Pyraclostrobin
CASRN:	175013-18-0
DTXSID:	DTXSID7032638
Use:	Very broad spectrum fungicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.000041

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	non-cancer effects	9	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	200	decreased body weight, kidney tubular casts and atrophy in both sexes; increased incidence of liver necrosis and erosion/ulceration of the glandular- stomach and fore-stomach in males	general population	OPP	2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.00825	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Pyraclostrobin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.034	mg/kg/day	OPP 2018	Mellert et al. 1999	decreased body weight, kidney tubular casts and atrophy in both sexes; increased incidence of liver necrosis and erosion/ulceration of the glandular- stomach and fore-stomach in males	general population	33.8	201	[406]	
Cancer Classification (CC)	NL		OPP 2018						[406]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Health-Based Guidance Value	0.1	mg/L	MN DOH	
Acute Health-Based Guidance Value	0.3	mg/L	MN DOH	
Acute Human Health Benchmark	1	mg/L	EPA HHBP	
Acute PAD	0.05	mg/kg/day	EPA HHBP	
Chronic Health-Based Guidance Value	0.1	mg/L	MN DOH	
Chronic Human Health Benchmark	0.22	mg/L	EPA HHBP	
Health-Based Screening Level	0.22	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.034	mg/kg/day	EPA HHBP	
Short-Term/Subchronic Health-Based Guidance Value	0.1	mg/L	MN DOH	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	5000	mg/kg	NIH HSDB	
LOAEL	50	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	9.1999998	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	25	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	4.7	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	28.72	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	10.8	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	34.700001	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	12.9	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	5.4	mg/kg/day	EPA Toxicity Reference Database	min

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity test	0.587	no units	TEST QSAR	
Developmental toxin test	0.41	no units	TEST QSAR	

Pyraclostrobin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
		Prevalence				Magnitude					
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	1,763	138	Sites	7.83	0.00011	0.00182	0.00825	0.389	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	324	136	Sites	42	0.00011	0.00182	0.00807	0.389	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	1,439	2	Sites	0.14	0.00021	0.123	0.196	0.245	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	48	2,471,066	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Ambient Water											
		Prevalence				Magnitude					
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	434	52	Sites	12	0.00025	0.00339	0.0782	3.33	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	531	1	Sites	0.19	0.00441	0.00441	0.00441	0.00441	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	965	53	Sites	5.49	0.00025	0.00341	0.0774	3.33	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	244	50	Sites	20	0.02	0.096	0.245	1.37	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	1	Sites	2.63	0.0383	0.0383	0.0383	0.0383	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	1	Sites	0.17	2e-04	2e-04	2e-04	2e-04	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		2.01E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.89847	days	
Boiling point	OPERA QSAR	336.014	degree C	
Boiling point	TEST QSAR	465.144	degree C	
Vapor pressure	OPERA QSAR	8.44E-09	mmHg	
Vapor pressure	TEST QSAR	1.5E-09	mmHg	
Solubility in water	OPERA QSAR	0.0000103	mol/L	
Solubility in water	TEST QSAR	0.0000209	mol/L	
Bioconcentration factor	OPERA QSAR	174.72	no units	
Bioconcentration factor	TEST QSAR			
Henry's Law constant	OPERA QSAR	0.000000108	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	4.00245	no units	

Pyraclostrobin

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
406	USEPA. 2018. Pyraclostrobin. Human Health Risk Assessment for a Petition for the Establishment of Use on Greenhouse-Grown Leafy Greens, Except Head Lettuce, Subgroup 4- 16A; Cucurbit Vegetables, Group 9; and Fruiting Vegetables, Group 8-10 and Crop Group Conversions and Expansion of Tolerances for Brassica, Leafy Greens, Subgroup 4-16B; Celtuce; Florence Fennel; Kohlrabi; Leaf Petiole Vegetables, Subgroup 22B; Tropical and Subtropical, Medium to Large Fruit, Inedible Peel, Subgroup 23B; and Brassica Head and Stem, Group 5-16 and a Revised Tolerance Level for Leafy Greens,
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Pyrene

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Pyrene
CASRN:	129-00-0
DTXSID:	DTXSID3024289
Use:	Occurs as a result of incomplete burning
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.00046

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	non-cancer effects	9	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	100	nephropathy (renal tubular pathology, decreased kidney weights)	general population	OW	1991

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.046	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Pyrene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.03	mg/kg/day	IRIS 1990	USEPA 1989	renal tubular pathology, decreased kidney weights	general population	33.8	178	[209]	
Reference Dose (RfD) or Equivalent	0.025	mg/kg/day	OW 1991	USEPA 1989	nephropathy (renal tubular pathology, decreased kidney weights)	general population	33.8	148	[212]	
Cancer Classification (CC)	NL		PPRTV 2007						[282]	
Cancer Classification (CC)	D		IRIS 1990						[209]	
Cancer Classification (CC)	D		OW 1991						[212]	
			ATSDR 1995						[10]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Reproductive	0.0075	Paltaviciene, 2006	Reproductive	0.00075	Paltaviciene, 2006	2006-09-01	2020-03-25	6765	2	16	1

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Cancer Classification (CC)	3	no units	WHO IARC	
Chronic Health-Based Guidance Value	0.05	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.2	mg/L	MN DOH	
Human Health Ambient Water Quality Criteria	0.02	mg/L	EPA Human Health Criteria for CWA	
Short-Term/Subchronic Health-Based Guidance Value	0.09	mg/L	MN DOH	
Subchronic Provisional RfD	0.3	mg/kg/day	EPA PPRTV	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	2700	mg/kg	NIH HSDB	
Percent of active toxcast in vitro assays tested	6.19	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0070469	mol/kg	TEST QSAR	
Ames mutagenicity test	0.842	no units	TEST QSAR	
Developmental toxin test	0.342	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Pyrene
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
		Prevalence				Magnitude					
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	588	38	Sites	6.46	0.003	0.01	0.046	0.14	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	101	30	Sites	30	0.003	0.01	0.0475	0.14	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	487	8	Sites	1.64	0.004	0.009	0.0388	0.046	ug/L	
Pesticide Application Data		Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data		Number of States	Amount Released (lbs/year)	Chemical Production Data		Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)					Toxic Release Inventory (TRI) Program (EPA) (2016)				Chemical Data Reporting (CDR) Results (EPA) (2016)		100K - 500K

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	28	1	Sites	3.57	0.001	0.001	0.001	0.001	ug/L	
Drinking Water Monitoring Data - WA (Finished)	2006 - 2011	481	0	Sites	0						
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
		Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	231	8	Sites	3.46	0.1	0.16	0.28	0.3	ug/L	
Drinking Water Monitoring Data - WA (Source)	2006 - 2011	634	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	867	275	Sites	32	0.002	0.03	0.37	25.6	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	1,095	71	Sites	6.48	0.001	0.0155	0.072	1.28	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,962	346	Sites	18	0.001	0.0295	0.34	25.6	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	14	Sites	37	0.0034	0.0092	0.0242	0.0447	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Waste Water Effluent											
		Prevalence				Magnitude					
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	5	Sites	24						
Estimated Concentration in Water		Date	Source	Value	Units	Model	Notes				

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg- bw/day)	Notes
ExpoCast exposure		0.00000147	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	255.189	days	
Boiling point	OPERA QSAR	392.038	degree C	
Boiling point	TEST QSAR	415.21	degree C	
Vapor pressure	OPERA QSAR	0.00000288	mmHg	
Vapor pressure	TEST QSAR	8.69E-08	mmHg	
Solubility in water	OPERA QSAR	0.000000659	mol/L	
Solubility in water	TEST QSAR	0.000000121	mol/L	
Bioconcentration factor	OPERA QSAR	2230.1	no units	
Bioconcentration factor	TEST QSAR	529.663	no units	
Henry's Law constant	OPERA QSAR	0.0000116	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	5.05118	no units	

Pyrene

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
10	ATSDR. 1995. Toxicological Profile for Polycyclic Aromatic Hydrocarbons. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
209	USEPA. 1990. Chemical Assessment Summary, Pyrene. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, D.C.
212	USEPA. 1991. Drinking Water Criteria Document for Polycyclic Aromatic Hydrocarbons (PAHs). U.S. Environmental Protection Agency, Office of Health and Environmental Assessment, Environmental Criteria and Assessment Office, Cincinnati, OH.
282	USEPA. 2007. Provisional Peer-Reviewed Toxicity Values for Pyrene. U.S. Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment, Superfund Health Risk Technical Support Center, Cincinnati, OH.

Pyridaben

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Pyridaben
CASRN:	96489-71-3
DTXSID:	DTXSID5032573
Use:	Insecticide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0054

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	reproductive and developmental effects	5	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	30	decreased parental and pup body weight	bottle-fed infants	OPP	2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.1614	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Pyridaben

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.022	mg/kg/day	OPP 2018	Tesh et al. 1989; Willoughby 1990	decreased parental and pup body weight	bottle-fed infants	151	29.1	[407]	
Cancer Classification (CC)	NL		OPP 2018						[407]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	2.9	mg/L	EPA HHBP	
Acute PAD	0.44	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.03	mg/L	EPA HHBP	
Health-Based Screening Level	0.03	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.005	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1100	mg/kg	NIH HSDB	max
LD50	383	mg/kg	NIH HSDB	min
LOAEL	0.5	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	30	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	13	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	2.41	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	21.96	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	13.02	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic LOAEL	4	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	1	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	4.92	mg/kg/day	EPA Toxicity Reference Database	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0015417	mol/kg	TEST QSAR	
Ames mutagenicity test	0.255	no units	TEST QSAR	
Developmental toxin test	0.152	no units	TEST QSAR	

Pyridaben

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	1,761	9	Sites	0.51	0.00033	0.00096	0.161	0.219	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	322	7	Sites	2.17	0.00038	0.00096	0.0475	0.155	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	1,439	2	Sites	0.14	0.00033	0.11	0.175	0.219	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	11	35,107	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	359	3	Sites	0.84	0.0042	0.195	0.215	0.223	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	528	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	887	3	Sites	0.34	0.0042	0.195	0.215	0.223	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	99	0	Sites	0						
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exposure exposure		0.000000139	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	12.6613	days	
Boiling point	OPERA QSAR	364.625	degree C	
Boiling point	TEST QSAR	421.721	degree C	
Vapor pressure	OPERA QSAR	0.00000141	mmHg	
Vapor pressure	TEST QSAR	8.67E-08	mmHg	
Solubility in water	OPERA QSAR	7.08E-08	mol/L	
Solubility in water	TEST QSAR	0.000000585	mol/L	
Bioconcentration factor	OPERA QSAR	599.145	no units	
Bioconcentration factor	TEST QSAR			
Henry's Law constant	OPERA QSAR	4.99E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	6.11525	no units	

Pyridaben

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
407	USEPA. 2018. Pyridaben. Human Health Draft Risk Assessment in Support of Registration Review. EPA-HQ-OPP-2010-0214-0015. DP No. D440297. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Quinoline

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Quinoline
CASRN:	91-22-5
DTXSID:	DTXSID1021798
Use:	Chemical intermediate; pharmaceutical (anti-malarial); flavoring
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	9.3

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	carcinogen with linear MOA	6	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.01	hepatic hemangioendotheliomas or hemangiosarcomas	general population	IRIS	2001

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.09312	90th Percentile	Finished Water	UCMR4	2018-2019

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
		X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Quinoline

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Cancer Slope Factor (CSF)	3	(mg/kg/day)^-1	IRIS 2001	Hirao et al. 1976	hepatic hemangioendotheliomas or hemangiosarcomas	general population	33.8	0.00986	[244]	
Cancer Classification (CC)	B2		IRIS 2001						[244]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Renal, Immune, Hepatic, Carcinogenicity, Systemic	8.8	Matsumoto, 2018	Hepatic	30	Uno, 2015	2005-07-01	2020-03-16	2041	2	2	2

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	331	mg/kg	NIH HSDB	min
LD50	460	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	0.89	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0046559	mol/kg	TEST QSAR	
Ames mutagenicity test	0.888	no units	TEST QSAR	
Developmental toxin test	0.468	no units	TEST QSAR	

Quinoline

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019	3,675	36	Sites	0.98	0.0201	0.0288	0.0931	1.5	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)	9	2,474	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Ambient Water											
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.00000309	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	13.3246	days	
Boiling point	OPERA QSAR	243.313	degree C	
Boiling point	TEST QSAR	239.117	degree C	
Vapor pressure	OPERA QSAR	0.0417085	mmHg	
Vapor pressure	TEST QSAR	0.0293765	mmHg	
Solubility in water	OPERA QSAR	0.0339207	mol/L	
Solubility in water	TEST QSAR	0.0323594	mol/L	
Bioconcentration factor	OPERA QSAR	4.69938	no units	
Bioconcentration factor	TEST QSAR	17.1396	no units	
Henry's Law constant	OPERA QSAR	0.0000365	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.11472	no units	

Quinoline

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
244	USEPA. 2001. Chemical Assessment Summary, Quinoline. U.S. Environmental Protection Agency, National Center for Environmental Assessment, Integrated Risk Information System (IRIS), Washington, D.C.

Silicon

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Silicon
CASRN:	7440-21-3
DTXSID:	DTXSID0051441
Use:	Chemical intermediate; alloys
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxics	
PubMed Neurotoxics	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
		10	10

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
42069	90th Percentile	Finished Water	NIRS	1984-1986

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Silicon

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
			IOM 2001						[108]	NOTE: No health assessments found, "there is no evidence that the silicon that naturally occurs in food and water produces adverse health outcomes"

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	3160	mg/kg	NIH HSDB	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity test			TEST QSAR	
Developmental toxin test			TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Silicon
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986	989	989	Sites	100	260	18139	42069	98916	ug/L	
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	1B - 5B

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	100		2930		22300	ug/L	
Community Water System Survey (CWSS) (Finished) [178]	2006	1	NA	Sites			5280	5280		ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	49	49	Sites	100	2	2800	5900	61000	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	81	78	Sites	96	8	4600	6190	23000	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	130	127	Sites	98	2	3800	6150	61000	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	100		2750		22400	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Silicon

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. Science of The Total Environment. v581-582, (909-922).
108	IOM. 2001. Dietary Reference Intakes for Vitamin A, Vitamin K, Arsenic, Boron, Chromium, Copper, Iodine, Iron, Manganese, Molybdenum, Nickel, Silicon, Vanadium, and Zinc. Institute of Medicine (IOM), National Academies of Science, Washington, D.C.
178	USEPA (US Environmental Protection Agency). (2009). 2006 Community Water System Survey. Overview, 57.

Sitagliptin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Sitagliptin
CASRN:	486460-32-6
DTXSID:	DTXSID70197572
Use:	Hypoglycemic agents
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.028

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	non-cancer effects	8	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	3	lowest therapeutic dose: improved glycemic control for patients with type 2 diabetes	bottle-fed infants	FDA; NIH	2018; 2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.08453	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Sitagliptin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.000416667	mg/kg/day	FDA 2018; NIH 2018	Merck Sharp & Dohme Corp.	lowest therapeutic dose:improve glycemic control for patients with type 2 diabetes	bottle-fed infants	151	2.80	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels
Reference Dose (RfD) or Equivalent	0.000416667	mg/kg/day	FDA 2018; NIH 2018	Merck Sharp & Dohme Corp.	lowest therapeutic dose:improve glycemic control for patients with type 2 diabetes	general population	33.8	9.80	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References Identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Screening level for pharmaceutical - general population	0.009803922	mg/L	EPA Office of Water	
Screening level for pharmaceutical - infants	0.002777778	mg/L	EPA Office of Water	

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	3000	mg/kg	NIH HSDB	min
LD50	4000	mg/kg	NIH HSDB	max

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0016596	mol/kg	TEST QSAR	
Ames mutagenicity test	0.299	no units	TEST QSAR	
Developmental toxin test	0.869	no units	TEST QSAR	

Sitagliptin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	557	12	Sites	2.15	0.00365	0.0268	0.0845	0.184	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	75	12	Sites	16	0.00365	0.0268	0.0845	0.184	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	482	0	Sites	0						

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	205	41	Sites	20	0.00263	0.0333	0.117	0.484	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	401	2	Sites	0.5	0.0432	0.219	0.325	0.395	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	606	43	Sites	7.1	0.00263	0.0369	0.12	0.484	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	12	Sites	32	0.002071	0.00841	0.153	0.2267841	ug/L	
Bexfield et al. 2019 (Groundwater) [49]	2013 - 2015	1,106	0	Sites	0						
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	20	Sites	95	0.0242164	0.261	4.9	5.184601	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.54479	days	
Boiling point	OPERA QSAR	328.816	degree C	
Boiling point	TEST QSAR	403.649	degree C	
Vapor pressure	OPERA QSAR	9.8E-10	mmHg	
Vapor pressure	TEST QSAR	2.52E-09	mmHg	
Solubility in water	OPERA QSAR	0.00000549	mol/L	
Solubility in water	TEST QSAR	0.00000646	mol/L	
Bioconcentration factor	OPERA QSAR	6.6312	no units	
Bioconcentration factor	TEST QSAR	22.6986	no units	
Henry's Law constant	OPERA QSAR	6.26E-11	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.82307	no units	

Sitagliptin

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Reference Number	Full Reference
49	Bexfield, L.M., P.L. Toccalino, K. Belitz, W.T. Foreman, and E.T. Furlong. 2019. Hormones and pharmaceuticals in groundwater used as a source of drinking water across the United States. Environmental Science and Technology 53: 2950-2960.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. Environmental science & technology, 51(9), 4792-4802.
77	FDA. 2018. Drugs @ FDA: FDA Approved Drug Products. U.S. Food and Drug Administration (FDA). https://www.accessdata.fda.gov/scripts/cder/daf/ .
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. Science of The Total Environment. v581-582, (909-922).
150	NIH. 2018. DailyMed Database. U.S. National Library of Medicine, National Institutes of Health (NIH). https://dailymed.nlm.nih.gov/dailymed/ .
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. Science of the Total Environment, 636, 69-79.

Sodium

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Sodium
CASRN:	7440-23-5
DTXSID:	DTXSID1049774
Use:	Chemical intermediate; alloys; semiconductors
Chemical Notes:	EPA requires periodic monitoring of sodium at the entry point to the distribution system. Monitoring is to be conducted annually for surface water systems and every 3 years for groundwater systems (40 CFR:141.41). The water supplier must report sodium test results to local and State public health officials by direct mail within 3 months of the analysis unless this responsibility is assumed by the State.

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxics	
PubMed Neurotoxics	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	8

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
	non-cancer effects	10	10

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	20000	organoleptic effects, risk to adults under strict low-sodium diets	general population	OW	2003

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
160240	90th Percentile	Finished Water	NIRS	1984-1986

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X			

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
X	Not Applicable	Not Applicable

Basis

Sodium generally occurs at low levels in drinking water, and when it occurs at high levels the taste may be expected to cause people to reduce their consumption [a,b]. In addition, drinking water is only a minor source of dietary sodium compared with food, and sodium is only one factor among many that contributes to hypertension and heart disease. Therefore, regulation of sodium in drinking water is unlikely to represent a meaningful opportunity for health risk reduction [a,c]. The most effective means to protect the health of PWS users is to identify groups who are more sensitive than the general population, and provide dietary guidance through the public health community [c].

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Sodium

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	6.25	mg/kg/day	HC 1992	WHO 1984	organoleptic effects, risk to adults under strict low-sodium	general population	33.8	37000	[91]	
Drinking Water Advisory	20	mg/L	OW 2003	USEPA 1996	organoleptic effects, risk to adults under strict low-sodium	general population	33.8	20000	[256]	
			OW 2003						[256]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	2300	mg/day	IOM 2005	Johnson et al., 2001; MacGregor et al., 1989; Sacks et al., 2001	increased blood pressure	lactating women	2720	169000	[110]	
Reference Dose (RfD) or Equivalent	2300	mg/day	IOM 2005	Johnson et al., 2001; MacGregor et al., 1989; Sacks et al., 2001	hypertensive disorders	pregnant women	2642	174000	[110]	
Reference Dose (RfD) or Equivalent	2300	mg/day	IOM 2005	Johnson et al., 2001; MacGregor et al., 1989; Sacks et al., 2001	increased blood pressure	general population	2413	191000	[110]	
Reference Dose (RfD) or Equivalent	2300	mg/day	IOM 2005	Johnson et al., 2001; MacGregor et al., 1989; Sacks et al., 2001	increased blood pressure	women of childbearing age	2430	189000	[110]	
			IOM 2019						[112]	

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity			TEST QSAR	
Developmental			TEST QSAR	
toxic test				

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Sodium
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986	989	989	Sites	100	907	16355	160240	1541000	ug/L	
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	12,093	12,092	Sites	100	70	13300	84600	1.90E+07	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	2,592	2,592	Sites	100	70	13100	76600	6.00E+06	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	9,502	9,501	Sites	100	80	14000	107000	1.90E+07	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	50M - 100M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	589	588	Sites	100	500	50000	103000	3.7e+07	ug/L	
Drinking Water Monitoring Data - DC (Finished)	2008 - 2009	1	1	Sites	100	10000	15500	19300	22000	ug/L	
Drinking Water Monitoring Data - MA (Finished)	2006 - 2020	1,778	1,777	Sites	100	190	23000	88260	5100000	ug/L	
Drinking Water Monitoring Data - WA (Finished)	2006 - 2011	936	893	Sites	95	710	9800	37240	830000	ug/L	
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	100		27800		128000	ug/L	
Community Water System Survey (CWSS) (Finished) [178]	2006	27	NA	Sites			19500	83000		ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	5,409	5,400	Sites	100	400	35000	120000	203500000	ug/L	
Drinking Water Monitoring Data - FL (Source)	2006 - 2011	105	100	Sites	95	7	9165	80860	860000	ug/L	
Drinking Water Monitoring Data - MA (Source)	2006 - 2020	159	159	Sites	100	2600	49000	196790	4100000	ug/L	
Drinking Water Monitoring Data - PA (Source)	2006 - 2011	1	1	Sites	100	18900	18900	18900	18900	ug/L	
Drinking Water Monitoring Data - WA (Source)	2006 - 2011	1,498	1,303	Sites	87	700	8900	37400	950000	ug/L	
Drinking Water Monitoring Data - WI (Source)	2012-2019	142	141	Sites	99	450	6500	36000	210000	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	100		24000		128000	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	758	757	Sites	100	450	15800	164000	682000	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model						Notes

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exposure exposure			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Sodium

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
91	HC. 1992. Guideline Technical Document - Sodium. Health Canada (HC), Water and Air Quality Bureau, Healthy Environments and Consumer Safety Branch, Ottawa, Ontario, Canada.
110	IOM. 2005. Dietary Reference Intakes for Water, Potassium, Sodium, Chloride, and Sulfate. Institute of Medicine (IOM), National Academy of Science, Washington, D.C.
112	IOM. 2019. Dietary Reference Intakes for Sodium and Potassium (2019). Institute of Medicine (IOM), National Academies of Science, Washington, D.C.
152	NRC. 1989. Recommended Dietary Allowances. Washington, DC: National Academy of Sciences, National Academy Press. pp. 247–261.
178	USEPA (US Environmental Protection Agency). (2009). 2006 Community Water System Survey. Overview, 57.
183	USEPA, 2001. Regulatory Determination Support Document for Sodium. EPA 815 R-01-014.
185	USEPA. 2003. Drinking Water Advisory: Consumer Acceptability Advice and Health Effects Analysis on Sodium. EPA 822-R-03-006. February 2003.
232	USEPA. 1999. A Review of Contaminant Occurrence in Public Water Systems. Office of Water. EPA Report 816-R-99-006. 78 pp.
256	USEPA. 2003. Drinking Water Advisory: Consumer Acceptability Advice and Health Effects Analysis on Sodium. U.S. Environmental Protection Agency, Office of Water, Health and Ecological Criteria Division, Washington, D.C.

Sulfamethoxazole

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Sulfamethoxazole
CASRN:	723-46-6
DTXSID:	DTXSID8026064
Use:	Antibacterial; antipneumocystic
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0098

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	non-cancer effects	9	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	20	lowest therapeutic dose: treat or prevent bacterial infections: urinary tract infections/acute otitis media/acute exacerbations of chronic bronchitis/Shigellosis/Pneumocystis jiroveci Pneumonia/Traveler's Diarrhea in Adults	bottle-fed infants	FDA; NIH	2018; 2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.1968	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Sulfamethoxazole

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.003333333	mg/kg/day	FDA 2018; NIH 2018	Mutual Pharmaceutical Company, Inc.	lowest therapeutic dose:treat or prevent bacterial infections: urinary tract infections/acute otitis media/acute exacerbations of chronic bronchitis/Shigellosis/Pneumocystis jiroveci Pneumonia/Traveler's Diarrhea in Adults	bottle-fed infants	151	22.0	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels
Reference Dose (RfD) or Equivalent	0.003333333	mg/kg/day	FDA 2018; NIH 2018	Mutual Pharmaceutical Company, Inc.	lowest therapeutic dose:treat or prevent bacterial infections: urinary tract infections/acute otitis media/acute exacerbations of chronic bronchitis/Shigellosis/Pneumocystis jiroveci Pneumonia/Traveler's Diarrhea in Adults	general population	33.8	78.0	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Health-Based Guidance Value	0.1	mg/L	MN DOH	
Cancer Classification (CC)	3	no units	WHO IARC	
Chronic Health-Based Guidance Value	0.1	mg/L	MN DOH	
Screening level for pharmaceutical - general population	0.078431373	mg/L	EPA Office of Water	
Screening level for pharmaceutical - infants	0.022222222	mg/L	EPA Office of Water	
Short-Term/Subchronic Health-Based Guidance Value	0.1	mg/L	MN DOH	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	2650	mg/kg	NIH HSDB	min
LD50	6370	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	1.28	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0337287	mol/kg	TEST QSAR	
Ames mutagenicity test	-0.038	no units	TEST QSAR	
Developmental toxin test	0.853	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

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EPA - Office of Water

Sulfamethoxazole

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water			Prevalence			Magnitude					
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water			Prevalence			Magnitude					
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	619	30	Sites	4.85	0.0016	0.0408	0.197	1.46	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	75	15	Sites	20	0.0016	0.0527	0.305	1.46	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	544	15	Sites	2.76	0.00483	0.0169	0.0814	0.12	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water			Prevalence			Magnitude					
Bradley et al. 2018 (Finished) [53]	2016	26	1	Sites	3.85	0.005	0.005	0.005	0.005	ug/L	
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	4		0.0082		0.0082	ug/L	
Community Water System Survey (CWSS) (Finished) [178]	2006	1	NA	Sites			0.002	0.002		ug/L	
Padhye et al. 2013 (Finished) [155]	2009 - 2010	8	1	Samples	12	0	0		1.27e-05 +/- 3.6e-06	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Kleywegt et al. (2011) via Uslu et al. (2013) (Finished) [433]	2011	NA	NA						0.002	ug/L	
IL EPA (2008) via Uslu et al. (2013) (Finished) [433]	2008	NA	NA						0.005	ug/L	
Ambient Water			Prevalence			Magnitude					
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	502	179	Sites	36	0.00171	0.029	0.216	1.58	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	940	73	Sites	7.77	0.00275	0.0245	0.2	0.965	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,441	252	Sites	17	0.00171	0.029	0.202	1.58	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	40		0.0501		0.1611	ug/L	
Batt et al. 2016 (Ambient) [46]	2008 - 2009	182	141	Sites	77	0.0016	0.0289	0.11	0.5764	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	20	Sites	53	0.005	0.115	0.895	1.5	ug/L	
Bexfield et al. 2019 (Groundwater) [49]	2013 - 2015	1,100	12	Sites	1.09	0.019022	0.0338	0.0644	0.1198271	ug/L	
Padhye et al. 2013 (Ambient) [155]	2009 - 2010	8	7	Samples	88	0	2.4e-06		7.4e-06 +/- 8e-07	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	2	Sites	100	0.006	0.022	0.0448	0.052	ug/L	
Kleywegt et al. (2011) via Uslu et al. (2013) (Ambient) [433]	2011	NA	NA						0.284	ug/L	
Tabe et al. (2009) via Uslu et al. (2013) (Ambient) [433]	2009	NA	NA						0.002	ug/L	
Kormos et al. (2007) via Uslu et al. (2013) (Ambient) [433]	2007	NA	NA						0.035	ug/L	
IL EPA (2008) via Uslu et al. (2013) (Ambient) [433]	2008	NA	NA						0.012	ug/L	
Alvarez et al. (2005) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.034	ug/L	
Barnes et al. (2008) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						1.11	ug/L	
Batt et al. (2006) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.45	ug/L	
Batt et al. (2008) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.14	ug/L	
Benotti et al. (2007) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.081	ug/L	
Benotti et al. (2009) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.11	ug/L	
Brown et al. (2006) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.3	ug/L	
Conkle et al. (2008) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.369	ug/L	
Conley et al. (2008) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.033	ug/L	
Conley et al. (2008b) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.01	ug/L	
Focazio et al. (2008) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.023	ug/L	

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Glassmeyer et al. (2005) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.763	ug/L	
Haggard et al. (2006) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.5	ug/L	
Karthikeyan et al. (2006) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.08	ug/L	
Kim et al. (2007) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.32	ug/L	
Kolpin et al. (2002) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						1.9	ug/L	
Kolpin et al. (2004) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.07	ug/L	
Lindsey et al. (2001) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						1.02	ug/L	
Shelver et al. (2008) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.09	ug/L	
Stackelberg et al. (2004) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.05	ug/L	
Stackelberg et al. (2007) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.06	ug/L	
Standley et al. (2008) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.0022	ug/L	
Trenholm et al. (2006) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.0049	ug/L	
Vanderford et al. (2003) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.033	ug/L	
Vanderford et al. (2006) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.672	ug/L	
Yang et al. (2003) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.16	ug/L	
Waste Water Effluent				Prevalence				Magnitude			
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	20	Sites	95	0.014029	0.474	0.945	2.082509	ug/L	
Kostich et al. 2014 (Wastewater) [126]	not reported	50	48	Sites	96	0.0026	0.447	1.32	2.8725	ug/L	
Batt et al. (2005) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						1.3	ug/L	
Batt et al. (2006) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						6	ug/L	
Batt et al. (2007) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						2.8	ug/L	
Batt et al. (2008) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						2.2	ug/L	
Benotti et al. (2007) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						0.626	ug/L	
Conkle et al. (2008) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						4.09	ug/L	
Glassmeyer et al. (2005) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						0.589	ug/L	
Karthikeyan et al. (2006) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						1.25	ug/L	
Renew et al. (2004) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						2.14	ug/L	
Shelver et al. (2008) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						3.1	ug/L	
Spongberg et al. (2008) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						0.472	ug/L	
Trenholm et al. (2006) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						0.36	ug/L	
Vanderford et al. (2006) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						2.06	ug/L	
Yang et al. (2003) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						0.52	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg- bw/day)	Notes
Expocast exposure		2.48E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.34495	days	
Boiling point	OPERA QSAR	290.681	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	6.8E-10	mmHg	
Vapor pressure	TEST QSAR	4.63E-09	mmHg	
Solubility in water	OPERA QSAR	0.000989291	mol/L	
Solubility in water	TEST QSAR	0.00126183	mol/L	
Bioconcentration factor	OPERA QSAR	2.73669	no units	
Bioconcentration factor	TEST QSAR	17.1002	no units	
Henry's law constant	OPERA QSAR	7.84E-11	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	0.948532	no units	

Sulfamethoxazole

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Reference Number	Full Reference
46	Batt, A. L., Kincaid, T. M., Kostich, M. S., Lazorchak, J. M., & Olsen, A. R. (2016). Evaluating the extent of pharmaceuticals in surface waters of the United States using a National-scale Rivers and Streams Assessment survey. <i>Environmental toxicology and chemistry</i> , 35(4), 874-881.
49	Bexfield, L.M., P.L. Toccalino, K. Belitz, W.T. Foreman, and E.T. Furlong. 2019. Hormones and pharmaceuticals in groundwater used as a source of drinking water across the United States. <i>Environmental Science and Technology</i> 53: 2950-2960.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
53	Bradley, P. M., Kolpin, D. W., Romanok, K. M., Smalling, K. L., Focazio, M. J., Brown, J. B., ... & Dietze, J. E. (2018). Reconnaissance of mixed organic and inorganic chemicals in private and public supply tapwaters at selected residential and workplace sites in the United States. <i>Environmental science & technology</i> , 52(23), 13972-13985.
77	FDA. 2018. Drugs @ FDA: FDA Approved Drug Products. U.S. Food and Drug Administration (FDA). https://www.accessdata.fda.gov/scripts/cder/daf/ .
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
126	Kostich MS, et al. 2014 Concentrations of prioritized pharmaceuticals in effluents from 50 large wastewater treatment plants in the US and implications for risk estimation. <i>Environ Pollut</i> . 2014 Jan;184:354-9. doi: 10.1016/j.envpol.2013.09.013. Epub 2013 Oct 3. PMID: 24095705.
127	Kostich, MS, et al., 2010. Predicting variability of aquatic concentrations of human pharmaceuticals. <i>Sci. Total Environ</i> . 408 (20), 4504e4510.
150	NIH. 2018. DailyMed Database. U.S. National Library of Medicine, National Institutes of Health (NIH). https://dailymed.nlm.nih.gov/dailymed/ .
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
155	Padhye, L.P., Yao, H., Kung'u, F.T., and Huang, C.H. Year-long evaluation on the occurrence and fate of pharmaceuticals, personal care products, and endocrine disrupting chemicals in an urban drinking water treatment plant. 2014. <i>Water Research</i> 51 (2014) 266-276.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
178	USEPA (US Environmental Protection Agency). (2009). 2006 Community Water System Survey. Overview, 57.
433	Uslu, M., Jasim, S., Arvai, A., Bewtra, J. and Biswas, N., 2013. A Survey of Occurrence and Risk Assessment of Pharmaceutical Substances in the Great Lakes Basin. <i>Ozone: Science & Engineering</i> , 35(4), pp.249-262.

Sulfentrazone

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Sulfentrazone
CASRN:	122836-35-5
DTXSID:	DTXSID6032645
Use:	Herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0009

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	reduced longevity	10	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	200	reduced prenatal viability (fetal and litter), reduced litter size, increased number of stillborn pups, reduced pup and litter postnatal survival, decreased pup body weights throughout lactation	bottle-fed infants	OPP	2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.1793	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.14	mg/kg/day	OPP 2018	Ponnock 1994	reduced prenatal viability (fetal and litter), reduced litter size, increased number of stillborn pups, reduced pup and litter postnatal survival, decreased pup body weights throughout lactation	bottle-fed infants	151	185	[409]	
Cancer Classification (CC)	NL		OPP 2018						[409]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	3.9	mg/L	EPA HHBP	
Acute PAD	0.14	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.9	mg/L	EPA HHBP	
Health-Based Screening Level	0.9	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.14	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	2855	mg/kg	NIH HSDB	
LOAEL	25	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	250	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	10	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	116.9	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	2.79	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	108.4	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic LOAEL	57	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	23.1	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	79.8	mg/kg/day	EPA Toxicity Reference Database	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0012274	mol/kg	TEST QSAR	
Ames mutagenicity test	0.709	no units	TEST QSAR	
Developmental toxin test	1.271	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

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EPA - Office of Water

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	1,762	230	Sites	13	0.00055	0.0224	0.179	4.1	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	322	198	Sites	61	0.00055	0.0224	0.178	4.1	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	1,440	32	Sites	2.22	0.0015	0.0166	0.201	0.26	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	39	4,031,687	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	307	72	Sites	23	0.00133	0.0226	0.25	2.42	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	530	15	Sites	2.83	0.00548	0.0158	0.0304	0.0594	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	837	87	Sites	10	0.00133	0.0215	0.244	2.42	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	6	Sites	1.03	0.0015	0.007	0.109	0.199	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.000000118	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.65135	days	
Boiling point	OPERA QSAR	342.454	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	7.86E-10	mmHg	
Vapor pressure	TEST QSAR	2.59E-08	mmHg	
Solubility in water	OPERA QSAR	0.0001917	mol/L	
Solubility in water	TEST QSAR	0.000125314	mol/L	
Bioconcentration factor	OPERA QSAR	7.66859	no units	
Bioconcentration factor	TEST QSAR	6.91831	no units	
Henry's Law constant	OPERA QSAR	8.59E-11	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.3198	no units	

Sulfentrazone

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
409	USEPA. 2018. Sulfentrazone - Human Health Risk Assessment for a Section 3 Registration Request to Add New Uses on Chia and Teff; an Amended Use on Mint; and Crop Group Conversions for Tree Nut Group 14-12, Stalk and Stem Vegetable Subgroup 22A; Vegetable, Brassica, Head and Stem, Group 5-16; and Brassica, Leafy Greens, Subgroup 4-16B. EPA-HQ-OPP-2017-0072-0009. DP No. D443993. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.

Sulfometuron methyl

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Sulfometuron methyl
CASRN:	74222-97-2
DTXSID:	DTXSID0034936
Use:	Herbicide for annual, biennial, and perennial grasses and annual broadleaf weeds
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.000018

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	non-cancer effects	9	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	2000	decreased body weight gain, hemolytic anemia, increase in alkaline phosphatase	general population	OPP	2015

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.03624	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Sulfometuron methyl

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.275	mg/kg/day	OPP 2015	Wood and O'Neal 1983	decreased body weight gain, hemolytic anemia, increase in alkaline phosphatase -- decreased body weight gain seen at beginning of 4 weeks of exposure in adult dogs	general population	33.8	1630	[357]	
Cancer Classification (CC)	NL		OPP 2015						[357]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	1.83	mg/L	EPA HHBP	
Acute PAD	0.275	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	1.76	mg/L	EPA HHBP	
Health-Based Screening Level	1.76	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.275	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	5000	mg/kg	NIH HSDB	
Percent of active toxcast in vitro assays tested	0.75	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity test	0.116	no units	TEST QSAR	
Developmental toxin test	1.056	no units	TEST QSAR	

Scoring Data											
Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence					Magnitude				
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water							Magnitude				
		Prevalence					Magnitude				
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	4,167	261	Sites	6.26	9.00E - 05	0.00454	0.0362	3.51	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	471	228	Sites	48	2.00E - 04	0.00455	0.0363	3.51	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	3,696	33	Sites	0.89	9.00E - 05	0.004	0.0336	0.284	ug/L	

Non-Scoring Data												
Non-Nationally Representative Water Data		Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water			Prevalence				Magnitude					
USDA Pesticide Data Program (PDP) (Finished)		2001 - 2013	12	7	Sites	58	0.00127	0.0032	0.012	0.025	ug/L	
Ambient Water			Prevalence				Magnitude					
National Water Information System (USGS NWIS) (Surface Water)		2008 - 2017	475	119	Sites	25	2.00E - 04	0.00645	0.0348	1.79	ug/L	
National Water Information System (USGS NWIS) (Groundwater)		2008 - 2017	1,057	16	Sites	1.51	0.00137	0.0055	0.0474	0.101	ug/L	
National Water Information System (USGS NWIS) (All Water)		2008 - 2017	1,532	135	Sites	8.81	2.00E - 04	0.00645	0.0352	1.79	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)		2001 - 2013	229	9	Sites	3.93	0.00127	0.0038	0.0192	0.059	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)		2001 - 2013	219	2	Sites	0.91	0.00863	0.0105	0.0281	0.035	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)		2001 - 2013	12	7	Sites	58	0.00127	0.0032	0.0187	0.059	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]		1990 - 2018	26	0	Sites	0						
Bradley et al. 2017 (Ambient) [52]		2012 - 2014	38	5	Sites	13	0.0252	0.0349	0.177	0.248	ug/L	
Arnold et al. 2016 (Filtered) [7]		2012 - 2013	690	8	Sites	1.16	1e-04	0.00095	0.00325	0.0064	ug/L	
USGS, McKenzie River, Oregon, 2012 (Ambient) [158]		2002 - 2010	126	18	Samples	14				1.61	ug/L	
Waste Water Effluent			Prevalence				Magnitude					
Estimated Concentration in Water		Date	Source	Value	Units	Model	Notes					

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)	< 1.0D	µg/l	

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.63689	days	
Boiling point	OPERA QSAR	264.401	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	1.3E-10	mmHg	
Vapor pressure	TEST QSAR	2.21E-11	mmHg	
Solubility in water	OPERA QSAR	0.000446592	mol/L	
Solubility in water	TEST QSAR	0.000406443	mol/L	
Bioconcentration factor	OPERA QSAR	3.45799	no units	
Bioconcentration factor	TEST QSAR	0.907821	no units	
Henry's Law constant	OPERA QSAR	6.36E-10	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.21447	no units	

Sulfometuron methyl

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
158	Reconnaissance of Land-Use Sources of Pesticides in Drinking Water, McKenzie River, Oregon. U.S. Geological Survey Scientific Investigations Report 2012–5091, 46 p. plus appendixes.
357	USEPA. 2015. Sulfometuron Methyl. Draft Human Health Risk Assessment in Support of Registration Review. EPA-HQ-OPP-2012-0433-0026. DP No. D427028. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Tamoxifen

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Tamoxifen
CASRN:	10540-29-1
DTXSID:	DTXSID1034187
Use:	Antiestrogen; antineoplastic (hormonal)
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	X
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.31

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	non-cancer effects	1	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	0.6	lowest therapeutic dose: nonsteroidal antiestrogen/ treatment of metastatic breast cancer/adjuvant breast cancer treatment/ductal carcinoma in situ/prophylaxis in women at high risk for cancer	bottle-fed infants	FDA; NIH	2018; 2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.187	90th Percentile	All Ambient Water	NWIS	2008-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		
Not Applicable		

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Tamoxifen

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	8.33333E-05	mg/kg/day	FDA 2018; NIH 2018	Andrx Pharmaceuticals, Inc.	lowest therapeutic dose:nonsteroidal antiestrogen/ treatment of metastatic breast cancer/adjuvant breast cancer treatment/ductal carcinoma in situ/prophylaxis in women at high risk for cancer	bottle-fed infants	151	0.560	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels
Reference Dose (RfD) or Equivalent	8.33333E-05	mg/kg/day	FDA 2018; NIH 2018	Andrx Pharmaceuticals, Inc.	lowest therapeutic dose:nonsteroidal antiestrogen/ treatment of metastatic breast cancer/adjuvant breast cancer treatment/ductal carcinoma in situ/prophylaxis in women at high risk for cancer	general population	33.8	2.00	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Cancer Classification (CC)	1	no units	WHO IARC	
Screening level for pharmaceutical - general population	0.001960784	mg/L	EPA Office of Water	
Screening level for pharmaceutical - infants	0.000555556	mg/L	EPA Office of Water	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Percent of active toxcast in vitro assays tested	40.13	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0058345	mol/kg	TEST QSAR	
Ames mutagenicity test	0.096	no units	TEST QSAR	
Developmental toxin test	0.788	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Tamoxifen
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	531	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	75	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	456	0	Sites	0						

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	193	1	Sites	0.52	0.187	0.187	0.187	0.187	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	333	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	526	1	Sites	0.19	0.187	0.187	0.187	0.187	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Bexfield et al. 2019 (Groundwater) [49]	2013 - 2015	1,097	0	Sites	0						
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	20	0	Sites	0						
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		4.05E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.36164	days	
Boiling point	OPERA QSAR	419.341	degree C	
Boiling point	TEST QSAR	428.393	degree C	
Vapor pressure	OPERA QSAR	2.07E-08	mmHg	
Vapor pressure	TEST QSAR	5.27E-09	mmHg	
Solubility in water	OPERA QSAR	0.00000858	mol/L	
Solubility in water	TEST QSAR	0.00000274	mol/L	
Bioconcentration factor	OPERA QSAR	1210.92	no units	
Bioconcentration factor	TEST QSAR	345.144	no units	
Henry's Law constant	OPERA QSAR	2.21E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	6.2335	no units	

Tamoxifen

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
49	Bexfield, L.M., P.L. Toccalino, K. Belitz, W.T. Foreman, and E.T. Furlong. 2019. Hormones and pharmaceuticals in groundwater used as a source of drinking water across the United States. Environmental Science and Technology 53: 2950-2960.
77	FDA. 2018. Drugs @ FDA: FDA Approved Drug Products. U.S. Food and Drug Administration (FDA). https://www.accessdata.fda.gov/scripts/cder/daf/ .
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. Science of The Total Environment. v581-582, (909-922).
150	NIH. 2018. DailyMed Database. U.S. National Library of Medicine, National Institutes of Health (NIH). https://dailymed.nlm.nih.gov/dailymed/ .
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. Science of the Total Environment, 636, 69-79.

Tebuconazole

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Tebuconazole
CASRN:	107534-96-3
DTXSID:	DTXSID9032113
Use:	Fungicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	X

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.0058

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	reproductive and developmental effects	1	5

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	40	decreases in body weights, absolute brain weights, brain measurements, and motor activity in offspring	bottle-fed infants	OPP	2019

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.2307	90th Percentile	Finished Water	UCMR4	2018-2019

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
		X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Tebuconazole

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.029	mg/kg/day	OPP 2019	Parker 2000	decreases in body weights, absolute brain weights, brain measurements, and motor activity in offspring	bottle-fed infants	151	38.4	[427]	
Cancer Classification (CC)	C		OPP 2019						[427]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.19	mg/L	EPA HHBP	
Acute PAD	0.029	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.19	mg/L	EPA HHBP	
Health-Based Screening Level	0.19	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.029	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	5000	mg/kg	NIH HSDB	max
LD50	625	mg/kg	NIH HSDB	min
Percent of active toxcast in vitro assays tested	17.05	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0101391	mol/kg	TEST QSAR	
Ames mutagenicity test	0.499	no units	TEST QSAR	
Developmental toxin test	0.483	no units	TEST QSAR	

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019	3,648	2	Sites	0.05	0.21	0.222	0.231	0.233	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	1,788	165	Sites	9.23	0.00024	0.00735	0.0285	0.93	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	328	163	Sites	50	0.00024	0.00735	0.0284	0.93	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	1,460	2	Sites	0.14	0.00035	0.13	0.207	0.259	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	47	2,111,268	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	7	Sites	41	0.0035	0.0035	0.0165	0.15	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	435	69	Sites	16	0.00044	0.0118	0.0784	3.24	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	536	2	Sites	0.37	0.00584	0.0103	0.0702	0.0959	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	971	71	Sites	7.31	0.00044	0.0118	0.0859	3.24	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	12	Sites	5.24	0.0035	0.0058	0.0377	0.15	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	6	Sites	2.74	0.0035	0.014	0.061	0.083	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	6	Sites	50	0.0035	0.00465	0.026	0.15	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	50	0	Sites	0						
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	7	Sites	18	0.0173	0.0255	0.041	0.0421	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		1.58E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.17404	days	
Boiling point	OPERA QSAR	321.712	degree C	
Boiling point	TEST QSAR	344.862	degree C	
Vapor pressure	OPERA QSAR	0.000000022	mmHg	
Vapor pressure	TEST QSAR	9.29E-08	mmHg	
Solubility in water	OPERA QSAR	0.00010626	mol/L	
Solubility in water	TEST QSAR	0.0000893	mol/L	
Bioconcentration factor	OPERA QSAR	243.826	no units	
Bioconcentration factor	TEST QSAR	49.204	no units	
Henry's Law constant	OPERA QSAR	0.000000329	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.68215	no units	

Tebuconazole

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
427	USEPA. 2019. Tebuconazole: Acute and Chronic Aggregate Dietary Exposure and Risk Assessments for Petition for the Establishment of Registrations and Permanent Tolerances for Residues in/on Watercress; Add Green-House Grown Tomato to Label and Crop Group Conversions/Expansions for Brassica Leafy Greens, Subgroup 4-16B, Except Watercress; Cottonseed, Subgroup 20C; Pome Fruit, Group 11-10; Stone Fruit, Group 12-12, Except Cherry; Small Vine Climbing Fruit, Except Fuzzy Kiwifruit, Subgroup 13-07F; Tropical and Subtropical Small Fruit, Inedible Peel, Subgroup 24A; Tree Nut,
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Tebuthiuron

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Tebuthiuron
CASRN:	34014-18-1
DTXSID:	DTXSID3024316
Use:	Herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision

Not List

Final Hazard Quotient (HQ)

0.00024

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	reproductive and developmental effects	10	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	200	decreased body weights in F1 females; decreased up body weights in F1 and F2 generations	bottle-fed infants	OPP	2014

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.048	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		
Not Applicable		

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Tebuthiuron

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.14	mg/kg/day	OPP 2014	Hoyt et al. 1981	decreased body weights in F1 females; decreased pup body weights in F1 and F2 generations	bottle-fed infants	151	185	[336]	
Cancer Classification (CC)	D		OPP 2014						[336]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	3	mg/L	EPA DWSHA 2018	
Lifetime Health Advisory	0.5	mg/L	EPA DWSHA 2018	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	200	mg/kg	NIH HSDB	min
LD50	644	mg/kg	NIH HSDB	max
LOAEL	110	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	31	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	15	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	72	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	1.28	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0068865	mol/kg	TEST QSAR	
Ames mutagenicity test			TEST QSAR	
Developmental toxin test	0.583	no units	TEST QSAR	

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OCCURRENCE DATA

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Scoring Data											
Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
		Prevalence				Magnitude					
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	11,243	1,134	Sites	10	0	0.0106	0.048	17.3	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	2,224	813	Sites	37	0	0.01	0.044	6.4	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	9,019	321	Sites	3.56	0.00024	0.0205	0.146	17.3	ug/L	
Pesticide Application Data				Toxic Release Data				Chemical Production Data			
Number of States	Amount Applied (lbs/year)	Date		Number of States	Amount Released (lbs/year)			Production Volume (lbs/year)			
Estimated Annual Agricultural Pesticide Use (USGS)	13	22,610	2015	Toxic Release Inventory (TRI) Program (EPA) (2016)				Chemical Data Reporting (CDR) Results (EPA) (2016)			

Non-Scoring Data											
Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	2	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	10	Sites	59	0.00035	0.001	0.0037	0.055	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
		Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	1	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	918	185	Sites	20	0.00031	0.00667	0.0449	1.4	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3,084	130	Sites	4.22	3.00E - 04	0.016	0.13	0.516	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	4,001	315	Sites	7.87	3.00E - 04	0.00857	0.0603	1.4	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	47	Sites	21	0.00035	0.001	0.0046	0.43	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	41	Sites	19	0.00035	0.0011	0.05	0.43	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	6	Sites	50	0.00035	0.001	0.0044	0.22	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	1,757	31	Sites	1.76	0.0127	0.052	1.3	3	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	3	Sites	7.89	0.0125	0.015	0.0316	0.0358	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	24	Sites	3.48	5e-04	0.0026	0.0145	0.0317	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
USGS, McKenzie River, Oregon, 2012 (Ambient) [158]	2002 - 2010	134	6	Samples	4.5				3.47	ug/L	
Waste Water Effluent											
		Prevalence				Magnitude					
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Exposure exposure		8.13E-08	
Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.57479	days	
Boiling point	OPERA QSAR	334.1	degree C	
Boiling point	TEST QSAR	340.382	degree C	
Vapor pressure	OPERA QSAR	0.00000229	mmHg	
Vapor pressure	TEST QSAR	0.000000564	mmHg	
Solubility in water	OPERA QSAR	0.0110523	mol/L	
Solubility in water	TEST QSAR	0.00409261	mol/L	
Bioconcentration factor	OPERA QSAR	2.60494	no units	
Bioconcentration factor	TEST QSAR	9.18333	no units	
Henry's Law constant	OPERA QSAR	1.38E-10	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.65206	no units	

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
158	Reconnaissance of Land-Use Sources of Pesticides in Drinking Water, McKenzie River, Oregon. U.S. Geological Survey Scientific Investigations Report 2012–5091, 46 p. plus appendixes.
336	USEPA. 2014. Tebuthiuron: Draft Human Risk Assessment. EPA-HQ-OPP-2009-0327-0041. DP Nos. D414218 D418910 D418911. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Tefluthrin

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Tefluthrin
CASRN:	79538-32-2
DTXSID:	DTXSID5032577
Use:	Insecticide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	X
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.001

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	non-cancer effects	3	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	10	increased incidence of tremors	general population	OPP	2019

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.0101	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Tefluthrin

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0017	mg/kg/day	OPP 2019	Stonard 1986	increased incidence of tremors	general population	33.8	10.1	[428]	
Cancer Classification (CC)	NL		OPP 2019						[428]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.011	mg/L	EPA HHBP	
Acute PAD	0.0017	mg/kg/day	EPA HHBP	
Health-Based Screening Level	0.011	mg/L	Health-based screening levels from USGS	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	22	mg/kg	NIH HSDB	min
LD50	57	mg/kg	NIH HSDB	max
LOAEL	3	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	54.400002	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	1	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	13.5	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	9.38	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	7.5	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	2.5	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0001941	mol/kg	TEST QSAR	
Ames mutagenicity test	0.654	no units	TEST QSAR	
Developmental toxin test	0.96	no units	TEST QSAR	

Tefluthrin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	3,062	7	Sites	0.23	0.004	0.005	0.0101	0.015	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	197	6	Sites	3.05	0.004	0.005	0.0108	0.015	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	2,865	1	Sites	0.03	0.006	0.006	0.006	0.006	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	36	350,395	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	10	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	508	1	Sites	0.2	0.062	0.062	0.062	0.062	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	956	4	Sites	0.42	0.002	0.0035	0.004	0.004	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,463	5	Sites	0.34	0.002	0.004	0.033	0.062	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	123	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	113	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	10	0	Sites	0						
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	106	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.000000183	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.53756	days	
Boiling point	OPERA QSAR	306.216	degree C	
Boiling point	TEST QSAR	289.657	degree C	
Vapor pressure	OPERA QSAR	0.000042	mmHg	
Vapor pressure	TEST QSAR	0.00000345	mmHg	
Solubility in water	OPERA QSAR	8.52E-08	mol/L	
Solubility in water	TEST QSAR	0.000000104	mol/L	
Bioconcentration factor	OPERA QSAR	1246.21	no units	
Bioconcentration factor	TEST QSAR	567.545	no units	
Henry's Law constant	OPERA QSAR	4.43E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	6.47305	no units	

Tefluthrin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
428	USEPA. 2019. Tefluthrin: Updated Human Health Draft Risk Assessment in Support of Registration Review. DP No. D453462. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.

Terbacil

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Terbacil
CASRN:	5902-51-2
DTXSID:	DTXSID8024317
Use:	Herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.00035

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	reproductive and developmental effects	1	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	400	decreased pup body weights pnd 7-21	bottle-fed infants	OPP	2019

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.1418	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X	X		

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	X	Not Applicable

Basis

Terbacil does not appear to occur at health levels of concern in PWSs and EPA has made a determination that terbacil does not present a meaningful opportunity for health risk reduction. While terbacil has been found in ambient waters at the levels less than the HRL of 90 µg/L (as well as ½ the HRL) [a,b], it was not found in the UCMR 1 survey of public water supplies [c].

[a] Kolpin & Martin, 2003 [123]; [b] Martin, Crawford, & Larson, 2003 [134]; [c] USEPA, 2008 [297]; as cited in USEPA, 2008 [296]

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Terbacil

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.33	mg/kg/day	OPP 2019	Edwards 2017	decreased pup body weights pnd 7-21	bottle-fed infants	151	437	[429]	
Cancer Classification (CC)	NL		OPP 2019						[429]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	0.3	mg/L	EPA DWSHA 2018	
Lifetime Health Advisory	0.09	mg/L	EPA DWSHA 2018	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	5000	mg/kg	NIH HSDB	min
LD50	7500	mg/kg	NIH HSDB	max
LOAEL	6.25	mg/kg/day	EPA Toxicity Reference Database	
NOAEL	1.25	mg/kg/day	EPA Toxicity Reference Database	
Percent of active toxcast in vitro assays tested	5.54	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0100231	mol/kg	TEST QSAR	
Ames mutagenicity test	0.196	no units	TEST QSAR	
Developmental toxin test	0.982	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Terbacil
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003	3,873	0	Sites	0					ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	10,088	235	Sites	2.33	0.0018	0.024	0.142	1.52	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	2,037	181	Sites	8.89	0.0018	0.024	0.126	1.52	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	8,052	54	Sites	0.67	0.003	0.0195	0.27	1.05	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	17	13,550	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	67	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	13	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	402	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	671	8	Sites	1.19	0.0129	0.0255	0.135	0.275	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	1,587	6	Sites	0.38	0.006	0.063	0.177	0.245	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	2,258	14	Sites	0.62	0.006	0.0264	0.192	0.275	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	121	3	Sites	2.48	0.00118	0.00118	0.00237	0.002664	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	114	1	Sites	0.88	0.002664	0.00266	0.00266	0.002664	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	8	2	Sites	25	0.00118	0.00118	0.00118	0.00118	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	501	2	Sites	0.4	0.008	0.021	0.0314	0.034	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	1	Sites	2.63	0.0154	0.0154	0.0154	0.0154	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	1	Sites	0.14	0.0072	0.0072	0.0072	0.0072	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg-bw/day)	Notes
Expcast exposure		7.54E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.32238	days	
Boiling point	OPERA QSAR	277.667	degree C	
Boiling point	TEST QSAR	300.294	degree C	
Vapor pressure	OPERA QSAR	0.00607559	mmHg	
Vapor pressure	TEST QSAR	0.000000202	mmHg	
Solubility in water	OPERA QSAR	0.0968241	mol/L	
Solubility in water	TEST QSAR	0.0038815	mol/L	
Bioconcentration factor	OPERA QSAR	2.47838	no units	
Bioconcentration factor	TEST QSAR	4.57088	no units	
Henry's Law constant	OPERA QSAR	0.00000155	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.05194	no units	

Terbacil

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
123	Kolpin, D.W. and J.D. Martin. 2003. Pesticides in Ground Water: Summary Statistics; Preliminary Results from Cycle I of the National Water Quality Assessment Program (NAWQA), 1992-2001. Available on the Internet at: http://ca.water.usgs.gov/pnsp/pestgw/Pest-GW_2001_Text.html .
134	Martin, J.D., C.G. Crawford, and S.J. Larson. 2003. Pesticides in Streams: Summary Statistics; Preliminary Results from Cycle I of the National Water Quality Assessment Program (NAWQA), 1992-2001. Available on the Internet at: http://ca.water.usgs.gov/pnsp/pestsw/Pest-SW_2001_Text.html .
296	USEPA. 2008. Regulatory Determinations Support Document for Selected Contaminants from the Second Drinking Water Contaminant Candidate List (CCL 2). EPA Report 815-R-08-012. June 2008.
297	USEPA. 2008. The Analysis of Occurrence Data from the First Unregulated Contaminant Monitoring Regulation (UCMR 1) in Support of Regulatory Determinations for the Second Drinking Water Contaminant Candidate List. EPA 815-R-08-013. June.
429	USEPA. 2019. Terbacil: Human Health Draft Risk Assessment for Registration Review. EPA-HQ-OPP-2011-0054-0038. DP No. D446169. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Terbufos

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Terbufos
CASRN:	13071-79-9
DTXSID:	DTXSID2022254
Use:	Insecticide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	X
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.66

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
8	non-cancer effects	1	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.3	plasma cholinesterase inhibition	general population	OPP	2006

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.1984	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X	X	X	

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	X

Basis

Terbufos regulation does not represent a meaningful opportunity for health risk reduction for persons served by PWSs. Although terbufos has the potential to cause adverse health effects, including ChE inhibition and reproductive effects [a,b,c], it does not appear to occur in PWSs with a frequency and at levels of public health concern [c,d]. Terbufos was not detected in any UCMR 1 samples collected by PWSs, using an MRL of 0.5 µg/L, which is slightly higher than the HRL (0.35 µg/L) [e,f,g,h].

[a] Shellenberger, 1984 [163]; [b] Shellenberger & Billups, 1986 [164]; [c] USEPA, 2006 [274]; [d] Bailey, 1988 [39]; [e] USEPA, 2007 [284]; [f] USEPA, 2008 [297]; [g] USEPA, 2010 [310]; [h] USEPA, 2015 [350]; as cited in USEPA, 2014 [334]

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Terbufos

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.00005	mg/kg/day	OPP 2006	American Cyanamid Co. 1986; Shellenberger 1984	plasma cholinesterase inhibition	general population	33.8	0.296	[267]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	0.005	mg/L	EPA DWSHA 2018	
Lifetime Health Advisory	0.0004	mg/L	EPA DWSHA 2018	
Maximum Allowable Concentration (MAC)	0.001	mg/L	Canadian Drinking Water Guidelines	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	2	mg/kg	NIH HSDB	min
LD50	9.2	mg/kg	NIH HSDB	max
LOAEL	0.2188	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	0.015	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	0.0854	mg/kg/day	EPA Toxicity Reference Database	
Percent of active toxcast in vitro assays tested	8.45	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	5.78E-06	mol/kg	TEST QSAR	
Ames mutagenicity test	0.005	no units	TEST QSAR	
Developmental toxin test	-0.779	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

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EPA - Office of Water

Terbufos
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003	295	0	Sites	0					ug/L	
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	11,234	33	Sites	0.29	0.002	0.017	0.198	0.56	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	2,224	29	Sites	1.3	0.002	0.023	0.194	0.56	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	9,010	4	Sites	0.04	0.007	0.01	0.126	0.202	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	23	2,259,511	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	4	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	1	Sites	5.88	0.089	0.089	0.089	0.089	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	44	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	898	4	Sites	0.45	0.006	0.146	0.212	0.226	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	3,037	1	Sites	0.03	0.009	0.009	0.009	0.009	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	3,934	5	Sites	0.13	0.006	0.103	0.208	0.226	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	495	1	Sites	0.2	0.04	0.04	0.04	0.04	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.00000011	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	403.714	days	
Boiling point	OPERA QSAR	315.407	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.000228304	mmHg	
Vapor pressure	TEST QSAR	0.000148594	mmHg	
Solubility in water	OPERA QSAR	0.0000298	mol/L	
Solubility in water	TEST QSAR	0.0000625	mol/L	
Bioconcentration factor	OPERA QSAR	64.5795	no units	
Bioconcentration factor	TEST QSAR	125.893	no units	
Henry's Law constant	OPERA QSAR	0.00000263	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	4.32209	no units	

Terbufos

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EPA-OGWDW and OST

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
39	Bailey, D.E. 1988. 14-Day oral toxicity study in the dog with AC 92 100 and its metabolites, CL 94 301 and CL94320. Unpublished report on HLA Study No. 362-190 (BASF RDI No.TE-420-007) from Hazleton Laboratories America, Inc., Vienna, VA, USA (as cited in USEPA, 2003).
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
163	Shellenberger, T. 1984. 28-Day Oral Toxicity in the Dog with AC 92,100: Report No. 87019. Unpublished study prepared by Tegeris Laboratories Inc. 89 p. (as cited in USEPA,2006).
164	Shellenberger, T., and L.H. Billups. 1986. One-year oral toxicity study in purebred beagle dogs with AC 92 100. Unpublished report No. 8414 (BASF RDI No. TE-427-002) from Tegeris Laboratories, Inc., Laurel, MD, USA (as cited in USEPA, 2003).
267	USEPA. 2006. Finalization of Interim Reregistration Eligibility Decisions (IREDs) and Interim Tolerance Reassessment and Risk Management Decisions (TREDs) for the Organophosphate Pesticides, and Completion of the Tolerance Reassessment and Reregistration Eligibility Process for the Organophosphate Pesticides. Reregistration Eligibility Decision for Terbufos. U.S. Environmental Protection Agency, Office of Prevention, Pesticides and Toxic Substances, Washington, D.C.
274	USEPA. 2006. Reregistration Eligibility Decision for Terbufos. Office of Pesticide Programs. Available on the Internet at: http://www.epa.gov/pesticides/reregistration/REDs/terbufos_red.pdf .
284	USEPA. 2007. Unregulated Contaminant Monitoring Regulation (UCMR) for Public Water Systems Revisions. Federal Register. Vol. 72, No. 2, p. 367, January 4, 2007.
297	USEPA. 2008. The Analysis of Occurrence Data from the First Unregulated Contaminant Monitoring Regulation (UCMR 1) in Support of Regulatory Determinations for the Second Drinking Water Contaminant Candidate List. EPA 815-R-08-013. June.
310	USEPA. 2010. Data Management and Analytical Plan for the Second Unregulated Contaminant Monitoring Regulation (UCMR 2) Data. June 2010 Draft Report Submitted to EPA.
334	USEPA. 2014. Regulatory Determinations 3 Support Document. April 2014. EPA Publication # 815-R14-003.
350	USEPA. 2015. Occurrence Data from the Second Unregulated Contaminant Monitoring Regulation (UCMR 2). Including Appendices A-C. EPA 815-R-15-013. December 2015.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Testosterone

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Testosterone
CASRN:	58-22-0
DTXSID:	DTXSID8022371
Use:	Medication (human and veterinary) and in research
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	X
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0018

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
8	non-cancer effects	9	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	0.3	lowest therapeutic dose: replacement therapy in conditions associated with deficiency or absence of endogenous testosterone/antiestrogen therapy	bottle-fed infants	FDA; NIH	2018; 2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.000527	90th Percentile	Finished Water	UCMR3	2013-2015

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Testosterone

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	4.16667E-05	mg/kg/day	FDA 2018; NIH 2018	Impax Generics	lowest therapeutic dose: replacement therapy in conditions associated with deficiency or absence of endogenous testosterone/antiestrogen therapy	bottle-fed infants	151	0.280	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels
Reference Dose (RfD) or Equivalent	4.16667E-05	mg/kg/day	FDA 2018; NIH 2018	Impax Generics	lowest therapeutic dose: replacement therapy in conditions associated with deficiency or absence of endogenous testosterone/antiestrogen therapy	general population	33.8	0.980	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Screening level for pharmaceutical - general population	0.000980392	mg/L	EPA Office of Water	
Screening level for pharmaceutical - infants	0.000277778	mg/L	EPA Office of Water	

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Percent of active toxicant in vitro assays tested	15.74	percent	EPA Chemistry Dashboard	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0135207	mol/kg	TEST QSAR	
Ames mutagenicity test	-0.018	no units	TEST QSAR	
Developmental toxin test	1.04	no units	TEST QSAR	

Testosterone

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015	1,201	65	Sites	5.41	1.00E - 04	0.00017	0.000527	0.0053	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	527	4	Sites	0.76	0.00042	0.00069	0.00122	0.00149	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	29	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	498	4	Sites	0.8	0.00042	0.00069	0.00122	0.00149	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	4		0.00015		0.00015	ug/L	
Batt et al. 2016 (Ambient) [46]	2008 - 2009	182	3	Sites	1.65	0.0037	0.0064	0.29	0.3614	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	1	Sites	2.63	0.0011	0.0011	0.0011	0.0011	ug/L	
Bexfield et al. 2019 (Groundwater) [49]	2013 - 2015	1,091	1	Sites	0.09	0.003038	0.00304	0.00304	0.003038	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	2	Sites	9.52	0.000973	0.000973	0.000973	0.000973	ug/L	
Kostich et al. 2014 (Wastewater) [126]	not reported	50	0	Sites	0						
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		3.14E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	68.9239	days	
Boiling point	OPERA QSAR	295.416	degree C	
Boiling point	TEST QSAR	357.585	degree C	
Vapor pressure	OPERA QSAR	0.000000187	mmHg	
Vapor pressure	TEST QSAR	0.000000245	mmHg	
Solubility in water	OPERA QSAR	0.000277495	mol/L	
Solubility in water	TEST QSAR	0.000130317	mol/L	
Bioconcentration factor	OPERA QSAR	52.7161	no units	
Bioconcentration factor	TEST QSAR	80.5378	no units	
Henry's Law constant	OPERA QSAR	2.46E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.24993	no units	

Testosterone

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
46	Batt, A. L., Kincaid, T. M., Kostich, M. S., Lazorchak, J. M., & Olsen, A. R. (2016). Evaluating the extent of pharmaceuticals in surface waters of the United States using a National-scale Rivers and Streams Assessment survey. <i>Environmental toxicology and chemistry</i> , 35(4), 874-881.
49	Bexfield, L.M., P.L. Toccalino, K. Belitz, W.T. Foreman, and E.T. Furlong. 2019. Hormones and pharmaceuticals in groundwater used as a source of drinking water across the United States. <i>Environmental Science and Technology</i> 53: 2950-2960.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
77	FDA. 2018. Drugs @ FDA: FDA Approved Drug Products. U.S. Food and Drug Administration (FDA). https://www.accessdata.fda.gov/scripts/cder/daf/ .
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
126	Kostich MS, et al. 2014 Concentrations of prioritized pharmaceuticals in effluents from 50 large wastewater treatment plants in the US and implications for risk estimation. <i>Environ Pollut</i> . 2014 Jan;184:354-9. doi: 10.1016/j.envpol.2013.09.013. Epub 2013 Oct 3. PMID: 24095705.
150	NIH. 2018. DailyMed Database. U.S. National Library of Medicine, National Institutes of Health (NIH). https://dailymed.nlm.nih.gov/dailymed/ .
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.

Tetraconazole

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Tetraconazole
CASRN:	112281-77-3
DTXSID:	DTXSID8034956
Use:	Fungicide used on blueberries, cereals, grapes, ornamentals, peanuts among others
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.00066

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	non-cancer effects	9	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	40	increased kidney weight and altered histopathology of the kidney	general population	OPP	2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.02644	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Tetraconazole

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0073	mg/kg/day	OPP 2018	Makin et al. 1990	increased kidney weight and altered histopathology of the kidney	general population	33.8	43.2	[410]	
Cancer Classification (CC)	NL		OPP 2018						[410]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	3	mg/L	EPA HHBP	
Acute PAD	0.5	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.047	mg/L	EPA HHBP	
Health-Based Screening Level	0.047	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.0073	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LOAEL	100	mg/kg/day	EPA Toxicity Reference Database	max
LOAEL	2.95	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	0.8	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	30	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	28.78	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	23.9	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	5.5	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity test	0.138	no units	TEST QSAR	
Developmental toxin test	0.626	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Tetraconazole

CCL 5 Contaminant Information Sheet

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	1,763	60	Sites	3.4	0.00035	0.00509	0.0264	0.254	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	324	55	Sites	17	0.00035	0.00514	0.026	0.208	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	1,439	5	Sites	0.35	0.00075	0.00158	0.13	0.254	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	31	134,273	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	15	6	Sites	40	0.002	0.0032	0.0096	0.084	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	433	19	Sites	4.39	1.00E - 04	0.0089	0.206	0.462	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	531	1	Sites	0.19	0.00359	0.00359	0.00359	0.00359	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	964	20	Sites	2.07	1.00E - 04	0.0082	0.204	0.462	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	227	6	Sites	2.64	0.002	0.0047	0.0178	0.03	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	1	Sites	0.46	0.003164	0.00316	0.00316	0.003164	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	10	5	Sites	50	0.002	0.0062	0.018	0.03	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	1	Sites	2.63	0.0219	0.0219	0.0219	0.0219	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	4	Sites	0.68	8e-04	0.00135	0.00454	0.0058	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.000000105	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.48195	days	
Boiling point	OPERA QSAR	339.08	degree C	
Boiling point	TEST QSAR	344.772	degree C	
Vapor pressure	OPERA QSAR	0.00000175	mmHg	
Vapor pressure	TEST QSAR	0.00000171	mmHg	
Solubility in water	OPERA QSAR	0.000928927	mol/L	
Solubility in water	TEST QSAR	0.0000151	mol/L	
Bioconcentration factor	OPERA QSAR	309.071	no units	
Bioconcentration factor	TEST QSAR	131.22	no units	
Henry's Law constant	OPERA QSAR	0.00000273	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.52679	no units	

Tetraconazole

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. Environmental science & technology, 51(9), 4792-4802.
410	USEPA. 2018. Tetraconazole: Human Health Risk Assessment for the Section 3 Registration for Application to add Crop Subgroup 6C; Dried Shelled Pea and Bean (except soybean) Subgroup 6C; Barley; Rapeseed Subgroup 20A; Wheat; and Forage, Fodder, and Straw of Cereal Grains Group 16. EPA-HQ-OPP-2016-0573-0005. DP No. D435706. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.

Thiabendazole

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Thiabendazole
CASRN:	148-79-8
DTXSID:	DTXSID0021337
Use:	Fungicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.000027

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	non-cancer effects	9	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	600	decreased body weight in males	general population	OPP	2019

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.0164	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Thiabendazole

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.1	mg/kg/day	OPP 2019	Merck Research Labs. 1993	decreased body weight in males	general population	33.8	592	[430]	
Cancer Classification (CC)	L/NL		OPP 2019						[430]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.3	mg/L	EPA HHBP	
Acute PAD	0.05	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.21	mg/L	EPA HHBP	
Health-Based Screening Level	0.21	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.033	mg/kg/day	EPA HHBP	
Screening level for pharmaceutical - general population	0.156862745	mg/L	EPA Office of Water	
Screening level for pharmaceutical - infants	0.044444444	mg/L	EPA Office of Water	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1300	mg/kg	NIH HSDB	min
LD50	4000	mg/kg	NIH HSDB	max
LOAEL	28.1	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	600	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	150	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	9.8	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	6.87	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	100	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic LOAEL	37	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	25	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	9.4	mg/kg/day	EPA Toxicity Reference Database	min

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity test	0.575	no units	TEST QSAR	
Developmental toxin test	0.486	no units	TEST QSAR	

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EPA - Office of Water

Thiabendazole

CCL 5 Contaminant Information Sheet

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
			Prevalence					Magnitude			
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
			Prevalence					Magnitude			
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	627	20	Sites	3.19	0.00098	0.00488	0.0164	0.115	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	76	17	Sites	22	0.00098	0.00453	0.0168	0.115	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	551	3	Sites	0.54	0.00187	0.00673	0.00774	0.00818	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	1	23,140	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	5	13,653	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
			Prevalence					Magnitude			
Furlong et al 2017 (Finished) [83]	2007 - 2012	NA	NA	Sites	0					ug/L	
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
			Prevalence					Magnitude			
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	501	33	Sites	6.59	0.00101	0.00491	0.019	0.176	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	841	4	Sites	0.48	0.00641	0.015	0.0826	0.127	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,341	37	Sites	2.76	0.00101	0.00518	0.0191	0.176	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	41	0	Sites	0						
Furlong et al 2017 (Ambient) [83]	2007 - 2012	NA	NA	Sites	0					ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	12	Sites	32	0.0039721	0.0117	0.0161	0.0421837	ug/L	
Bexfield et al. 2019 (Groundwater) [49]	2013 - 2015	1,106	2	Sites	0.18	0.0064082	0.169	0.3	0.3324209	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Stackelberg et al. (2004) via Kostich et al. 2010 (Ambient) [127]	2010	NA	NA						0.011	ug/L	
Waste Water Effluent											
			Prevalence					Magnitude			
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	19	Sites	90	0.0030236	0.0169	0.0262	0.1126352	ug/L	
Glassmeyer et al. (2005) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						0.515	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg- bw/day)	Notes
ExpoCast exposure		7.28E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	2.58879	days	
Boiling point	OPERA QSAR	326.584	degree C	
Boiling point	TEST QSAR	403.909	degree C	
Vapor pressure	OPERA QSAR	6.6E-09	mmHg	
Vapor pressure	TEST QSAR	0.000000706	mmHg	
Solubility in water	OPERA QSAR	0.000311564	mol/L	
Solubility in water	TEST QSAR	0.000156675	mol/L	
Bioconcentration factor	OPERA QSAR	7.89835	no units	
Bioconcentration factor	TEST QSAR	18.197	no units	
Henry's Law constant	OPERA QSAR	6.93E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.37325	no units	

Thiabendazole

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Reference Number	Full Reference
49	Bexfield, L.M., P.L. Toccalino, K. Belitz, W.T. Foreman, and E.T. Furlong. 2019. Hormones and pharmaceuticals in groundwater used as a source of drinking water across the United States. <i>Environmental Science and Technology</i> 53: 2950-2960.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
83	Furlong, E.T., Batt, A.L., Glassmeyer, S.T., Noriega, M.C., Kolpin, D.W., Mash, H., Schenck, K.M. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States: Pharmaceuticals. <i>Science of The Total Environment</i> . 579 (1629-1642).
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
127	Kostich, MS, et al., 2010. Predicting variability of aquatic concentrations of human pharmaceuticals. <i>Sci. Total Environ</i> . 408 (20), 4504e4510.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
430	USEPA. 2019. Thiabendazole. Acute and Chronic Aggregate (Food and Drinking Water) Dietary Exposure and Risk Assessments in Support of Registration Review. EPA-HQ-OPP-2014-0175-0028. DP No. D450527. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Thiamethoxam

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Thiamethoxam
CASRN:	153719-23-4
DTXSID:	DTXSID2034962
Use:	Insecticide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	6.6

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	reproductive and developmental effects	1	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	20	increased incidence and severity of tubular atrophy in testes of F1 males, sperm abnormalities in F1 males	bottle-fed infants	OPP	2016

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
131.77		EDWC SW (acute)	OPP	2016

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Thiamethoxam

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.012	mg/kg/day	OPP 2016	Winkler et al. 1998	increased incidence and severity of tubular atrophy in testes of F1 males (pups)	bottle-fed infants	151	15.9	[372]	
Cancer Classification (CC)	NL		OPP 2016						[372]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Health-Based Guidance Value	0.4	mg/L	MN DOH	
Acute Human Health Benchmark	2.3	mg/L	EPA HHBP	
Acute PAD	0.35	mg/kg/day	EPA HHBP	
Chronic Health-Based Guidance Value	0.2	mg/L	MN DOH	
Chronic Human Health Benchmark	0.077	mg/L	EPA HHBP	
Health-Based Screening Level	0.077	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.012	mg/kg/day	EPA HHBP	
Short-Term/Subchronic Health-Based Guidance Value	0.2	mg/L	MN DOH	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1563	mg/kg	NIH HSDB	
LOAEL	1.84	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	1000	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	0.8	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	500	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	0.64	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	14.3	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	32	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	1.879	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	9.27	mg/kg/day	EPA Toxicity Reference Database	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.003656	mol/kg	TEST QSAR	
Ames mutagenicity test	0.998	no units	TEST QSAR	
Developmental toxin test	1.036	no units	TEST QSAR	

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Draft Fifth Contaminant Candidate List (CCL 5)
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EPA - Office of Water

Thiamethoxam
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	5	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	5	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	48	353,487	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	10	3	Sites	30	0.0102	0.0102	0.0102	0.0102	ug/L	
Klarich et al. 2017 (Finished) [117]	2016	20	19	Sites	95	0.00026	0.00084	0.00215	0.00415	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	131	49	Sites	37	9.00E - 04	0.007	0.126	4.37	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	12	1	Sites	8.33	0.0031	0.0031	0.0031	0.0031	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	143	50	Sites	35	9.00E - 04	0.00695	0.126	4.37	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	227	2	Sites	0.88	0.0102	0.0102	0.0102	0.025	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	218	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	10	2	Sites	20	0.0102	0.0102	0.0102	0.025	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	281	43	Sites	15	0.0068	0.113	0.407	2.06	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	8	Sites	21	0.0019	0.016	0.0795	0.1904	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					
Estimated Drinking Water Concentration (EDWC) in Surface Water (acute)	2016	OPP	131.77	ug/L	Tier II Rice Model in Tailwater	The critical effect of male reproductive issues in F1 generation pups is considered a less-than-chronic response in a sensitive population. To be protective of this population, the modeled surface water acute concentration was selected as the occurrence concentration for thiamethoxam.					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		1.25E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.54394	days	
Boiling point	OPERA QSAR	278.329	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.00000154	mmHg	
Vapor pressure	TEST QSAR			
Solubility in water	OPERA QSAR	0.000322793	mol/L	
Solubility in water	TEST QSAR	0.00732825	mol/L	
Bioconcentration factor	OPERA QSAR	16.1043	no units	
Bioconcentration factor	TEST QSAR			
Henry's Law constant	OPERA QSAR	6.73E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	-0.144367	no units	

Thiamethoxam

CCL 5 Contaminant Information Sheet

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Reference Number	Full Reference
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
117	Klarich, K.L., Pflug, N.C., DeWald, E.M., Hladik, M.L., Kolpin, D.W., Cwiertny, D.M. and LeFevre, G.H., 2017. Occurrence of neonicotinoid insecticides in finished drinking water and fate during drinking water treatment. <i>Environmental Science & Technology Letters</i> , 4(5), pp.168-173.
372	USEPA. 2016. Thiamethoxam. Acute and Chronic Aggregate Dietary (Food and Drinking Water) Exposure and Risk Assessments for Residues of Thiarnethoxam on Imported Banana. EPA-HQ-OPP-2015-0705-0007. DP No. D429717. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Thiobencarb

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Thiobencarb
CASRN:	28249-77-6
DTXSID:	DTXSID6024337
Use:	Pre-emergent to early post-emergent herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0019

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	non-cancer effects	6	3

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	60	decreased body weights	general population	OPP	2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.1156	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Thiobencarb

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.01	mg/kg/day	OPP 2018	Cummins 1984	decreased body weights	general population	33.8	59.2	[411]	
Cancer Classification (CC)	D		OPP 2018						[411]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	7	mg/L	EPA HHBP	
Acute PAD	1	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.06	mg/L	EPA HHBP	
Health-Based Screening Level	0.06	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.01	mg/kg/day	EPA HHBP	
Public Health Goal	0.042	mg/L	CalEPA OEHHA Public Health Goals	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1903	mg/kg	NIH HSDB	max
LD50	560	mg/kg	NIH HSDB	min
LOAEL	2	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	200	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	100	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	25	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	9.39	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0057412	mol/kg	TEST QSAR	
Ames mutagenicity test	0.269	no units	TEST QSAR	
Developmental toxin test	0.403	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Thiobencarb

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
		Prevalence				Magnitude					
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	10,703	84	Sites	0.78	2.00E - 05	0.011	0.116	4.38	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	2,055	76	Sites	3.7	2.00E - 05	0.011	0.115	4.38	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	8,648	8	Sites	0.09	0.004	0.014	0.056	0.25	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	6	2,372,729	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	2	3,385	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	265	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	15	5	Sites	33	0.029	0.0745	0.151	0.19	ug/L	
Ambient Water											
		Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	2,975	2	Sites	0.07	0.097	0.848	1.45	1.6	ug/L	
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	936	33	Sites	3.53	0.00093	0.0369	0.346	12.4	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	2,045	2	Sites	0.1	0.003	0.007	0.0094	0.011	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	2,980	35	Sites	1.17	0.00093	0.0359	0.342	12.4	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	227	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	10	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	7,197	635	Sites	8.82	0.004	0.949	4.84	150	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	1	Sites	2.63	0.3429	0.343	0.343	0.3429	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	0	Sites	0						
Waste Water Effluent											
		Prevalence				Magnitude					
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg- bw/day)	Notes
Expocast exposure		8.52E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	2.94541	days	
Boiling point	OPERA QSAR	305.691	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.0000201	mmHg	
Vapor pressure	TEST QSAR	0.000147571	mmHg	
Solubility in water	OPERA QSAR	0.000168437	mol/L	
Solubility in water	TEST QSAR	0.0000845	mol/L	
Bioconcentration factor	OPERA QSAR	130.611	no units	
Bioconcentration factor	TEST QSAR	25.0611	no units	
Henry's Law constant	OPERA QSAR	0.000000019	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.37599	no units	

Thiobencarb

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
411	USEPA. 2018. Thiobencarb - Registration Review Draft Human Health Risk Assessment. EPA-HQ-OPP-2011-0932-0037. DP No. D439288. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Thiram

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Thiram
CASRN:	137-26-8
DTXSID:	DTXSID5021332
Use:	Pesticide; rubber accelerator; antiseptic
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	X
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.028

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	non-cancer effects	3	5

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	90	changes in hematology, clinical chemistry, incidences of bile duct hyperplasia, reduction in mean body weight gain, elevated cholesterol levels and increased liver weight	general population	OPP	2015

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
2.5		EDWC SW 30-Year	OPP	2015

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		
Not Applicable		

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Thiram

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.015	mg/kg/day	OPP 2015	Kehoe 1991a and 1991b	changes in hematology, clinical chemistry, incidences of bile duct hyperplasia, reduction in mean body weight gain, elevated cholesterol levels and increased liver weight	general population	33.8	88.8	[358]	
Cancer Classification (CC)	NL		OPP 2015						[358]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.39	mg/L	EPA HHBP	
Acute PAD	0.014	mg/kg/day	EPA HHBP	
Cancer Classification (CC)	3	no units	WHO IARC	
Chronic Human Health Benchmark	0.096	mg/L	EPA HHBP	
Population-Adjusted Dose (PAD)	0.015	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1350	mg/kg	NIH HSDB	max
LD50	210	mg/kg	NIH HSDB	min
LOAEL	0.84	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	24	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	1.8	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	7.5	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	33.64	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	7.0100002	mg/kg/day	EPA Toxicity Reference Database	
Subchronic NOAEL	2.35	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0038107	mol/kg	TEST QSAR	
Ames mutagenicity test	0.476	no units	TEST QSAR	
Developmental toxin test	0.772	no units	TEST QSAR	

Thiram

CCL 5 Contaminant Information Sheet

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017										
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	3	125,378	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	19	29,783	Chemical Data Reporting (CDR) Results (EPA) (2016)	1M - 10M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Ambient Water											
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	16	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					
Estimated Drinking Water Concentration (EDWC) in Surface Water, 30-Year Mean (chronic, non-cancer)	2015	OPP	2.5	ug/L	Pesticide Root Zone Model (PRZM) - Exposure Analysis Modeling System (EXAMS)	The modeled surface water chronic, non-cancer concentration provided by the most recent available EPA OPP health assessment was selected as the occurrence concentration for thiram. This value coincides with the chronic critical effects of multiple signs of systemic toxicity and hematological alterations provided within the health effects report.					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		3.58E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	90.9543	days	
Boiling point	OPERA QSAR	305.681	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.0000166	mmHg	
Vapor pressure	TEST QSAR			
Solubility in water	OPERA QSAR	0.000151428	mol/L	
Solubility in water	TEST QSAR	0.000587489	mol/L	
Bioconcentration factor	OPERA QSAR	3.67366	no units	
Bioconcentration factor	TEST QSAR	10.4954	no units	
Henry's Law constant	OPERA QSAR	2.01E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.65192	no units	

Thiram

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
358	USEPA. 2015. Thiram. Revised Human Health Risk Assessment for the Import Use of Thiram on Avocado, PP#4E8250 and Banana, PP#4E8268. EPA-HQ-OPP-2014-0249-0004. DP No. D427383. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Tin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Tin
CASRN:	7440-31-5
DTXSID:	DTXSID1049801
Use:	Metal; used in alloys and solder. Block tin is used to coat copper cooking utensils and lead sheet, or to line lead pipe for distilled water, beer, carbonated beverages, and some chemicals.
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxics	
PubMed Neurotoxics	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
		8	8

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
23	90th Percentile	Finished Water	NIRS	1984-1986

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis
Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Tin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
			ATSDR 2005						[24]	NOTE: ATSDR declined to quantify chronic oral toxicity

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Developmental	2	El-Makawy, 2008	Reproductive	2	El-Makawy, 2008	2004-08-01	2020-03-25	3052	1	23	1

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Chronic Health-Based Guidance Value	4	mg/L	MN DOH	
Intermediate Minimal Risk Level (MRL)	0.3	mg/kg/day	CDC ATSDR	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity test			TEST QSAR	
Developmental toxin test			TEST QSAR	

Tin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986	989	14	Sites	1.42	3	5	23	32	ug/L	
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	1	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	1	0	Sites	0						
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017										

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	10M - 50M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	36		6.4		15.9	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	80	15	Sites	19	0.02	1.83	200	200	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	126	47	Sites	37	0.01	0.5	5.3	22	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	206	62	Sites	30	0.01	1	20	200	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	40		3.55		17.4	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)	2.42	ug/l	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Tin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
24	ATSDR. 2005. Toxicological Profile for Tin and Tin Compounds. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. Science of The Total Environment. v581-582, (909-922).

Triallate

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Triallate
CASRN:	2303-17-5
DTXSID:	DTXSID5024344
Use:	Pre-emergent selective herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.15

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	carcinogen with linear MOA	6	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.4	hepatocellular carcinomas and renal tubular cell adenomas	general population	OPP	2019

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.059	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Triallate
CCL 5 Contaminant Information Sheet
HEALTH EFFECTS DATA

EPA-OGWDW and OST

July 2021

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.025	mg/kg/day	OPP 2019	Stout and Thake 1987; Vigneault 1988	decreased survival; decreased mean body weights and increased adrenal weight in males	general population	33.8	148	[431]	
Cancer Slope Factor (CSF)	0.0717	(mg/kg/day)^-1	OPP 2019	Stout et al. 1983	hepatocellular carcinomas and renal tubular cell adenomas	general population	33.8	0.413	[431]	
Cancer Classification (CC)	C		OPP 2019						[431]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	1	mg/L	EPA HHBP	
Acute PAD	0.05	mg/kg/day	EPA HHBP	
Cancer Slope Factor (CSF)	0.0717	(mg/kg/day)^-1	EPA HHBP	
Chronic Human Health Benchmark	0.16	mg/L	EPA HHBP	
Chronic Human Health Benchmark	0.000446	mg/L	EPA HHBP	
Health-Based Screening Level	0.16	mg/L	Health-based screening levels from USGS	
Health-Based Screening Level	0.000446	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.025	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
The full citation for the critical study is provided in the corresponding health assessment.
PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	2700	mg/kg	NIH HSDB	max
LD50	800	mg/kg	NIH HSDB	min
LOAEL	5	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	90	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	1.5	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	30	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxicant in vitro assays tested	15.9	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0144544	mol/kg	TEST QSAR	
Ames mutagenicity test	0.687	no units	TEST QSAR	
Developmental toxin test	0.189	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Triallate
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	9,433	92	Sites	0.98	0.001	0.008	0.059	0.65	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	2,030	82	Sites	4.04	0.001	0.008	0.059	0.65	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	7,403	10	Sites	0.14	0.0011	0.002	0.021	0.23	ug/L	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	1	Sites	5.88	0.12	0.12	0.12	0.12	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	549	2	Sites	0.36	0.219	0.236	0.247	0.254	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	1,094	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,643	2	Sites	0.12	0.219	0.236	0.247	0.254	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	590	1	Sites	0.17	0.003	0.003	0.003	0.003	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	0	Sites	0						
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.000000102	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.39965	days	
Boiling point	OPERA QSAR	293.256	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.00012696	mmHg	
Vapor pressure	TEST QSAR	0.000402717	mmHg	
Solubility in water	OPERA QSAR	0.0000293	mol/L	
Solubility in water	TEST QSAR	0.0000345	mol/L	
Bioconcentration factor	OPERA QSAR	453.67	no units	
Bioconcentration factor	TEST QSAR	90.7821	no units	
Henry's Law constant	OPERA QSAR	0.000154671	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	4.51044	no units	

Triallate

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
431	USEPA. 2019. Triallate. Human Health Draft Risk Assessment Scoping Document in Support of Registration Review. EPA-HQ-OPP-2014-0573-0018. DP No. D452964. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Tribufos

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Tribufos
CASRN:	78-48-8
DTXSID:	DTXSID1024174
Use:	Insecticide; cotton defoliant
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	1.2

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	non-cancer effects	1	5

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.3	inhibition of red blood cell cholinesterase in females	bottle-fed infants	OPP	2015

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.36742	90th Percentile	Finished Water	UCMR4	2018-2019

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
		X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Tribufos

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0002	mg/kg/day	OPP 2015	Sheets and Gilmore 2001	inhibition of red blood cell cholinesterase in females	bottle-fed infants	151	0.265	[359]	
Cancer Classification (CC)	L/NL		OPP 2015						[359]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	0.007	mg/L	EPA HHBP	
Acute PAD	0.001	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.0006	mg/L	EPA HHBP	
Health-Based Screening Level	0.0006	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.0001	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	435	mg/kg	NIH HSDB	max
LD50	77	mg/kg	NIH HSDB	min
LOAEL	0.4	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	9	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	0.1	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	3	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	15.68	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0004487	mol/kg	TEST QSAR	
Ames mutagenicity test	0.199	no units	TEST QSAR	
Developmental toxin test	0.084	no units	TEST QSAR	

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019	3,647	2	Sites	0.05	0.0742	0.237	0.367	0.4	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Study (NIRS)	1984 - 1986										
Ambient Water											
		Prevalence				Magnitude					
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	4,417	21	Sites	0.48	0.00313	0.016	0.102	0.246	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	430	19	Sites	4.42	0.00313	0.016	0.0766	0.176	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	3,987	2	Sites	0.05	0.009	0.128	0.199	0.246	ug/L	

Non-Nationally Representative Water Data												Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water													Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Finished)												2006 - 2020	1	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)												2001 - 2013	13	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Finished) [153]												2009 - 2010	1	0	Sites	0						
Ambient Water													Prevalence				Magnitude					
Drinking Water Monitoring Data - CA (Source)												2006 - 2020	1	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)												2008 - 2017	779	8	Sites	1.03	0.005	0.0255	0.219	0.227	ug/L	
National Water Information System (USGS NWIS) (Groundwater)												2008 - 2017	2,510	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)												2008 - 2017	3,288	8	Sites	0.24	0.005	0.0255	0.219	0.227	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)												2001 - 2013	6	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)												2001 - 2013	6	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]												1990 - 2018	1,773	2	Sites	0.11	0.01	0.01	0.01	0.01	ug/L	
Arnold et al. 2016 (Filtered) [7]												2012 - 2013	690	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Ambient) [153]												2009 - 2010	2	0	Sites	0						
Waste Water Effluent													Prevalence				Magnitude					
Estimated Concentration in Water		Date	Source	Value	Units	Model	Notes															

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	273.028	days	
Boiling point	OPERA QSAR	343.854	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	0.00000738	mmHg	
Vapor pressure	TEST QSAR	0.0000101	mmHg	
Solubility in water	OPERA QSAR	0.00000337	mol/L	
Solubility in water	TEST QSAR	0.000178238	mol/L	
Bioconcentration factor	OPERA QSAR	333.052	no units	
Bioconcentration factor	TEST QSAR	42.462	no units	
Henry's Law constant	OPERA QSAR	0.000000412	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	5.67262	no units	

Tribufos

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
359	USEPA. 2015. Tribufos: Human Health Draft Risk Assessment for Registration Review. EPA-HQ-OPP-2008-0883-0011. DP No. D357537. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management (pp. 215-232). American Chemical Society.

Tributyl phosphate (TNBP)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Tributyl phosphate (TNBP)
CASRN:	126-73-8
DTXSID:	DTXSID3021986
Use:	Flame-retardant component of aircraft hydraulic fluid; solvent
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxics	X
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.057

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
3	carcinogen with linear MOA	9	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	3	bladder neoplasia (combined incidence of transitional cell and squamous cell carcinomas, and papillomas)	general population	PPRTV	2010

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.17	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Tributyl phosphate (TNBP)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.011	mg/kg/day	PPRTV 2010	Bio/dynamics Inc., 1991b	"cholinergic salivation"	general population	33.8	65.1	[316]	
Reference Dose (RfD) or Equivalent	0.08	mg/kg/day	ATSDR 2012	Arnold et al. 1997	"urinary bladder hyperplasia"	general population	33.8	473	[31]	
Cancer Slope Factor (CSF)	0.009	(mg/kg/day)^-1	PPRTV 2010	Auletta et al. 1998a	bladder neoplasia (combined incidence of transitional cell and squamous cell carcinomas, and papillomas)	general population	33.8	3.29	[316]	
Cancer Classification (CC)	L		PPRTV 2010						[316]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
						2011-09-01	2019-12-17	454	0	0	

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Minimal Risk Level (MRL)	1.1	mg/kg/day	CDC ATSDR	
Intermediate Minimal Risk Level (MRL)	0.08	mg/kg/day	CDC ATSDR	
Subchronic Provisional RfD	0.03	mg/kg/day	EPA PPRTV	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	20000	mg/kg	NIH HSDB	max
LD50	400	mg/kg	NIH HSDB	min
Percent of active toxcast in vitro assays tested	5.4	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0151705	mol/kg	TEST QSAR	
Ames mutagenicity test	0.08	no units	TEST QSAR	
Developmental toxin test	0.354	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Tributyl phosphate (TNBP)
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	571	36	Sites	6.3	0.006	0.06	0.17	0.92	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	88	28	Sites	32	0.006	0.06	0.17	0.92	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	483	8	Sites	1.66	0.02	0.05	0.161	0.17	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	1M - 10M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	1	Sites	100						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	724	233	Sites	32	0.004	0.027	0.092	4.69	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	692	47	Sites	6.79	0.007	0.0315	0.352	0.98	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,416	280	Sites	20	0.004	0.027	0.1	4.69	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	4		0.087		0.087	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	14	Sites	37	0.0116	0.0601	0.114	0.503	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	2	Sites	100	0.1	0.1	0.1	0.1	ug/L	
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	20	Sites	95	0.082	0.14	0.27	1.1	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.0000471	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.67987	days	
Boiling point	OPERA QSAR	284.939	degree C	
Boiling point	TEST QSAR	281.321	degree C	
Vapor pressure	OPERA QSAR	0.00171598	mmHg	
Vapor pressure	TEST QSAR	0.000174985	mmHg	
Solubility in water	OPERA QSAR	0.00139101	mol/L	
Solubility in water	TEST QSAR	0.00312608	mol/L	
Bioconcentration factor	OPERA QSAR	29.4881	no units	
Bioconcentration factor	TEST QSAR	8.26038	no units	
Henry's Law constant	OPERA QSAR	0.00000113	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.76206	no units	

Tributyl phosphate (TNBP)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
31	ATSDR. 2012. Toxicological Profile for Phosphate Ester Flame Retardants. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
316	USEPA. 2010. Provisional Peer-Reviewed Toxicity Values for Tributyl phosphate. EPA/690/R-20/024F. U.S. Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment, Superfund Health Risk Technical Support Center, Cincinnati, OH.

Triclopyr

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Triclopyr
CASRN:	55335-06-3
DTXSID:	DTXSID0032497
Use:	Herbicide; woody plants and many broad-leaved weeds in grassland, uncultivated land, industrial areas, coniferous forests, plantation crops and rice fields.
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.001

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	non-cancer effects	9	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	300	proximal renal tube degeneration	general population	OPP	2016

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.3	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Triclopyr

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.05	mg/kg/day	OPP 2016	Vedula et al., 1995	proximal renal tube degeneration	general population	33.8	296	[374]	
Cancer Classification (CC)	D		OPP 2016						[374]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	1	mg/L	EPA HHBP	
Acute PAD	0.05	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.3	mg/L	EPA HHBP	
Health-Based Screening Level	0.3	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.05	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	2140	mg/kg	NIH HSDB	max
LD50	310	mg/kg	NIH HSDB	min
LOAEL	2.5	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	200	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	0.5	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	100	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	1.89	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	2.5	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	20	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	0.5	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	5	mg/kg/day	EPA Toxicity Reference Database	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.002729	mol/kg	TEST QSAR	
Ames mutagenicity test	0.049	no units	TEST QSAR	
Developmental toxin test	0.559	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
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EPA - Office of Water

Triclopyr
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	7,742	257	Sites	3.32	0.0028	0.075	0.3	16	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	1,196	248	Sites	21	0.0028	0.0748	0.3	16	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	6,546	9	Sites	0.14	0.01	0.16	0.362	1.1	ug/L	
Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data			Number of States	Amount Released (lbs/year)	Chemical Production Data		Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	43	1,790,323	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)					Chemical Data Reporting (CDR) Results (EPA) (2016)		

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	17	7	Sites	41	0.0027	0.01	0.0393	0.566	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	479	117	Sites	24	0.0057	0.0723	0.289	13	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	1,059	3	Sites	0.28	0.04	0.31	0.314	0.316	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,538	120	Sites	7.8	0.0057	0.0728	0.299	13	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	229	28	Sites	12	0.002664	0.00965	0.0493	3.6	ug/L	
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	219	21	Sites	9.59	0.002664	0.00266	0.0164	3.6	ug/L	
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	12	7	Sites	58	0.0027	0.00999	0.0507	0.847	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	1,372	524	Sites	38	0.05	0.208	1.8	250	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	6	Sites	16	0.0198	0.148	2.9	5.6413	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	690	1	Sites	0.14	0.246	0.246	0.246	0.246	ug/L	
USGS, McKenzie River, Oregon, 2012 (Ambient) [158]	2002 - 2010	126	13	Samples	10				3.1	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.00000104	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.53784	days	
Boiling point	OPERA QSAR	307.12	degree C	
Boiling point	TEST QSAR	325.714	degree C	
Vapor pressure	OPERA QSAR	0.00000216	mmHg	
Vapor pressure	TEST QSAR	0.00000741	mmHg	
Solubility in water	OPERA QSAR	0.00157866	mol/L	
Solubility in water	TEST QSAR	0.00113501	mol/L	
Bioconcentration factor	OPERA QSAR	3.14686	no units	
Bioconcentration factor	TEST QSAR	6.223	no units	
Henry's Law constant	OPERA QSAR	1.36E-09	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	2.51566	no units	

Triclopyr

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
158	Reconnaissance of Land-Use Sources of Pesticides in Drinking Water, McKenzie River, Oregon. U.S. Geological Survey Scientific Investigations Report 2012–5091, 46 p. plus appendixes.
374	USEPA. 2016. Triclopyr. Revised Human Health Risk Assessment for Section 18 Emergency Exemption Request for Use on Sugarcane in Louisiana (LA). EPA-HQ-OPP-2017-0036-0002. DP No. D436366. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Triclosan

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Triclosan
CASRN:	3380-34-5
DTXSID:	DTXSID5032498
Use:	Antiseptic/disinfectant/antimicrobial in personal care products and household goods; pesticide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	X
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.000068

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	reproductive and developmental effects	9	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	2000	20% decrease in T4 and associations with neurodevelopmental and cognitive deficits	women of childbearing age	OPP	2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.135	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Triclosan

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.27	mg/kg/day	OPP 2018	Stoker et al., 2010; Zorilla et al., 2010	20% decrease in T4 and associations with neurodevelopmental and cognitive deficits	women of childbearing age	35.4	1530	[408]	
Cancer Classification (CC)	NL		OPP 2018						[408]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Health-Based Guidance Value	0.05	mg/L	MN DOH	
Acute Human Health Benchmark	2	mg/L	EPA HHBP	
Acute PAD	0.3	mg/kg/day	EPA HHBP	
Chronic Health-Based Guidance Value	0.05	mg/L	MN DOH	
Chronic Human Health Benchmark	2	mg/L	EPA HHBP	
Health-Based Screening Level	2	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.3	mg/kg/day	EPA HHBP	
Short-Term/Subchronic Health-Based Guidance Value	0.05	mg/L	MN DOH	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	3700	mg/kg	NIH HSDB	min
LD50	4530	mg/kg	NIH HSDB	max
LOAEL	15	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	300	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	100	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	50	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	36.79	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	25	mg/kg/day	EPA Toxicity Reference Database	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0000468	mol/kg	TEST QSAR	
Ames mutagenicity test	0.402	no units	TEST QSAR	
Developmental toxin test	0.627	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Triclosan
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	567	31	Sites	5.47	0.01	0.04	0.135	0.56	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	88	29	Sites	33	0.01	0.04	0.149	0.56	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	479	2	Sites	0.42	0.02	0.045	0.06	0.07	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	2	1	Sites	50	3	3	3	3	ug/L	
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Padhye et al. 2013 (Finished) [155]	2009 - 2010	8	5	Samples	62	0	1.4e-06		5.96e-05 +/- 2.57e-05	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	3	1	Sites	33	3	3	3	3	ug/L	
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	725	117	Sites	16	0.02	0.09	0.26	15.6	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	690	9	Sites	1.3	0.03	0.06	0.071	0.08	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,415	126	Sites	8.9	0.02	0.09	0.254	15.6	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	12		0.00271		0.0035	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	23	Sites	61	0.00152	0.0146	0.0928	0.534	ug/L	
Padhye et al. 2013 (Ambient) [155]	2009 - 2010	8	5	Samples	62	0	3.3e-06		0.0001058 +/- 6.31e-05	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	8	Sites	38	0.12	0.28	0.949	0.97	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.00000141	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)	172	ug/l	

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.47143	days	
Boiling point	OPERA QSAR	342.344	degree C	
Boiling point	TEST QSAR	369.746	degree C	
Vapor pressure	OPERA QSAR	0.000000453	mmHg	
Vapor pressure	TEST QSAR	0.00000453	mmHg	
Solubility in water	OPERA QSAR	0.0000298	mol/L	
Solubility in water	TEST QSAR	0.00000454	mol/L	
Bioconcentration factor	OPERA QSAR	94.8967	no units	
Bioconcentration factor	TEST QSAR	1698.24	no units	
Henry's Law constant	OPERA QSAR	6.29E-10	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	4.94675	no units	

Triclosan

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
155	Padhye, L.P., Yao, H., Kung'u, F.T., and Huang, C.H. Year-long evaluation on the occurrence and fate of pharmaceuticals, personal care products, and endocrine disrupting chemicals in an urban drinking water treatment plant. 2014. <i>Water Research</i> 51 (2014) 266-276.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
408	USEPA. 2018. Registration Review Draft Risk Assessment for Triclosan. EPA-HQ-OPP-2012-0811-0020. DP Nos. 449415, 449416. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.

Trifloxystrobin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Trifloxystrobin
CASRN:	141517-21-7
DTXSID:	DTXSID4032580
Use:	Fungicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	X
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.00017

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	reproductive and developmental effects	9	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	50	maternal decreased body weight and lesions in the liver, kidney and spleen; offspring decreased body weight during lactation	bottle-fed infants	OPP	2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.008552	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis
Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Trifloxystrobin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.038	mg/kg/day	OPP 2018	Khalil 1997	maternal decreased body weight and lesions in the liver, kidney and spleen; offspring decreased body weight during lactation	bottle-fed infants	151	50.3	[412]	
Cancer Classification (CC)	NL		OPP 2018						[412]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Human Health Benchmark	69	mg/L	EPA HHBP	
Acute PAD	2.5	mg/kg/day	EPA HHBP	
Chronic Human Health Benchmark	0.24	mg/L	EPA HHBP	
Health-Based Screening Level	0.24	mg/L	Health-based screening levels from USGS	
Population-Adjusted Dose (PAD)	0.038	mg/kg/day	EPA HHBP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	4000	mg/kg	NIH HSDB	min
LD50	5000	mg/kg	NIH HSDB	max
LOAEL	29.700001	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	500	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	250	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	3.9	mg/kg/day	EPA Toxicity Reference Database	min
Percent of active toxcast in vitro assays tested	24.02	percent	EPA Chemistry Dashboard	
Subchronic LOAEL	127	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic LOAEL	150	mg/kg/day	EPA Toxicity Reference Database	max
Subchronic NOAEL	30	mg/kg/day	EPA Toxicity Reference Database	min
Subchronic NOAEL	32.8	mg/kg/day	EPA Toxicity Reference Database	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0014555	mol/kg	TEST QSAR	
Ames mutagenicity test	0.189	no units	TEST QSAR	
Developmental toxin test	0.886	no units	TEST QSAR	

Trifloxystrobin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
		Prevalence				Magnitude					
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	1,763	100	Sites	5.67	0.00011	0.00115	0.00855	0.486	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	324	98	Sites	30	0.00011	0.00115	0.00807	0.486	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	1,439	2	Sites	0.14	0.00065	0.12	0.192	0.24	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	48	796,042	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Ambient Water											
		Prevalence				Magnitude					
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	433	14	Sites	3.23	0.00014	0.00475	0.0638	0.216	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	531	1	Sites	0.19	0.00226	0.00226	0.00226	0.00226	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	964	15	Sites	1.56	0.00014	0.00468	0.0495	0.216	ug/L	
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	254	1	Sites	0.39	0.067	0.067	0.067	0.067	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	1	Sites	2.63	0.045	0.045	0.045	0.045	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	584	1	Sites	0.17	6e-04	6e-04	6e-04	6e-04	ug/L	
Waste Water Effluent											
		Prevalence				Magnitude					
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		1.91E-08	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.54712	days	
Boiling point	OPERA QSAR	358.422	degree C	
Boiling point	TEST QSAR			
Vapor pressure	OPERA QSAR	2.48E-08	mmHg	
Vapor pressure	TEST QSAR	0.0000109	mmHg	
Solubility in water	OPERA QSAR	0.00000387	mol/L	
Solubility in water	TEST QSAR	0.00000448	mol/L	
Bioconcentration factor	OPERA QSAR	99.2112	no units	
Bioconcentration factor	TEST QSAR	83.1764	no units	
Henry's Law constant	OPERA QSAR	1.28E-08	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	4.31154	no units	

Trifloxystrobin

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
412	USEPA. 2018. Trifloxystrobin. Human Health Risk Assessment for the Proposed New Use on Flax Seed and Increase of Established Tolerance on Aspirated Grain Fractions. EPA-HQ-OPP-2013-0074-0049. DP Nos. D442038 D444241. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

Trifluralin

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Trifluralin
CASRN:	1582-09-8
DTXSID:	DTXSID4021395
Use:	Herbicide
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	X
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0025

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
3	carcinogen with linear MOA	9	2

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	10	thyroid follicular cell combined adenoma, papillary adenoma, cystadenoma, and carcinoma in males	general population	OPP	2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.025	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Trifluralin

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.024	mg/kg/day	OPP 2018	Adams et al. 1992	increased frequency of abnormal stool, decreased body weight and weight gain, decreased erythrocyte and hemoglobin, increased thrombocytes	general population	33.8	142	[413]	
Cancer Slope Factor (CSF)	0.00296	(mg/kg/day)^-1	OPP 2018	Emmerson et al. 1980	thyroid follicular cell combined adenoma, papillary adenoma, cystadenoma, and carcinoma in males	general population	33.8	10.0	[413]	
Cancer Classification (CC)	C		OPP 2018						[413]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
10-day Health Advisory	0.08	mg/L	EPA DWSHA 2018	
Cancer Classification (CC)	3	no units	WHO IARC	
Drinking Water Guideline Value	0.02	mg/L	WHO Drinking Water Quality Guidelines	
Lifetime Health Advisory	0.01	mg/L	EPA DWSHA 2018	
Lifetime Health Advisory	0.004	mg/L	EPA DWSHA 2018	
Maximum Allowable Concentration (MAC)	0.045	mg/L	Canadian Drinking Water Guidelines	
Cancer Classification (CC)	Female.Mice P	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats N	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice N	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats N	no units	HHS NTP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	10000	mg/kg	NIH HSDB	max
LD50	500	mg/kg	NIH HSDB	min
LOAEL	3.8	mg/kg/day	EPA Toxicity Reference Database	min
LOAEL	500	mg/kg/day	EPA Toxicity Reference Database	max
NOAEL	0.8	mg/kg/day	EPA Toxicity Reference Database	min
NOAEL	225	mg/kg/day	EPA Toxicity Reference Database	max
Percent of active toxcast in vitro assays tested	10.44	percent	EPA Chemistry Dashboard	
TD50	263	mg/kg/day	NIH CPDB	min
TD50	5440	mg/kg/day	NIH CPDB	max

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0136773	mol/kg	TEST QSAR	
Ames mutagenicity test	0.445	no units	TEST QSAR	
Developmental toxin test	1.145	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
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EPA - Office of Water

Trifluralin
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	10,201	485	Sites	4.75	0.001	0.005	0.025	1.74	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	2,075	421	Sites	20	0.001	0.005	0.025	1.74	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	8,127	64	Sites	0.79	0.001	0.005	0.014	0.057	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)	47	8,578,613	2016	Toxic Release Inventory (TRI) Program (EPA) (2016)	13	11,482	Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	60	0	Sites	0						
Drinking Water Monitoring Data - WA (Finished)	2006 - 2011	481	0	Sites	0						
USDA Pesticide Data Program (PDP) (Finished)	2001 - 2013	15	1	Sites	6.67	0.0025	0.0025	0.0025	0.0025	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	604	3	Sites	0.5	0.5	31	174	210	ug/L	
Drinking Water Monitoring Data - WA (Source)	2006 - 2011	635	0	Sites	0						
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	811	121	Sites	15	6.00E - 05	0.003	0.0147	0.323	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	2,670	28	Sites	1.05	0.001	0.003	0.0164	0.113	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	3,480	149	Sites	4.28	6.00E - 05	0.003	0.015	0.323	ug/L	
USDA Pesticide Data Program (PDP) (Combined Groundwater And Untreated)	2001 - 2013	225	0	Sites	0						
USDA Pesticide Data Program (PDP) (Groundwater)	2001 - 2013	218	0	Sites	0						
USDA Pesticide Data Program (PDP) (Untreated)	2001 - 2013	8	0	Sites	0						
Surface Water Database (SURF) California Dept. of Pesticide Regulation (Ambient) [451]	1990 - 2018	2,711	254	Sites	9.37	0.003	0.024	0.234	3.3	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	15	Sites	39	2.75e-05	0.000138	0.0188	0.0473	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	106	0	Sites	0						
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
USGS, McKenzie River, Oregon, 2012 (Ambient) [158]	2002 - 2010	133	3	Samples	2.3				0.002	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Exposure exposure		0.00000157	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.54291	days	
Boiling point	OPERA QSAR	365.036	degree C	
Boiling point	TEST QSAR	369.442	degree C	
Vapor pressure	OPERA QSAR	0.0000523	mmHg	
Vapor pressure	TEST QSAR	0.00000292	mmHg	
Solubility in water	OPERA QSAR	0.000000496	mol/L	
Solubility in water	TEST QSAR	0.000002	mol/L	
Bioconcentration factor	OPERA QSAR	1513.15	no units	
Bioconcentration factor	TEST QSAR	149.624	no units	
Henry's Law constant	OPERA QSAR	0.0000755	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	5.27633	no units	

Trifluralin

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
158	Reconnaissance of Land-Use Sources of Pesticides in Drinking Water, McKenzie River, Oregon. U.S. Geological Survey Scientific Investigations Report 2012–5091, 46 p. plus appendixes.
413	USEPA. 2018. Trifluralin: Acute, Chronic, and Cancer Aggregate Dietary (Food and Drinking Water) Exposure and Risk Assessment for the Section 3 Registration Action on Rosemary and Crop Group Conversions to Support Registration Review. EPA-HQ-OPP-2017-0420-0006. DP Nos. D445916 D447175. U.S. Environmental Protection Agency, Office of Chemical Safety and Pollution Prevention, Washington, D.C.
451	Zhang, X., Ensminger, M., Deng, X., Budd, R., Xie, Y., Wang, D., ... & Goh, K. S. (2019). The Surface Water Database (SURF): A California Database for Surface Water Pesticide Monitoring Data. In <i>Pesticides in Surface Water: Monitoring, Modeling, Risk Assessment, and Management</i> (pp. 215-232). American Chemical Society.

tris(1,3-dichloro-2-propyl) phosphate (TDCP)

CCL 5 Contaminant Information Sheet

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CONTAMINANT IDENTIFYING INFORMATION

Name:	tris(1,3-dichloro-2-propyl) phosphate (TDCP)
CASRN:	13674-87-8
DTXSID:	DTXSID9026261
Use:	Flame-retardant in plastics and as a secondary plasticizer
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.0016

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
5	non-cancer effects	9	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	100	renal tubule epithelial hyperplasia	general population	ATSDR	2012

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.157	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

tris(1,3-dichloro-2-propyl) phosphate (TDCP)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.02	mg/kg/day	ATSDR 2012	Stauffer Chemical Co. 1981	renal tubule epithelial hyperplasia	general population	33.8	118	[31]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Hepatic	0.0026	Deng, 2018	Cardiovascular, Respiratory	500	Wang, 2019	2011-09-01	2020-02-13	233	5	8	5

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Chronic Health-Based Guidance Value	0.00008	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.009	mg/L	MN DOH	
Intermediate Minimal Risk Level (MRL)	0.05	mg/kg/day	CDC ATSDR	
Short-Term/Subchronic Health-Based Guidance Value	0.02	mg/L	MN DOH	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1850	mg/kg	NIH HSDB	min
LD50	2670	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	24.79	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.004529	mol/kg	TEST QSAR	
Ames mutagenicity test	0.601	no units	TEST QSAR	
Developmental toxin test	0.546	no units	TEST QSAR	

tris(1,3-dichloro-2-propyl) phosphate (TDCP)

CCL 5 Contaminant Information Sheet

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OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	567	39	Sites	6.88	0.01	0.07	0.157	0.52	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	88	33	Sites	38	0.01	0.08	0.163	0.52	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	479	6	Sites	1.25	0.02	0.03	0.068	0.08	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	10M - 50M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	720	278	Sites	39	0.01	0.08	0.21	14.9	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	687	64	Sites	9.32	0.02	0.095	0.266	0.44	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,407	342	Sites	24	0.01	0.08	0.23	14.9	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	12	Sites	32	0.11	0.336	0.501	0.583	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	19	Sites	90	0.13	0.22	0.317	0.4	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.00000181	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	4.07587	days	
Boiling point	OPERA QSAR	313.35	degree C	
Boiling point	TEST QSAR	373.105	degree C	
Vapor pressure	OPERA QSAR	0.00000524	mmHg	
Vapor pressure	TEST QSAR	0.0000164	mmHg	
Solubility in water	OPERA QSAR	0.0000446	mol/L	
Solubility in water	TEST QSAR	0.0000881	mol/L	
Bioconcentration factor	OPERA QSAR	12.6458	no units	
Bioconcentration factor	TEST QSAR	14.9279	no units	
Henry's Law constant	OPERA QSAR	0.00000168	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.64426	no units	

tris(1,3-dichloro-2-propyl) phosphate (TDCP)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
31	ATSDR. 2012. Toxicological Profile for Phosphate Ester Flame Retardants. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.

Tris(2-butoxyethyl) phosphate (TBEP)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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CONTAMINANT IDENTIFYING INFORMATION

Name:	Tris(2-butoxyethyl) phosphate (TBEP)
CASRN:	78-51-3
DTXSID:	DTXSID5021758
Use:	Primary plasticizer for most resins and elastomers; floor finishes and waxes; flame-retarding agent.
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxics	
PubMed Neurotoxics	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
		9	5

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.98	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Tris(2-butoylethyl) phosphate (TBEP)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
			ATSDR 2012						[31]	NOTE: Though there is no chronic duration MRL available, the intermediate duration MRL is 0.09 mg/kg/day based on hepatocyte vacuolization seen in an 18-week rat study. The ECHA DNEL value appears to be based on the same subchronic duration study

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.25	mg/kg/day	ECHA 2010	Reyna 1987	liver effects	general population	33.8	1.48	[74]	

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
						2011-09-01	2019-10-22	148	0	4	

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Minimal Risk Level (MRL)	4.8	mg/kg/day	CDC ATSDR	
Intermediate Minimal Risk Level (MRL)	0.09	mg/kg/day	CDC ATSDR	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	3000	mg/kg	NIH HSDB	
Percent of active toxcast in vitro assays tested	10.9	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0127938	mol/kg	TEST QSAR	
Ames mutagenicity test	0.045	no units	TEST QSAR	
Developmental toxin test	0.501	no units	TEST QSAR	

Tris(2-butoylethyl) phosphate (TBEP)
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	566	36	Sites	6.36	0.1	0.2	0.98	9.9	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	88	26	Sites	30	0.1	0.3	1.18	9.9	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	478	10	Sites	2.09	0.1	0.1	0.3	0.5	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	1M - 10M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	725	291	Sites	40	0.04	0.36	1.03	31.9	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	690	58	Sites	8.41	0.07	0.4	0.9	8	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,415	349	Sites	25	0.04	0.36	1.02	31.9	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	4		0.47		0.47	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	10	Sites	26	0.244	0.488	0.835	1.11	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	0	Sites	0						
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	17	Sites	81	0.4	2.9	14.4	19	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.0000929	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.67989	days	
Boiling point	OPERA QSAR	345.446	degree C	
Boiling point	TEST QSAR	353.92	degree C	
Vapor pressure	OPERA QSAR	0.0000171	mmHg	
Vapor pressure	TEST QSAR	0.00000378	mmHg	
Solubility in water	OPERA QSAR	0.00231797	mol/L	
Solubility in water	TEST QSAR	0.000592925	mol/L	
Bioconcentration factor	OPERA QSAR	6.05572	no units	
Bioconcentration factor	TEST QSAR	6.09537	no units	
Henry's Law constant	OPERA QSAR	0.00000725	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.61399	no units	

Tris(2-butoylethyl) phosphate (TBEP)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
31	ATSDR. 2012. Toxicological Profile for Phosphate Ester Flame Retardants. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
74	ECHA. Registration Dossier for Tris(2-butoxyethyl) phosphate. European Chemicals Agency (ECHA), Helsinki, Finland. https://echa.europa.eu/registration-dossier/-/registered-dossier/14166/10 Accessed 2/5/2020.
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.

Tris(chloroethyl)phosphate (TCEP)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Tris(chloroethyl)phosphate (TCEP)
CASRN:	115-96-8
DTXSID:	DTXSID5021411
Use:	Flame-retardant in plastics and urethanes
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.14

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
4	carcinogen with linear MOA	9	4

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	1	renal tubular cell adenomas and carcinomas	general population	PPRTV	2009

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.142	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Tris(chloroethyl)phosphate (TCEP)
CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA**Qualifying Assessments, Exposure Factors, and HRL Determination**

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.2	mg/kg/day	ATSDR 2012	NTP 1991	renal tubule epithelial hyperplasia	general population	33.8	1180	[31]	
Reference Dose (RfD) or Equivalent	0.007	mg/kg/day	PPRTV 2009	Matthews et al., 1990; NTP, 1991	increased absolute and relative liver and kidney weights	general population	33.8	41.4	[304]	
Cancer Slope Factor (CSF)	0.02	(mg/kg/day) ⁻¹	PPRTV 2009	NTP, 1991; Matthews et al., 1993	combined incidence of renal tubular cell adenomas and carcinomas	general population	33.8	1.48	[304]	
Cancer Classification (CC)	L		PPRTV 2009						[304]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Gastrointestinal, Hepatic	0.0256	Deng, 2018	Systemic	100	Yang, 2018	2011-09-01	2020-01-28	357	5	3	4

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute Health-Based Guidance Value	0.3	mg/L	MN DOH	
Cancer Classification (CC)	3	no units	WHO IARC	
Chronic Health-Based Guidance Value	0.2	mg/L	MN DOH	
Chronic Health-Based Guidance Value	0.0005	mg/L	MN DOH	
Intermediate Minimal Risk Level (MRL)	0.6	mg/kg/day	CDC ATSDR	
Short-Term/Subchronic Health-Based Guidance Value	0.2	mg/L	MN DOH	
Subchronic Provisional RfD	0.02	mg/kg/day	EPA PPRTV	
Cancer Classification (CC)	Female.Mice EE	no units	HHS NTP	
Cancer Classification (CC)	Female.Rats P	no units	HHS NTP	
Cancer Classification (CC)	Male.Mice EE	no units	HHS NTP	
Cancer Classification (CC)	Male.Rats P	no units	HHS NTP	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	1866	mg/kg	NIH HSDB	max
LD50	430	mg/kg	NIH HSDB	min
Percent of active toxcast in vitro assays tested	0.29	percent	EPA Chemistry Dashboard	
TD50	23600000	mg/kg/day	NIH CPDB	max
TD50	39.9	mg/kg/day	NIH CPDB	min

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0015704	mol/kg	TEST QSAR	
Ames mutagenicity test	0.976	no units	TEST QSAR	
Developmental toxin test	0.483	no units	TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Tris(chloroethyl)phosphate (TCEP)
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
		Prevalence				Magnitude					
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	567	56	Sites	9.88	0.01	0.07	0.142	0.44	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	88	42	Sites	48	0.01	0.07	0.16	0.44	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	479	14	Sites	2.92	0.01	0.04	0.086	0.13	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	25K - 100K

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
		Prevalence				Magnitude					
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	0					ug/L	
Padhye et al. 2013 (Finished) [155]	2009 - 2010	8	7	Samples	88	0	3.7e-06		2.04e-05 +/- 5.8e-06	ug/L	
USGS, Sioux Falls Area, 2012 (Finished) [153]	2009 - 2010	1	0	Sites	0						
Ambient Water											
		Prevalence				Magnitude					
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	725	291	Sites	40	0.01	0.07	0.21	7.66	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	690	62	Sites	8.99	0.01	0.06	0.195	1.88	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,415	353	Sites	25	0.01	0.07	0.21	7.66	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	4		0.065		0.065	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	15	Sites	39	0.0416	0.18	0.282	0.487	ug/L	
Padhye et al. 2013 (Ambient) [155]	2009 - 2010	8	7	Samples	88	0	5.6e-06		5.17e-05 +/- 1.9e-06	ug/L	
USGS, Sioux Falls Area, 2012 (Ambient) [153]	2009 - 2010	2	2	Sites	100						
Waste Water Effluent											
		Prevalence				Magnitude					
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	21	Sites	100	0.2	0.415	0.57	0.73	ug/L	
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure		0.00000696	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.
Blank fields indicate there were no data available.
“All Water” data from NWIS and NAWQA are combined surface water and groundwater data.
Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.
State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.
UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	3.67993	days	
Boiling point	OPERA QSAR	321.803	degree C	
Boiling point	TEST QSAR	295.075	degree C	
Vapor pressure	OPERA QSAR	0.0350806	mmHg	
Vapor pressure	TEST QSAR	0.000645654	mmHg	
Solubility in water	OPERA QSAR	0.0265137	mol/L	
Solubility in water	TEST QSAR	0.00506991	mol/L	
Bioconcentration factor	OPERA QSAR	1.32172	no units	
Bioconcentration factor	TEST QSAR	5.01187	no units	
Henry's Law constant	OPERA QSAR	0.000000128	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	1.52722	no units	

Tris(chloroethyl)phosphate (TCEP)

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
31	ATSDR. 2012. Toxicological Profile for Phosphate Ester Flame Retardants. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
52	Bradley, P. M., Journey, C. A., Romanok, K. M., Barber, L. B., Buxton, H. T., Foreman, W. T., ... & Jones, D. K. (2017). Expanded target-chemical analysis reveals extensive mixed-organic-contaminant exposure in US streams. <i>Environmental science & technology</i> , 51(9), 4792-4802.
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. <i>Science of The Total Environment</i> . v581-582, (909-922).
153	Occurrence of anthropogenic organic compounds and nutrients in source and finished water in the Sioux Falls area, South Dakota, 2009–10: U.S. Geological Survey Scientific Investigations Report 2012–5098, 21 p. plus appendixes.
155	Padhye, L.P., Yao, H., Kung'u, F.T., and Huang, C.H. Year-long evaluation on the occurrence and fate of pharmaceuticals, personal care products, and endocrine disrupting chemicals in an urban drinking water treatment plant. 2014. <i>Water Research</i> 51 (2014) 266-276.
161	Scott, T. M., Phillips, P. J., Kolpin, D. W., Colella, K. M., Furlong, E. T., Foreman, W. T., & Gray, J. L. (2018). Pharmaceutical manufacturing facility discharges can substantially increase the pharmaceutical load to US wastewaters. <i>Science of the Total Environment</i> , 636, 69-79.
304	USEPA. 2009. Provisional Peer-Reviewed Toxicity Values for Tris(2-chloroethyl)phosphate (TCEP) (CASRN 115-96-8). U.S. Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment, Superfund Health Risk Technical Support Center, Cincinnati, OH.

Tungsten

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Tungsten
CASRN:	7440-33-7
DTXSID:	DTXSID8052481
Use:	Metal, in plating material and textiles
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	0.8

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	non-cancer effects	10	6

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	5	glandular stomach goblet cell metaplasia	general population	PPRTV	2015

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
3.99	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable
Basis		

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Tungsten

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.0008	mg/kg/day	PPRTV 2015	USACHPPM 2007a and b	glandular stomach goblet cell metaplasia	general population	33.8	4.73	[356]	
Cancer Classification (CC)	I		PPRTV 2015						[356]	
			ATSDR 2005						[25]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Immune, Renal, Hematologic	17.7	Frawley, 2016	Respiratory, Systemic	284	Frawley, 2016	2014-09-01	2020-01-21	805	2	29	2

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Subchronic Provisional RfD	0.008	mg/kg/day	EPA PPRTV	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity test			TEST QSAR	
Developmental toxin test			TEST QSAR	

Tungsten

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

OCCURRENCE DATA

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	21	17	Sites	81	0.06	0.376	3.99	22.1	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	4	3	Sites	75	0.1	0.7	1.88	2.3	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	17	14	Sites	82	0.06	0.376	4.4	22.1	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	10M - 50M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	82	49	Sites	60	0.003	1.04	3.01	42.2	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	1,175	722	Sites	61	0.001	0.232	8.32	5060	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	1,257	771	Sites	61	0.001	0.26	5.9	5060	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expcast exposure			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)	0.263	ug/l	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Tungsten

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

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Reference Number	Full Reference
25	ATSDR. 2005. Toxicological Profile for Tungsten. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
356	USEPA. 2015. Provisional Peer-Reviewed Toxicity Values for Soluble Tungsten Compounds. U.S. Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment, Superfund Health Risk Technical Support Center, Cincinnati, OH.

Vanadium

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Vanadium
CASRN:	7440-62-2
DTXSID:	DTXSID2040282
Use:	Use data are for vanadium pentoxide: Chemical intermediate; catalyst;; naturally-occurring
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	X
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
List	31

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
7	non-cancer effects	10	7

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
HRL	0.4	"kidney toxicity"	general population	PPRTV	2009

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
12.4	90th Percentile	Finished Water	UCMR3	2013-2015

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4
X	X	X	X

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis
Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Vanadium

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.00007	mg/kg/day	PPRTV 2009	Boscolo et al. 1994	"kidney toxicity"	general population	33.8	0.414	[305]	
Cancer Classification (CC)	I		PPRTV 2009 ATSDR 2012						[305] [32]	

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review
Neurological	38.51	Sun, 2017	Hepatic, Renal	83.7	Wang, 2016	2011-09-01	2019-10-22	1233	19	53	2

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Acute inhalation Minimal Risk Level (MRL)	0.0008	mg/m ³	CDC ATSDR	
Benchmark	0.015	mg/L	CalEPA OEHHA Chemical Database	
Chronic Health-Based Guidance Value	0.05	mg/L	MN DOH	
Chronic inhalation Minimal Risk Level (MRL)	0.0001	mg/m ³	CDC ATSDR	
Intermediate Minimal Risk Level (MRL)	0.01	mg/kg/day	CDC ATSDR	
Subchronic Provisional RfD	0.0007	mg/kg/day	EPA PPRTV	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	2000	mg/kg	NIH HSDB	max
LD50	23	mg/kg	NIH HSDB	min

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50			TEST QSAR	
Ames mutagenicity test			TEST QSAR	
Developmental toxin test			TEST QSAR	

Technical Support Document for the
Draft Fifth Contaminant Candidate List (CCL 5)
Contaminant Information Sheets

EPA 815-R-21-006
July 2021

EPA - Office of Water

Vanadium
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

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Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015	4,922	3,625	Sites	74	0.2	1.3	12.4	193	ug/L	
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986	989	146	Sites	15	3	7	23	70	ug/L	
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	5,985	4,753	Sites	79	0.02	1.5	8.8	294	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	274	176	Sites	64	0.04	1.5	5.9	54.8	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	5,711	4,577	Sites	80	0.02	1.4	17.5	294	ug/L	

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)	12	692,638	Chemical Data Reporting (CDR) Results (EPA) (2016)	10M - 50M

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Drinking Water Monitoring Data - CA (Finished)	2006 - 2020	213	123	Sites	58	0.844	5	12	76	ug/L	
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	16		3.4		4.9	ug/L	
Community Water System Survey (CWSS) (Finished) [178]	2006	3	NA	Sites			2.225	4.1		ug/L	
Ambient Water											
Drinking Water Monitoring Data - CA (Source)	2006 - 2020	1,704	1,279	Sites	75	0.0044	6.68	26	262	ug/L	
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	1,056	964	Sites	91	0.01	1.8	8.3	801	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	5,214	3,986	Sites	76	0.01	3.7	27.2	1000	ug/L	
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	6,258	4,941	Sites	79	0.01	2.4	17.7	1000	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	44		2.3		5.8	ug/L	
Arnold et al. 2016 (Filtered) [7]	2012 - 2013	757	510	Sites	67	0.08	0.48	13	62.3	ug/L	
Waste Water Effluent											
Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes					

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure			

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Vanadium

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Reference Number	Full Reference
7	Arnold, T.L., DeSimone, L.A., Bexfield, L.M., Lindsey, B.D., Barlow, J.R., Kulongoski, J.T., Musgrove, MaryLynn, Kingsbury, J.A., and Belitz, Kenneth, 2016, Groundwater quality data from the National Water-Quality Assessment Project, May 2012 through December 2013 (ver. 1.1, November 2016): U.S. Geological Survey Data Series 997, 56 p., http://dx.doi.org/10.3133/ds997 .
32	ATSDR. 2012. Toxicological Profile for Vanadium. U.S. Department of Health and Human Services, Public Health Service, Agency for Toxic Substances and Disease Registry (ATSDR), Atlanta, GA.
86	Glassmeyer, S.T., Furlong, E.T., Kolpin, D.W., Batt, A.L., Benson, R., Boone, J.S., ... & Wilson, V.S. (2017). Nationwide reconnaissance of contaminants of emerging concern in source and treated drinking waters of the United States. Science of The Total Environment. v581-582, (909-922).
178	USEPA (US Environmental Protection Agency). (2009). 2006 Community Water System Survey. Overview, 57.
305	USEPA. 2009. Provisional Peer-Reviewed Toxicity Values for Vanadium and Its Soluble Inorganic Compounds Other Than Vanadium Pentoxide (CASRN 7440-62-2 and Others), Derivation of Subchronic and Chronic Oral RfDs. EPA/690/R-09/070F. U.S. Environmental Protection Agency, Office of Research and Development, National Center for Environmental Assessment, Superfund Health Risk Technical Support Center, Cincinnati, OH.

Verapamil

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

CONTAMINANT IDENTIFYING INFORMATION

Name:	Verapamil
CASRN:	52-53-9
DTXSID:	DTXSID9041152
Use:	Anti-arrhythmia agent
Chemical Notes:	

Is the contaminant on any lists?	
CERCLA	
FIFRA	
Human Neurotoxicants	
PubMed Neurotoxicants	X
Neurodev. Disruptors	
Androgen Receptors in vitro	
Compounds with neurodev effects, Mundy et al 2015	

CONTAMINANT SUMMARY & DECISION

Draft CCL5 List Decision	Final Hazard Quotient (HQ)
Not List	0.00038

ATTRIBUTE SCORE & FINAL HAZARD QUOTIENT INFORMATION

Potency	Severity	Prevalence	Magnitude
6	non-cancer effects	4	1

Health Reference Level (HRL) or CCL Screening Level (SL)	HRL or SL value (ug/L)	Critical Effect	Target Pop.	Assessment Source	Assessment Pub. Date
SL	5	lowest therapeutic dose: management of hypertension	bottle-fed infants	FDA; NIH	2018; 2018

Conc. in water for HQ (ug/L)	90th Percentile or Maximum (if measured conc)	Finished or Ambient (FW, SW, GW, WW)	Source	Date
0.001886	90th Percentile	All Ambient Water	NAWQA	1991-2017

PUBLIC NOMINATION STATUS

Public Nomination

PAST CCL STATUS

CCL 1	CCL 2	CCL 3	CCL 4

PAST NEGATIVE REGULATORY DETERMINATION STATUS

RD 1	RD 2	RD 3
Not Applicable	Not Applicable	Not Applicable

Basis

Not Applicable

Notes: The final hazard quotient is the ratio of the contaminant's concentration in water to its Health Reference Level (HRL) or CCL Screening Level.

The HRL or CCL Screening Level for carcinogens is equivalent to the one-in-a-million cancer risk expressed as a drinking water concentration. For non-carcinogens, the toxicity value (RfD or equivalent) is divided by an exposure factor (i.e. drinking water intake level) relevant to the target population and critical effect and multiplied by a Relative Source Contribution of 20%.

Verapamil

CCL 5 Contaminant Information Sheet

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HEALTH EFFECTS DATA

Qualifying Assessments, Exposure Factors, and HRL Determination

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	HRL (ug/L)	Assessment Full Citation	Notes

Non-Qualifying Assessments, Exposure Factors, and CCL Screening Level Determinations

Data Element	Value	Units	Assessment Source	Critical Study	Critical Effect	Target Population	Exposure Factor (mL/kg-day)	CCL Screening Level (ug/L)	Assessment Full Citation	Notes
Reference Dose (RfD) or Equivalent	0.00075	mg/kg/day	FDA 2018; NIH 2018	Ranbaxy Laboratories Inc.	lowest therapeutic dose:management of hypertension	bottle-fed infants	151	0.993	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels
Reference Dose (RfD) or Equivalent	0.00075	mg/kg/day	FDA 2018; NIH 2018	Ranbaxy Laboratories Inc.	lowest therapeutic dose:management of hypertension	general population	33.8	4.44	[77] [150]	NOTE: (Lowest Therapeutic Dose/3000x UF) is used in place of an RfD; LTDs were obtained from FDA-approved drug labels

Literature Search Summary

Lowest LOAEL Health Effects	Lowest LOAEL (mg/kg bw/day)	Lowest LOAEL Study	Highest NOAEL Health Effects	Highest NOAEL (mg/kg bw/day)	Highest NOAEL Study	Start Date of Search	End Date of Search	No. Unique References identified in lit search	No. Animal Studies passed Title-abstract Screen	No. Human Studies passed Title-abstract Screen	No. PECO Relevant Studies passed full-text review

Other Health Data

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
Screening level for pharmaceutical - general population	0.017647059	mg/L	EPA Office of Water	
Screening level for pharmaceutical - infants	0.005	mg/L	EPA Office of Water	

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

The full citation for the critical study is provided in the corresponding health assessment.

PECO = Population, Exposure, Comparator, Outcome.

Data Element	Value	Units	Source	Notes
Measured Data and Assessment Results				
LD50	108	mg/kg	NIH HSDB	min
LD50	163	mg/kg	NIH HSDB	max
Percent of active toxcast in vitro assays tested	14.04	percent	EPA Chemistry Dashboard	

Data Element	Value	Units	Source	Notes
Modeled Data				
LD50	0.0010568	mol/kg	TEST QSAR	
Ames mutagenicity test	-0.173	no units	TEST QSAR	
Developmental toxin test	0.641	no units	TEST QSAR	

Verapamil
CCL 5 Contaminant Information Sheet
OCCURRENCE DATA

EPA-OGWDW and OST

July 2021

Scoring Data

Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Unregulated Contaminant Monitoring Rule (UCMR) 4	2018 - 2019										
Unregulated Contaminant Monitoring Rule (UCMR) 3	2013 - 2015										
Unregulated Contaminant Monitoring Rule (UCMR) 2	2008 - 2010										
Unregulated Contaminant Monitoring Rule (UCMR) 1	2001 - 2003										
Unregulated Contaminant Monitoring-State (UCM-State) Round 2	1993 - 1997										
Unregulated Contaminant Monitoring-State (UCM-State) Round 1	1988 - 1992										
National Inorganics and Radionuclides Survey (NIRS)	1984 - 1986										
Ambient Water											
National Water Quality Assessment (USGS NAWQA) (All Water)	1991 - 2017	557	2	Sites	0.36	0.00031	0.0013	0.00189	0.00228	ug/L	
National Water Quality Assessment (USGS NAWQA) (Surface Water)	1991 - 2017	75	2	Sites	2.67	0.00031	0.0013	0.00189	0.00228	ug/L	
National Water Quality Assessment (USGS NAWQA) (Ground Water)	1991 - 2017	482	0	Sites	0						

Pesticide Application Data	Number of States	Amount Applied (lbs/year)	Date	Toxic Release Data	Number of States	Amount Released (lbs/year)	Chemical Production Data	Production Volume (lbs/year)
Estimated Annual Agricultural Pesticide Use (USGS)				Toxic Release Inventory (TRI) Program (EPA) (2016)			Chemical Data Reporting (CDR) Results (EPA) (2016)	

Non-Scoring Data

Non-Nationally Representative Water Data	Date	Number of PWS/ Sites/ Samples	Number of Detects	PWS/ Sites/ Samples	Percent with Detects	Minimum Conc. (Detects)	Median Conc. (Detects)	90th Percentile (Detects)	Maximum Conc. (Detects)	Conc. Units	Notes
Finished Water											
Glassmeyer et al 2017 (Finished) [86]	2007 - 2012	25	NA	Sites	4		0.0267		0.0267	ug/L	
Ambient Water											
National Water Information System (USGS NWIS) (Surface Water)	2008 - 2017	210	9	Sites	4.29	4.00E - 04	0.0184	0.0541	0.161	ug/L	
National Water Information System (USGS NWIS) (Groundwater)	2008 - 2017	401	0	Sites	0						
National Water Information System (USGS NWIS) (All Water)	2008 - 2017	611	9	Sites	1.47	4.00E - 04	0.0184	0.0541	0.161	ug/L	
Glassmeyer et al 2017 (Ambient) [86]	2007 - 2012	25	NA	Sites	4		0.0459		0.0459	ug/L	
Batt et al. 2016 (Ambient) [46]	2008 - 2009	182	39	Sites	21	9e-04	0.0032	0.015	0.0358	ug/L	
Bradley et al. 2017 (Ambient) [52]	2012 - 2014	38	6	Sites	16	0.0007812	0.00358	0.0099	0.0129033	ug/L	
Bexfield et al. 2019 (Groundwater) [49]	2013 - 2015	1,106	0	Sites	0						
Waste Water Effluent											
Scott et al. 2018 (Wastewater) [161]	2011 - 2017	21	12	Sites	57	0.0095317	0.0228	0.132	4.119285	ug/L	
Kostich et al. 2014 (Wastewater) [126]	not reported	49	39	Sites	80	0.0053	0.021	0.0502	0.0971	ug/L	
Batt et al. (2008) via Kostich et al. 2010 (Wastewater) [127]	2010	NA	NA						0.19	ug/L	

Estimated Concentration in Water	Date	Source	Value	Units	Model	Notes

Predicted Exposure Data (EPA CompTox Dashboard)	Date	Total Predicted Exposure (mg/kg bw/day)	Notes
Expocast exposure		0.000000276	

Biomonitoring Data	Detection at 90th Percentile	Units	Notes
NHANES biomonitoring detection in serum (1999-2016)			
NHANES biomonitoring detection in blood (1999-2016)			
NHANES biomonitoring detection in urine (1999-2016)			

Notes: Highlighted data indicate value was used in attribute scoring.

Blank fields indicate there were no data available.

"All Water" data from NWIS and NAWQA are combined surface water and groundwater data.

Monitoring dates for non-scoring data and NAWQA are not chemical-specific and may not contain samples for all years listed.

State Drinking Water Monitoring Data with a max date range of 2020 may contain few samples from early 2020.

UCMR 4 data used in the draft CCL5 is a partial dataset and will be complete in Dec. 2020.

Modelled Environmental Fate Parameters (EPA CompTox Dashboard)	Source	Value	Units	Notes
Biodegradation half-life	OPERA QSAR	7.28169	days	
Boiling point	OPERA QSAR	425.134	degree C	
Boiling point	TEST QSAR	489.98	degree C	
Vapor pressure	OPERA QSAR	6.02E-10	mmHg	
Vapor pressure	TEST QSAR	1.22E-09	mmHg	
Solubility in water	OPERA QSAR	0.000000569	mol/L	
Solubility in water	TEST QSAR	0.000000891	mol/L	
Bioconcentration factor	OPERA QSAR	200.744	no units	
Bioconcentration factor	TEST QSAR	197.242	no units	
Henry's Law constant	OPERA QSAR	0.000000428	atm-m ³ /mol	
Octanol/water partitioning coeff. (log Kow)	OPERA QSAR	3.88495	no units	

Verapamil

CCL 5 Contaminant Information Sheet

EPA-OGWDW and OST

July 2021

Reference Number	Full Reference
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Appendix B Contaminant Information Sheet References

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