

# How can the “PubChem PFAS Tree” Help Support the Regulation of PFAS?

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National Center for Biotechnology Information, National  
Library of Medicine, National Institutes of Health

Contact: [pubchem-help@ncbi.nlm.nih.gov](mailto:pubchem-help@ncbi.nlm.nih.gov)

PFAS and Fluorinated Compounds in PubChem	20,092,587
OECD PFAS definition	6,063,764
Organofluorine compounds	19,173,213
Other diverse fluorinated compounds	106,093
PFAS and fluorinated compound collections	1,784,338
PFAS by functional class	6,954,048
Regulatory PFAS collections	25,024
Long-chain PFCAs and related substances	17,716
PFHxS and related substances	649
PFOA and related substances	23,696
PFOA and related substances - exclusions	68
PFOS and related substances	1,301





# Outline

- Background and Motivation
- PubChem PFAS Tree
- How can this support regulation
- Live Demo
- Questions / Discussion

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What is PubChem? <https://pubchem.ncbi.nlm.nih.gov/>

Explore Chemistry

Quickly find chemical information from authoritative sources

Try covid-19 aspirin EGFR C9H8O4 57-27-2 C1=CC=C(C=C1)C=O InChI=1S/C3H6O/c1-3(2)4/h1-2H3

☐ Use Entrez ☒ Compounds ☐ Substances ☐ BioAssays

Draw Structure Upload ID List Browse Data Periodic Table

112M Compounds 297M Substances 297M Bioactivities 35M Literature 42M Patents 874 Data Sources

[See More Statistics >](#) [Explore Data Sources >](#)

<https://pubchem.ncbi.nlm.nih.gov/>



# What is PubChem?



## Explore Chemistry

Quickly find chemical information from

PFOA

Compound

PFOA

PFOS

PFDA

Gene

Ptma

Ptpa

Pura

## Explore Chemistry

Quickly find chemical information from authoritative sources

335-67-1

Compound

335-67-1

335161-24-5

335621-00-6

335161-19-8

Gene

snoRNA:Me285-C3351

zinc finger protein 335

CG3356

CG33557

Taxonomy

Prevotella buccae ATCC 33574

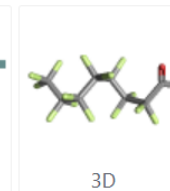
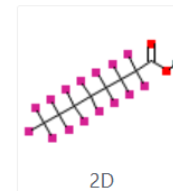
### COMPOUND SUMMARY

## Perfluorooctanoic acid

PubChem CID

9554

Structure



Find Similar Structures

Chemical Safety



Corrosive



Irritant



Health Hazard

Laboratory Chemical Safety Summary (LCSS) Datasheet

Molecular Formula

C<sub>8</sub>HF<sub>15</sub>O<sub>2</sub>



# What is PubChem? <https://pubchem.ncbi.nlm.nih.gov/>

▼ PubChem Compound TOC ? 63,097,836

- ▶ Agrochemical Information ? 3,105
- ▶ Associated Disorders and Diseases ? 23,799
- ▶ Biologic Description ? 2,236,718
- ▶ Biological Test Results ? 4,109,169
- ▶ Biomolecular Interactions and Pathways ? 140,468
- ▶ Chemical and Physical Properties ? 277,595
- ▶ Classification ? 21,252,957
- ▶ Drug and Medication Information ? 18,059
- ▶ Food Additives and Ingredients ? 7,411
- ▶ Identification ? 4,769
- ▶ Information Sources ? 42,423,777
- ▶ Literature ? 2,073,600
- ▶ Names and Identifiers ? 1,901,543
- ▶ Patents ? 37,419,039
- ▶ Pharmacology and Biochemistry ? 112,418
- ▶ Related Records ? 12,867,766
- ▶ Safety and Hazards ? 171,674
- ▶ Spectral Information ? 1,364,279
- ▶ Structures ? 11,772,818
- ▶ Toxicity ? 115,645
- ▶ Use and Manufacturing ? 104,096

## Perfluorohexanesulfonic acid

### Associated Disorders and Diseases

17 items

Download

#	Structure	CTD Chemical ID	Chemical Name	Disease Source	CTD Disease ID	Disease	Evidence Type	Evidence PMID
1		C471071	perfluorohexanesulfonic acid	MeSH	D001289	Attention Deficit Disorder with Hyperactivity	marker/mechanism	20551004
2		C471071	perfluorohexanesulfonic acid	MeSH	D000067877	Autism Spectrum Disorder	marker/mechanism	32353786

## PubChem Perfluorooctanoic acid (Compound)

### 8.1 Uses

EPA CPDat Chemical and Product Categories

4 items

Category	Category Description
Cleaning and safety	Products used for cleaning or safe occupational or industrial setting
Cleaning products and household care -> carpet and floor -> floor polish	Products that impart a shine to surface
nonfunctional ingredient	
used as a stain or water repellent.	

### 8.3 U.S. Production

Production volumes for non-confidential chemicals reported under the Inventory Update Rule.

Year	Production Range (pounds)
1986	10 thousand - 500 thousand
1990	No Reports
1994	10 thousand - 500 thousand
1998	10 thousand - 500 thousand
2002	10 thousand - 500 thousand

US EPA; Non-confidential Production Volume Information Submitted by Companies for Chemicals Under the 1986-2002 Inventory Update Rule (IUR). Octanoic acid, pentadecafluoro- (335-67-1). Available from, as of November 2, 2010: <https://www.epa.gov/oppt/iur/tools/data/2002-vol.html>

▶ Hazardous Substances Data Bank (HSDB)

Use

<https://pubchem.ncbi.nlm.nih.gov/classification/#hid=72>





# What is the NORMAN Suspect List Exchange?

<https://www.norman-network.com/nds/SLE/>



## NORMAN Database System



[NORMAN WEBSITE](#) | [NORMAN DATABASE SYSTEM](#) | [HOME](#) | [LOGIN](#)

NORMAN SUBSTANCE DATABASE

### NORMAN Suspect List Exchange – NORMAN SLE

The NORMAN Suspect List Exchange (NORMAN-SLE) was established in 2015 as a central access point for NORMAN members (and others) to find suspect lists relevant for their environmental monitoring questions. The NORMAN-SLE documents all individual collections that form a part of the merged collection [NORMAN SusDat](#). The original SLE lists should be consulted to verify SusDat information if necessary (see Source column in SusDat). NORMAN-SLE versions are tracked on [Zenodo](#).

Comments and contributions are welcome - please email us at [suspects@normandata.eu](mailto:suspects@normandata.eu).

Please refer to our [documentation](#) pages for: [citation](#) instructions, [credits](#), [updates](#), [license](#) details, [SDFs](#) and other useful tips!

No.	Abbreviation	Description	Link to full list	Link to InChIKey list	References
S0	SUSDAT	<b>Merged NORMAN Suspect List: SusDat</b>	<a href="#">Interactive Data table</a> SusDat with Haz and Expo scores as <a href="#">XLSX</a> , <a href="#">CSV</a> (18/01/2022) <a href="#">MetFrag CSV</a> (03/03/2020) <a href="#">CompTox SUSDAT List</a>	SusDat InChIKeys: <a href="#">All</a> , <a href="#">MS-ready</a> (18/01/2022)	A merged list of >111,000 structures from SLE suspect lists. See <a href="#">interactive version</a> . Compiled by Reza Aalizadeh, Nikiforos Alygizakis and Lubos Cirka, University of Athens/EI, including RTI and toxicity values, with Hazard and Exposure values provided by Stellan Fischer, KEMI, documented <a href="#">here</a> . <i>Work in progress ... please report any issues!</i>  DOI: <a href="#">10.5281/zenodo.2664077</a>



### SEARCH All Databases

Searching for individual substance or group(s) of substances

**Note:** Click on a link below to go to an individual database



### Substance Database

A merged list of NORMAN substances; Central Database to access various lists of substances for suspect screening and prioritisation



### Suspect List Exchange

Central Database to access various lists of substances for suspect screening and prioritisation



### Antibiotic Resistance Bacteria/Genes

A database of ARBs/ARGs in environmental matrices



### MassBank Europe

A database of mass spectra of emerging substances to support identification of unknown substances






# NORMAN-SLE in PubChem

The NORMAN network enhances the exchange of information on emerging environmental substances, and encourages the validation and harmonisation of common measurement methods and monitoring tools so that the requirements of risk assessors and risk managers can be better met. It specifically seeks both to promote and to benefit from the synergies between research teams from different countries in the field of emerging substances.



Organization	NORMAN Network (c/o UniLu)	
Category	Research and Development	
URL	<a href="https://www.norman-network.com/nds/SLE/">https://www.norman-network.com/nds/SLE/</a>	
License Note	Data: CC-BY 4.0; Code (hosted by ECI, LCSB): Artistic-2.0	
License URL	<a href="https://creativecommons.org/licenses/by/4.0/">https://creativecommons.org/licenses/by/4.0/</a>	
Contact Name	Emma Schymanski	
Address	6 avenue du Swing, Belvaux, Luxembourg, 4367	
Data Source ID	23819	
Data in PubChem	117,154 Live Substances 20,099 Annotations 1 Classification	
Last Updated	2022/09/14	



# NORMAN-SLE in PubChem



The NORMAN network enhances the exchange of information on emerging environmental substances, and encourages the validation and harmonisation of common measurement methods and monitoring tools so that the requirements of risk assessors and risk managers can be better met. It specifically seeks both to promote and to benefit from the synergies between research teams from different countries in the field of emerging substances.

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License Note	Data: CC-BY 4.0; Code (hosted by ECI, LCSB): Artistic-2.0
License URL	<a href="https://creativecommons.org/licenses/by/4.0/">https://creativecommons.org/licenses/by/4.0/</a>
Contact Name	Emma Schymanski
Address	6 avenue du Swing, Belvaux, Luxembourg, 4367
Data Source ID	23819
Data in PubChem	117,154 Live Substances 20,099 Annotations 1 Classification
Last Updated	2022/09/14

▼ NORMAN Suspect List Exchange Classification ? ↗ 113,735
▶ S13   EUCOSMETICS   Combined Inventory of Ingredients Employed in Cosmetic Products (2000) and Revised Inventory (2006) ? 3,801
▶ S25   OECDPFAS   List of PFAS from the OECD ? 3,677
▶ S36   UBAPMT   Potential Persistent, Mobile and Toxic (PMT) substances ? 254
▶ S47   ECHAPLASTICS   A list from the Plastic Additives Initiative Mapping Exercise by ECHA ? 241
▶ S50   CCSCOMPEND   The Unified Collision Cross Section (CCS) Compendium ? 869
▶ S60   SWISSPEST19   Swiss Pesticides and Metabolites from Kiefer et al 2019 ? 1,348
▶ S61   UJICCSLIB   Collision Cross Section (CCS) Library from UJI ? 574
▶ S66   EAWAGTPS   Parent-Transformation Product Pairs from Eawag ? 258
▶ S68   HSDBTPS   Transformation Products Extracted from HSDB Content in PubChem ? 102
▶ S69   LUXPEST   Pesticide Screening List for Luxembourg ? 386
▶ S72   NTUPHTW   Pharmaceutically Active Substances from National Taiwan University ? 1,068
▶ S75   CyanoMetDB   Comprehensive database of secondary metabolites from cyanobacteria ? 2,087
▶ S79   UACCSCEC   Collision Cross Section (CCS) Library from UAntwerp ? 148
▼ S80   PFASGLUEGE   Overview of PFAS Uses ? 1,250



# Adding PFAS to PubChem: Glüge *et al.* (2020)

## Environmental Science Processes & Impacts



### PAPER

View Article Online  
View Journal | View Issue



Cite this: *Environ. Sci.: Processes  
Impacts*, 2020, 22, 2345

## An overview of the uses of per- and polyfluoroalkyl substances (PFAS)<sup>†</sup>

Juliane Glüge,<sup>a</sup> Martin Scheringer,<sup>a</sup> Ian T. Cousins,<sup>b</sup> Jamie C. DeWitt,<sup>c</sup>  
Gretta Goldenman,<sup>d</sup> Dorte Herzke,<sup>e,f</sup> Rainer Lohmann,<sup>g</sup> Carla A. Ng,<sup>h</sup>  
Xenia Trier<sup>i</sup> and Zhanyun Wang<sup>j</sup>

Per- and polyfluoroalkyl substances (PFAS) are of concern because of their high persistence (or that of their degradation products) and their impacts on human and environmental health that are known or can be deduced from some well-studied PFAS. Currently, many different PFAS (on the order of several thousands) are used in a wide range of applications, and there is no comprehensive source of information on the many individual substances and their functions in different applications. Here we provide a broad overview of many use categories where PFAS have been employed and for which function; we also specify which PFAS have been used and discuss the magnitude of the uses. Despite being non-exhaustive, our study clearly demonstrates that PFAS are used in almost all industry branches and many consumer products. In total, more than 200 use categories and subcategories are identified for more than 1400 individual PFAS. In addition to well-known categories such as textile impregnation, fire-fighting foam, and electroplating, the identified use categories also include many categories not described in the scientific literature, including PFAS in ammunition, climbing ropes, guitar strings, artificial turf, and soil remediation. We further discuss several use categories that may be prioritised for finding PFAS-free alternatives. Besides the detailed description of use categories, the present study also provides a list of the identified PFAS per use category, including their exact masses for future analytical studies aiming to identify additional PFAS.

Received 2nd July 2020  
Accepted 23rd September 2020

DOI: 10.1039/d0em00291g

rsc.li/espi

### Environmental significance

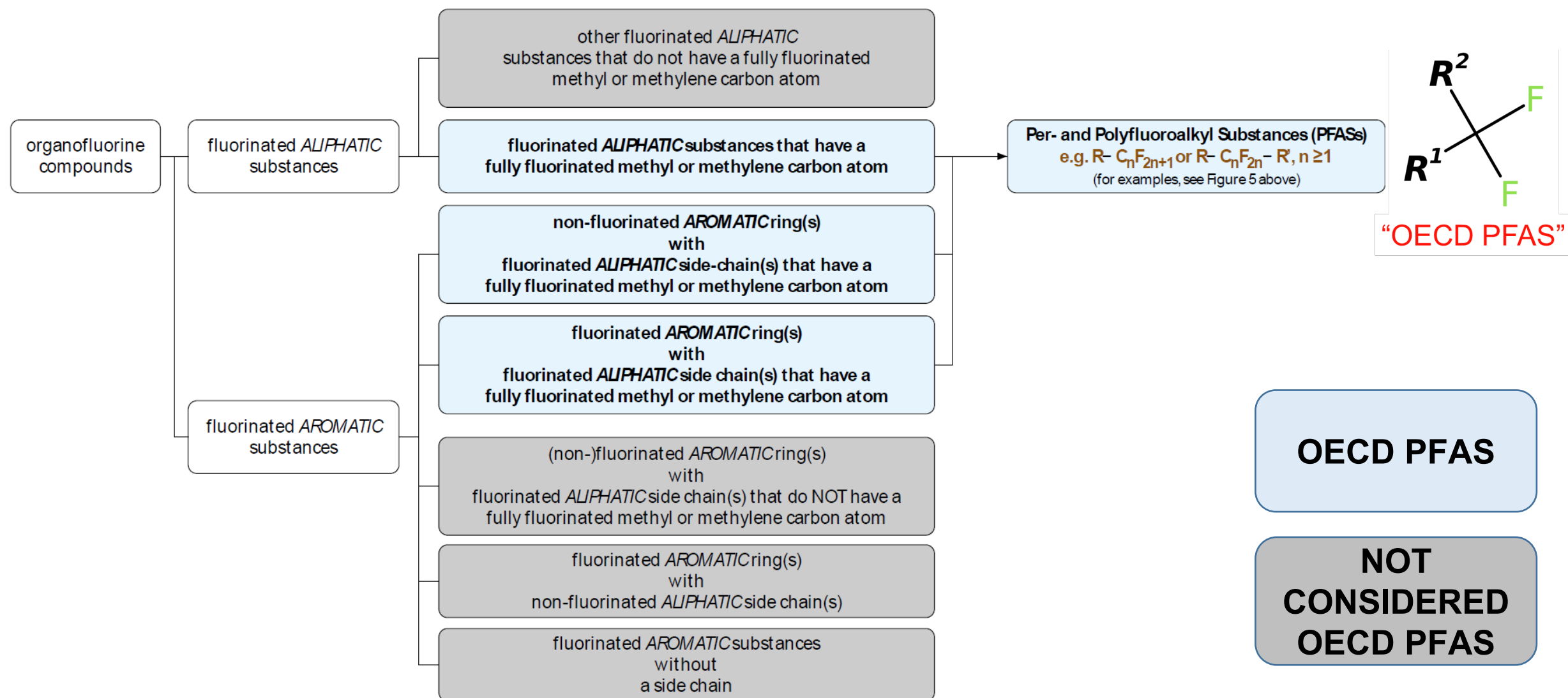
Per- and polyfluoroalkyl substances (PFAS) are a large group of more than 4700 substances that are used in a wide range of technical applications and consumer products. Releases of PFAS to the environment have caused large-scale contamination in many countries. For an effective management of PFAS, an overview of the use areas of PFAS, the functions of PFAS in these uses, and the chemical identity of the PFAS actually used is needed. Here we present a systematic description of more than 200 uses of PFAS and the individual substances associated with each of them (over 1400 PFAS in total). This large list of PFAS and their uses is intended to support the identification of essential and non-essential uses of PFAS.

▼ S80   PFASGLUEGE   Overview of PFAS Uses	?	1,250
▶ PFAS Polymer Type	?	489
▶ PFAS Structural Category	?	1,230
▶ PFAS Use Category	?	489
▼ Use Type Information Source	?	489
▶ Approved In The Past	?	4
▶ Detected Analytically	?	125
▶ In Current Use	?	36
▶ In Patent	?	285
▼ In Use	?	169
▶ Aerospace	?	2
▶ Automotive	?	7
▶ Biotechnology	?	5
▶ Building and Construction	?	10
▶ Chemical Industry	?	19
▶ Cleaning compositions	?	20

Glüge *et al.* (2020) ESPI, DOI: [10.1039/d0em00291g](https://pubchem.ncbi.nlm.nih.gov/classification/#hid=101)  
<https://pubchem.ncbi.nlm.nih.gov/classification/#hid=101>



# Motivation: PFAS Definition in OECD Monograph, Figure 8





# Motivation: How to scale this to PubChem?

Explore Chemistry

Quickly find chemical information from authoritative sources

PFAS

Try covid-19 aspirin EGFR C9H8O4 57-27-2 C1=CC=C(C=C1)C=O InChI=1S/C3H6O/c1-3(2)4/h1-2H3

☐ Use Entrez ☒ Compounds ☐ Substances ☐ BioAssays

Draw Structure Upload ID List Browse Data Periodic Table

112M Compounds 297M Substances 297M Bioactivities 35M Literature 42M Patents 874 Data Sources

See More Statistics > Explore Data Sources >

<https://pubchem.ncbi.nlm.nih.gov/>



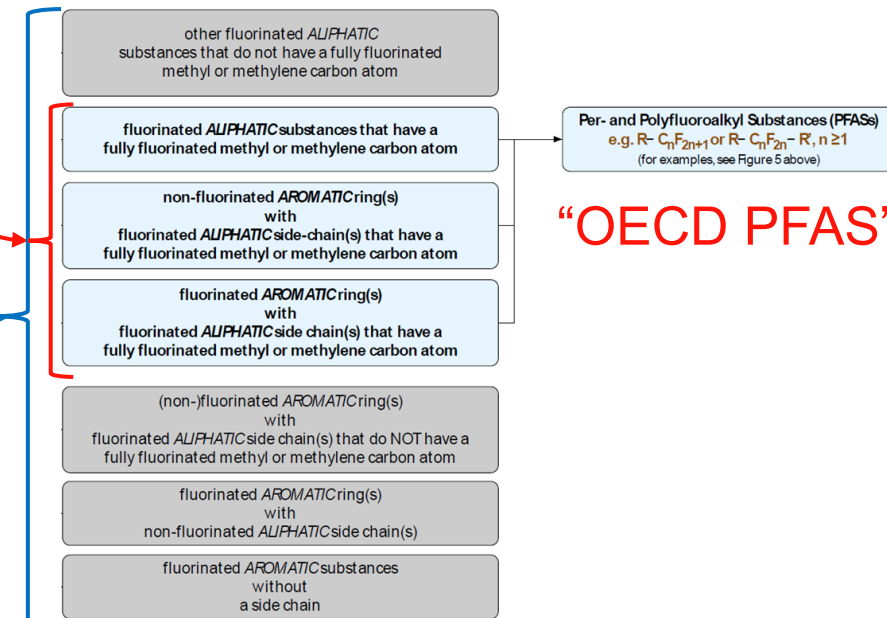
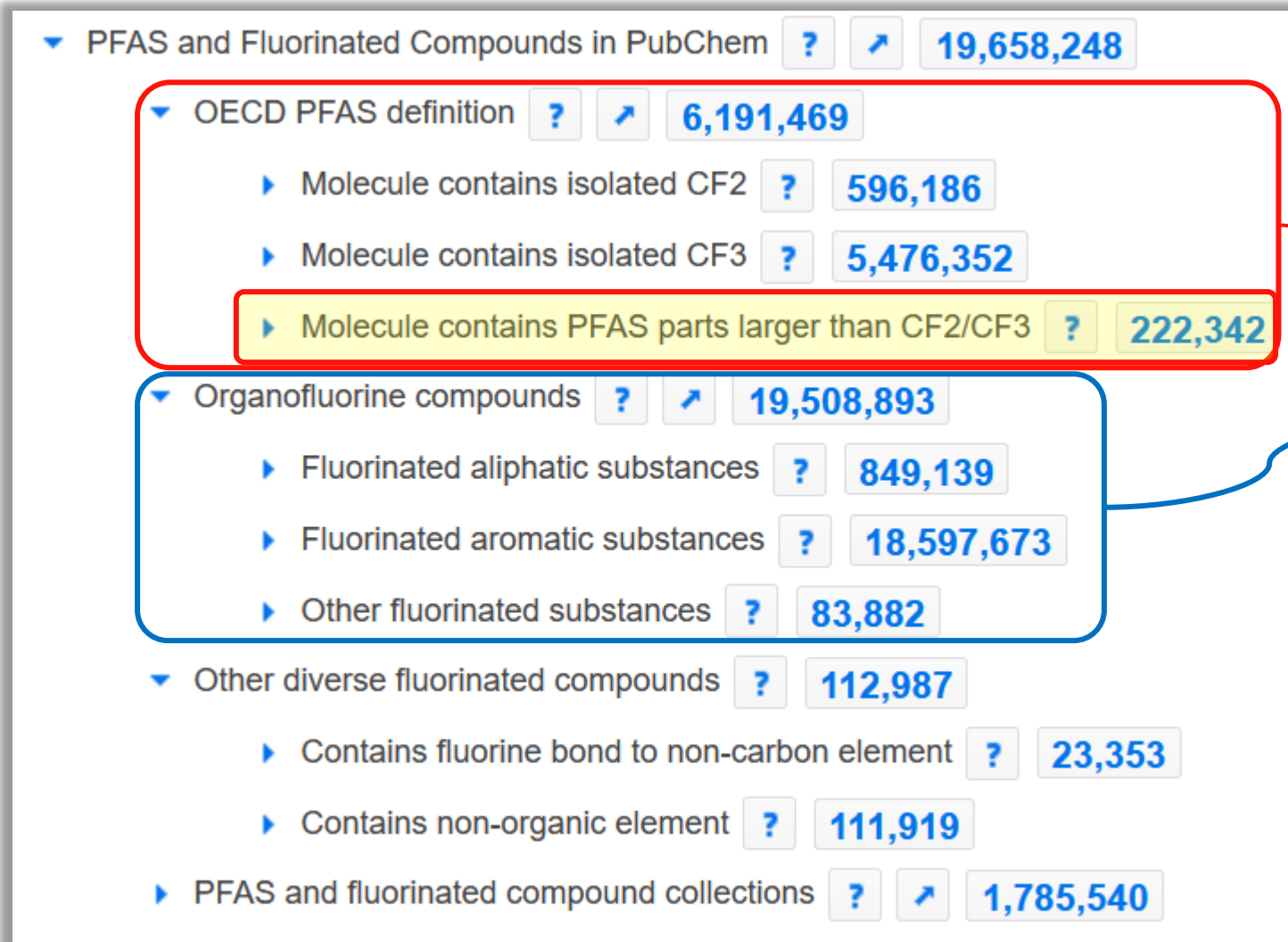
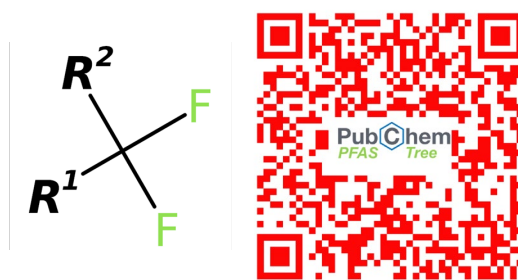
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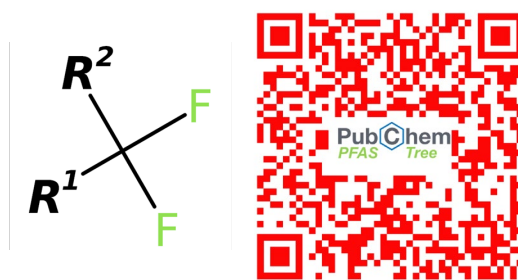


# The PubChem PFAS Tree





# The PubChem PFAS Tree



▼ PFAS and Fluorinated Compounds in PubChem ? ↗ 19,658,248

▼ OECD PFAS definition ? ↗ 6,191,469

▶ Molecule contains isolated CF2 ? 596,186

▶ Molecule contains isolated CF3 ? 5,476,352

▶ Molecule contains PFAS parts larger than CF2/CF3 ? 222,342

▼ Organofluorine compounds ? ↗ 19,508,893

▶ Fluorinated aliphatic substances ? 849,139

▶ Fluorinated aromatic substances ? 18,597,673

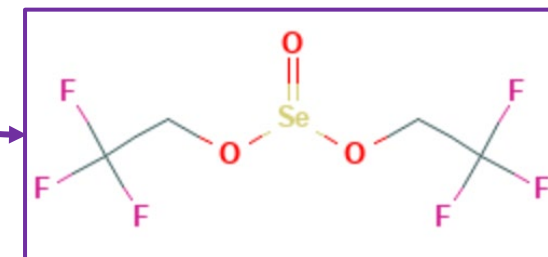
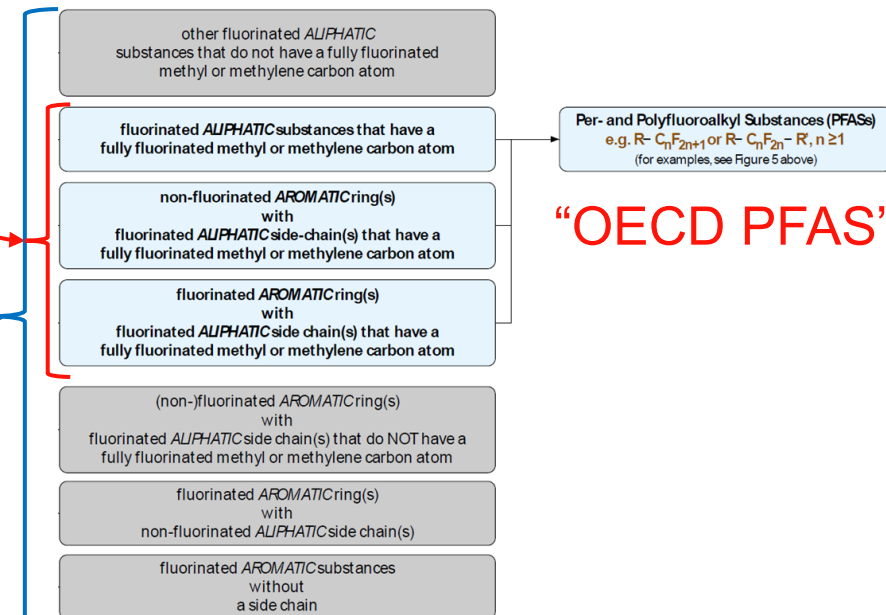
▶ Other fluorinated substances ? 83,882

▼ Other diverse fluorinated compounds ? 112,987

▶ Contains fluorine bond to non-carbon element ? 23,353

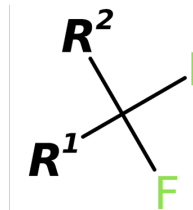
▶ Contains non-organic element ? 111,919

▶ PFAS and fluorinated compound collections ? ↗ 1,785,540

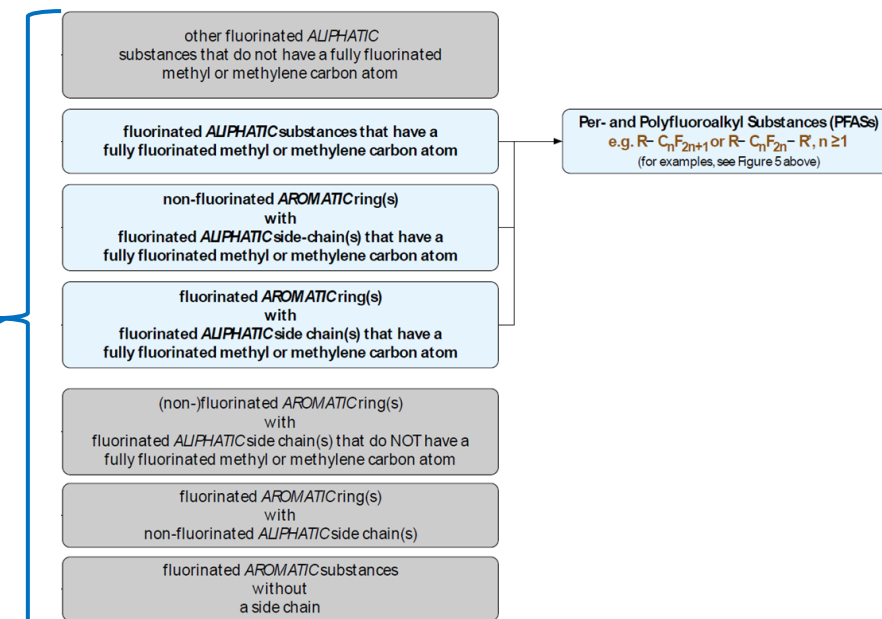




# The PubChem PFAS Tree - Organofluorine



▼ PFAS and Fluorinated Compounds in PubChem	?	↗	19,658,248
▼ OECD PFAS definition	?	↗	6,191,469
▶ Molecule contains isolated CF <sub>2</sub>	?		596,186
▶ Molecule contains isolated CF <sub>3</sub>	?		5,476,352
▶ Molecule contains PFAS parts larger than CF <sub>2</sub> /CF <sub>3</sub>	?		222,342
▼ Organofluorine compounds	?	↗	19,508,893
▶ Fluorinated aliphatic substances	?		849,139
▶ Fluorinated aromatic substances	?		18,597,673
▶ Other fluorinated substances	?		83,882
▼ Other diverse fluorinated compounds	?		112,987
▶ Contains fluorine bond to non-carbon element	?		23,353
▶ Contains non-organic element	?		111,919
▶ PFAS and fluorinated compound collections	?	↗	1,785,540



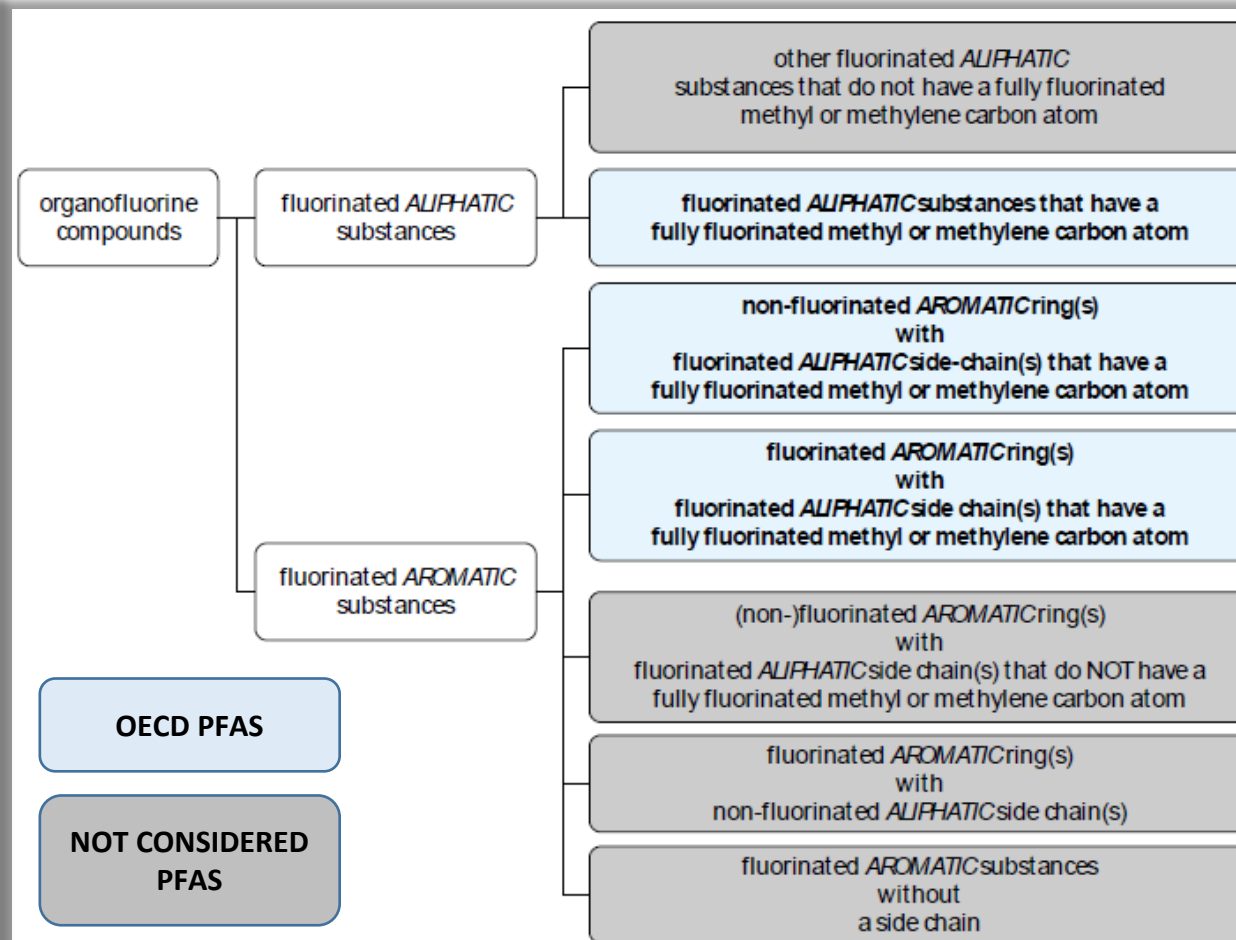


# >19 M Organofluorine compounds in PubChem

<https://pubchem.ncbi.nlm.nih.gov/classification/#hid=120>

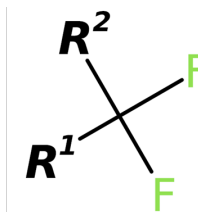


- ▼ Organofluorine compounds ? 19,508,893
  - ▼ Fluorinated aliphatic substances ? 849,139
    - ▶ Fluorinated aliphatic substances that have a fully fluorinated methyl or methylene carbon atom ? 566,903
    - ▶ Other fluorinated aliphatic substances that do NOT have a fully fluorinated methyl or methylene carbon atom ? 282,236
  - ▼ Fluorinated aromatic substances ? 18,597,673
    - ▶ (Non-)Fluorinated aromatic ring(s) with fluorinated aliphatic side chain(s) that do NOT have a fully fluorinated methyl or methylene carbon atom ? 1,448,549
    - ▶ Fluorinated aromatic ring(s) with fluorinated aliphatic side chain(s) that have a fully fluorinated methyl or methylene carbon atom ? 844,998
    - ▶ Fluorinated aromatic ring(s) with non-fluorinated aliphatic side chain(s) ? 11,489,706
    - ▶ Fluorinated aromatic substances without a side chain ? 34,851
    - ▶ Non-fluorinated aromatic ring(s) with fluorinated aliphatic side chain(s) that have fully fluorinated methyl or methylene carbon atom ? 4,779,569
  - ▶ Other fluorinated substances ? 83,882





# The PubChem PFAS Tree – OECD PFAS



▼ PFAS and Fluorinated Compounds in PubChem ? ↗ 19,658,248

▼ OECD PFAS definition ? ↗ 6,191,469

- ▶ Molecule contains isolated CF<sub>2</sub> ? 596,186
- ▶ Molecule contains isolated CF<sub>3</sub> ? 5,476,352
- ▶ Molecule contains PFAS parts larger than CF<sub>2</sub>/CF<sub>3</sub> ? 222,342

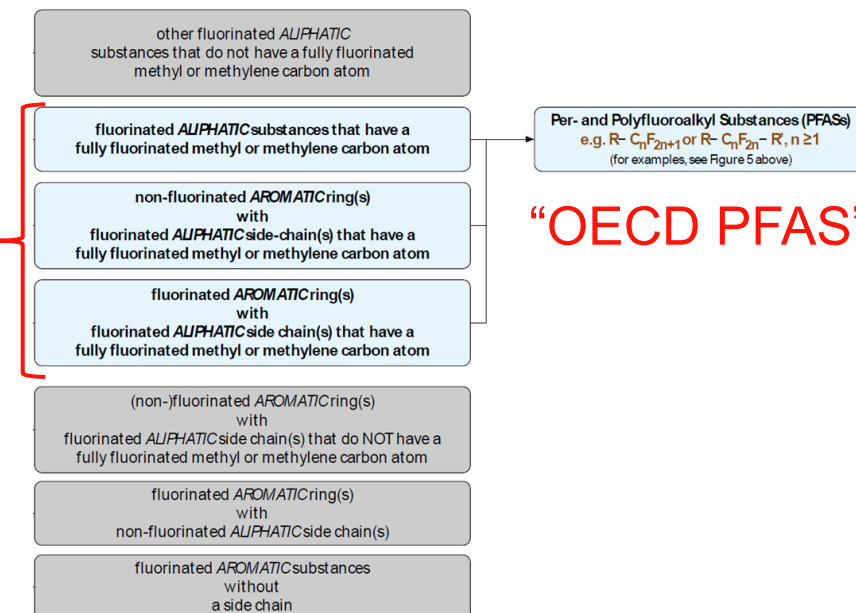
▼ Organofluorine compounds ? ↗ 19,508,893

- ▶ Fluorinated aliphatic substances ? 849,139
- ▶ Fluorinated aromatic substances ? 18,597,673
- ▶ Other fluorinated substances ? 83,882

▼ Other diverse fluorinated compounds ? 112,987

- ▶ Contains fluorine bond to non-carbon element ? 23,353
- ▶ Contains non-organic element ? 111,919

▶ PFAS and fluorinated compound collections ? ↗ 1,785,540





# Over 6 million OECD PFAS in PubChem !!!!!



▼ PFAS and Fluorinated Compounds in PubChem ? 19,658,248

▼ OECD PFAS definition ? 6,191,469

▼ Molecule contains isolated CF2 ? 596,186

▶ Contains CF2 and larger PFAS parts ? 8,783

▶ Contains only isolated CF2 ? 518,829

▶ Contains only isolated CF2/CF3 ? 68,574

▼ Molecule contains isolated CF3 ? 5,476,352

▶ Contains CF3 and larger PFAS parts ? 26,054

▶ Contains only isolated CF2/CF3 ? 68,574

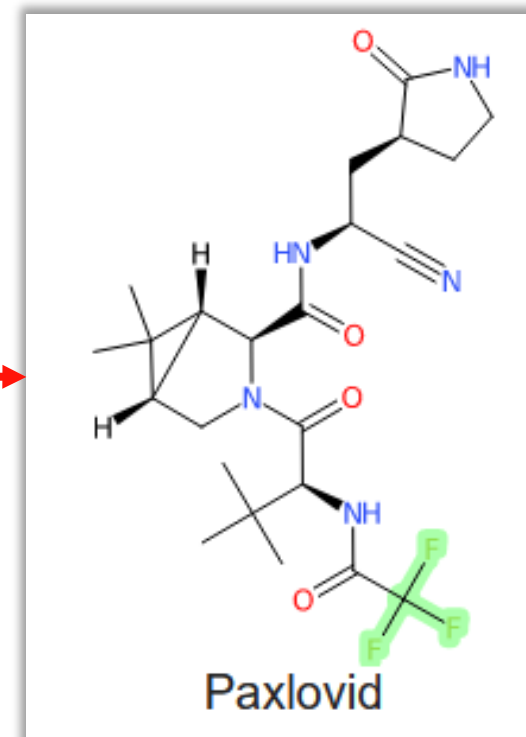
▶ Contains only isolated CF3 ? 5,381,724

▼ Molecule contains PFAS parts larger than CF2/CF3 ? 222,342

▶ Breakdown by isolated PFAS part count ? 222,342

▶ Breakdown by isolated PFAS part type ? 222,342

*Note: this does not include mixtures and salts ...*





# The PubChem PFAS Tree – Collection of Lists

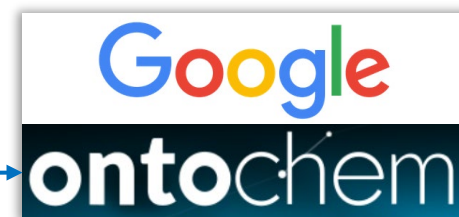


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- ▶ Other diverse fluorinated compounds ? 112,987
- ▼ PFAS and fluorinated compound collections ? ↗ 1,785,540
  - ▶ CompTox Chemicals Dashboard PFAS suspect lists ? ↗ 8,502
  - ▶ NORMAN-SLE PFAS suspect lists ? ↗ 6,040
  - ▶ OntoChem PFAS lists ? ↗ 1,777,052
  - ▶ Other fluorinated chemical content in PubChem ? ↗ 1,674
- NIST PFAS suspect list ? ↗ 4,948



CompTox Chemicals Dashboard



PubChem



<https://pubchem.ncbi.nlm.nih.gov/classification/#hid=120>



# Many different PFAS lists in the tree ...

## PFAS and fluorinated compound collections 1,785,540

CompTox Chemicals Dashboard PFAS suspect lists 8,502

NORMAN-SLE PFAS suspect lists 6,040



S09 | PFASTRIER | PFAS Suspect List

S14 | KEMIPFAS | PFAS Highly Fluorinated

S25 | OECDPFAS | List of PFAS from OECD

S46 | PFASNTREV19 | List of PFAS from NIST

S80 | PFASGLUEGE | Overview of PFAS

S89 | PRORISKPFAAS | List of PFAS from NORMAN

S92 | FLUOROPHARMA | List of 340 PFAS from Pharma

S94 | FLUOROPEST | List of 423 PFAS from Pesticides

S95 | PFASANEXCH | PFAS List from NORMAN

S96 | ECIPFAS | Updatable List to add new PFAS

OntoChem PFAS lists 1,777,052

Other fluorinated chemical content in PubChem

NIST PFAS suspect list 4,948



## OntoChem PFAS lists 1,777,052

OntoChem PFAS from CORE - Definition A

OntoChem PFAS from CORE - Definition B

OntoChem PFAS from CORE - Definition C

OntoChem PFAS from Google Patents - Definition A

OntoChem PFAS from Google Patents - Definition B

OntoChem PFAS from Google Patents - Definition C

## Other fluorinated chemical content in PubChem

MeSH: Fluorinated Hydrocarbons 295

MeSH: Chlorofluorocarbons 40

MeSH: Fluoroacetates 30

MeSH: Fluorobenzenes 104

MeSH: Fluorocarbons 121

CAMEO Chemicals: Fluorinated Organic Compounds

ChEBI: Organofluorine Compound 1,372

## CompTox Chemicals Dashboard PFAS suspect lists 8,502

[EPAPFAS75S1] PFAS[EPA: List of 75 Test Samples (Set 1)] 74

[EPAPFAS75S2] PFAS[EPA: List of 75 Test Samples (Set 2)] 76

[EPAPFASCAT] PFAS[EPA Structure-based Categories] 82

[EPAPFASDW537] PFAS[EPA|WATER: Existing EPA DW Method 537.1] 19

[EPAPFASDW] PFAS[EPA: New EPA Method Drinking Water] 26

[EPAPFASDWTREAT] PFAS[EPA|WATER: Drinking Water Treatment Technology] 9

[EPAPFASINSOL] PFAS[EPA: Chemical Inventory Insoluble in DMSO] 43

[EPAPFASINV] PFAS[EPA: ToxCast Chemical Inventory] 428

[EPAPFASINVIVO] PFAS[EPA: In Vivo Studies Available] 23

[EPAPFASLITSEARCH] PFAS[EPA: Literature Search Completed] 23

[EPAPFASNONDW] PFAS[EPA: New EPA Method Non-Drinking Water] 24

[EPAPFASRESEARCH] PFAS[EPA: EPA PFAS Research List] 165

[EPAPFASRL] PFAS

[EPAPFASTOX] PFAS

[EPAPFASVALDW] PFAS[EPA: Water Methods] 31

[EPASDEV1] PFAS[EPA: Developmental Toxicology] 45

[EPASGLUEGE] PFAS[EPA: Overview of PFAS] 483

[EPASINVITR] PFAS[EPA: In Vitro Studies Available] 182

[EPASKEMI] PFAS: List from the Swedish Chemicals Agency (KEMI) Report 1,473

[EPASLCMSGCMS] PFAS: Collection of GC-MS and LC-MS standards: Food Contact Materials 38

[EPASMASTER] PFAS Master List of PFAS Substances (Version 2) 8,117

[EPASNORDIC] PFAS: Nordic PFAS Report 2019 203

[EPASNTREV19] PFAS: PFAS in Non-Target HRMS Studies (Liu et al 2019) 127

[EPASOECD] PFAS: Listed in OECD Global Database 3,702

[EPASOECDNA] NORMAN: List of PFAS from the OECD Curated by Nikiforos Alygizakis 3,206

[EPASPACKAGING] PFAS[EPA PFAS Substances in Pesticide Packaging] 8

[EPASSTRUCT] Navigation Panel to PFAS Structure Lists 8,079

[EPASSTRUCTV1] PFAS[EPA: PFAS structures in DSSTox (update March 2018)] 4,351

[EPASSTRUCTV2] PFAS[EPA: PFAS structures in DSSTox (update November 2019)] 6,625

[EPASSTRUCTV3] PFAS[EPA: PFAS structures in DSSTox (update August 2020)] 8,137

[EPASSTRUCTV4] PFAS[EPA: PFAS structures in DSSTox (update August 2021)] 8,079

[EPASTDB] WATER|PFAS: PFAS Chemicals contained in the EPA Drinking Water Treatability Database 38

[EPASTOXDB] PFAS: PFAS-Tox Database 43

[EPASTRI] PFAS: PFAS to the Toxics Release Inventory (TRI) Program by the National Defense Authorization Act 100

[EPASTRIER] PFAS Community-Compiled List (Trier et al. 2015) 589

[EPASTRIER] NORMAN|List of PFAS Compiled from NORMAN-SusDat 3,372



CompTox  
Chemicals  
Dashboard





# Browse the PubChem PFAS Tree to find more!



PFAS and Fluorinated Compounds in PubChem ? ↗ 19,658,248

OECD PFAS definition ? ↗ 6,191,469

- ▶ Molecule contains isolated CF2 ? 596,186
- ▶ Molecule contains isolated CF3 ? 5,476,352
- ▼ Molecule contains PFAS parts larger than CF2/CF3 ? 222,342
  - ▼ Breakdown by isolated PFAS part count ? 222,342
    - ▼ Contains 01 isolated PFAS part ? 167,552
      - ▶ Count of molecules 00001-10 ? 873
      - ▶ Count of molecules 00011-100 ? 3,382
      - ▶ Count of molecules 00101-1000 ? 8,490
      - ▶ Count of molecules 01001-10000 ? 34,792
      - ▼ Count of molecules 10001-100000 ? 120,015
        - Contains 01xC02F04-linear 17,899
        - Contains 01xC02F05-linear 44,481
        - Contains 01xC03F06-linear 13,117
        - Contains 01xC03F07-linear 32,781
        - Contains 01xC04F09-linear 11,737
    - ▶ Contains 02 isolated PFAS parts ? 38,263
    - ▶ Contains 03 isolated PFAS parts ? 10,171

Molecules in this category contain 5 isolated PFAS parts

- ▶ Contains 05 isolated PFAS parts ? 869

SEARCH FOR

PFAS and Fluorinated Compounds in PubChem: Contains 01xC04F09-linear × 🔍

Treating this as a previously computed list of identifiers.

Compounds

11,737 results Filters SORT BY Relevance

Download

ACTIONS ON RESULTS WITH ID TYPE: Compounds

DOWNLOAD ×

Summary (Search Results)

CSV JSON XML

COMPRESSION: ☒ None ☐ GZip

Chemical Structure Records

SDF JSON XML ASNT

COORDINATE TYPE: ☒ 2D ☐ 3D

COMPRESSION: ☒ None ☐ GZip

375-62-2; Perfluorovaleryl Fluoride; Nonfluorovaleryl Fluoride; Perfluoropentanoyl Fluoride; Nonfluoropentanoyl Fluoride; ...

Compound CID: 67812

MF: C<sub>5</sub>F<sub>10</sub>O MW: 266.04g/mol

IUPAC Name: 2,2,3,3,4,4,5,5,5-nonafluoropentanoyl fluoride

Isomeric SMILES: C(=O)(C(C(C(C(F)(F)F)(F)(F)F)(F)(F)F)F)F

InChIKey: RUFSXELMOQBMOF-UHFFFAOYSA-N

InChI: InChI=1S/C5F10O/c6-1(16)2(7,8)3(9,10)4(11,12)5(13,14)15

Create Date: 2005-08-08

Summary Similar Structures Search Related Records

PubChem PFAS Tree:  
<https://pubchem.ncbi.nlm.nih.gov/classification/#hid=120>



# Download files contain additional information...



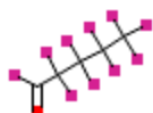
	A	B	C	D	E	F	G	H	I	J	K	L						
1	cid	cmpdnam	cmpdsyno	mw	mf	polararea	complexity	xlogp	heavycnt	hbondddor	hbondacc	rotbonds						
2	67812	Perfluorov	375-62-2	266.04	C5F10O	17.1	288	3.4	16	0	11	3						
3	67814	Nonafluor	375-72-4	302.09	C4F10O2S	42.5	386	3.4	17	0	12	3						
4	67815	Perfluorok	375-73-5	300.1	C4HF9	M	N	O	P	Q	R	S	T	U	V	W	X	
5	69494	Pentane, 1638-79-9		395.94	C5F11	inchi	isosmiles	inchikey	iupacnam	meshheac	annothits	annothitcr	aid	cidcdate	sidsrcnam	depcatg	annotation	
6	69939	1-Butanes	812-94-2	385.25	C9H12	InChI=1S/C(=O)(C(C	RUFSEXELV	2,2,3,3,4,4	NULL	Classificat	6	NULL	20050808	001Chemi	Chemical	NULL		
7	73893	2-Propenc	1492-87-1	439.3	C12H1	InChI=1S/C(C(C(F)(F	LUYQYZLE	1,1,2,2,3,3	NULL	Classificat	6	NULL	20050327	001Chemi	Chemical	NULL		
8	74534	3,3,4,4,5,5	1799-84-4	332.16	C10H9	InChI=1S/C(C(C(F)(F	JGTNAGYH	1,1,2,2,3,3	NULL	Biomolecu	11	NULL	20050326	001Chemi	Chemical	NULL		
9	74883	1-Hexanol	2043-47-2	264.09	C6H5F	InChI=1S/C(C(C(F)(F	KCEJSGJN	1,1,1,2,2,3	NULL	Chemical	7	NULL	20050808	3WAY PHA	Chemical	NULL		
10	74887	1,1,1,2,2,3	2043-55-2	373.99	C6H4F	InChI=1S/CN(CCCCC	ZDKQQLGI	1,1,2,2,3,3	NULL	Classificat	4	NULL	20050808	AAA Cher	Chemical	NULL		
11	75921	Perfluorov	Perfluorop	264.05	C5HF9	InChI=1S/CN(CCCCC	PGYDZCBT	4-[methyl	NULL	Classificat	4	NULL	20050808	AAA Cher	Chemical	NULL		
12	88054	3,3,4,4,5,5	19430-93-	246.07	C6H3F	InChI=1S/CC(=C)C(=	TYNRPOFA	3,3,4,4,5,5	NULL	Classificat	6	NULL	20050719	3B Scientif	Chemical	NULL		
13	100925	Methacryl	SCHEMBLE	304.11	C8H5F	InChI=1S/C(CO)C(C	JCMNMOE	3,3,4,4,5,5	NULL	Chemical	8	NULL	20050327	001Chemi	Chemical	NULL		
14	101642	2,2,3,3,4,4	308-26-9	304.11	C8H5F	InChI=1S/C(CI)C(C	CXHFIVFP	1,1,1,2,2,3	NULL	Biological	10	651631 65	20050719	001Chemi	Chemical	NULL		
15	104247	2-(Perflu	2-(Perflu	318.14	C9H7F	InChI=1S/C(=O)(C	CXZGQIAC	2,2,3,3,4,4	NULL	Biological	10	111187	20050326	001Chemi	Chemical	NULL		
						InChI=1S/C=CC(C(C	GVEUEBXI	3,3,4,4,5,5	NULL	Chemical	8	NULL	20050327	001Chemi	Chemical	NULL		
						InChI=1S/CC(=C)C(=	DYMLOJJA	1,1,2,2,3,3	NULL	Patents	1	NULL	20050808	ECI Group	Curation E	NULL		
						InChI=1S/C=CC(=O)	UOKXSSAM	2,2,3,3,4,4	NULL	Chemical	5	NULL	20050808	A2B Chem	Chemical	NULL		
						InChI=1S/C=CC(=O)	GYUPEJST	3,3,4,4,5,5	NULL	Classificat	6	NULL	20050719	3B Scientif	Chemical	NULL		



# Download files contain additional information...



	A	B	C	D	E	F	G	H	I	J	K	L						
1	cid	cmpdnam	cmpdsyno	mw	mf	polararea	complexity	xlogp	heavycnt	hbonddor	hbondacc	rotbonds						
2	67812	Perfluorov	375-62-2	266.04	C5F10O	17.1	288	3.4	16	0	11	3						
3	67814	Nonafluor	375-72-4	302.09	C4F10O2S	42.5	386	3.4	17	0	12	3						
4	67815	Perfluorok	375-73-5	300.1	C4HF9													
5	69494	Pentane,	1638-79-9	395.94	C5F11													
6	69939	1-Butanes	812-94-2	385.25	C9H12	InChI=1S/C(=O)(C(C	RUFSEXELV	2,2,3,3,4,4	NULL	Classificat	6	NULL	20050808	001Chemi	Chemical	NULL		
7	73893	2-Propenc	1492-87-1	439.3	C12H1	InChI=1S/C(C(C(F)(F	LUYQYZLE	1,1,2,2,3,3	NULL	Classificat	6	NULL	20050327	001Chemi	Chemical	NULL		
8	74534	3,3,4,4,5,5	1799-84-4	332.16	C10H9	InChI=1S/C(C(C(F)(F	JGTNAGYH	1,1,2,2,3,3	NULL	Biomolecu	11	NULL	20050326	001Chemi	Chemical	NULL		
9	74883	1-Hexanol	2043-47-2	264.09	C6H5F	InChI=1S/C(C(C(F)(F	KCEJSGJN	1,1,1,2,2,3	NULL	Chemical	7	NULL	20050808	3WAY PHA	Chemical	NULL		
10	74887	1,1,1,2,2,2	2043-55-2	272.09	C6H4F5	InChI=1S/CN(CCCCC	ZDKOQLGI	1,1,2,2,3,3	NULL	Classificat	4	NULL	20050808	AAA Chem	Chemical	NULL		
11																		
12																		
13																		
14																		
15																		



375-62-2; Perfluorovaleryl Fluoride; Nonafluorovaleryl Fluoride; Nonafluoropentanoyl Fluoride; Perfluoropentanoyl Fluoride; Pentanoyl Fluoride, Nonafluoro-; Perfluoropentanoyl Fluoride 98; 2,2,3,3,4,4,5,5,5-nonafluoropentanoyl Fluoride; ...

Compound CID: [67812](#)

MF:  $C_5F_{10}O$  MW: 266.04g/mol

IUPAC Name: 2,2,3,3,4,4,5,5,5-nonafluoropentanoyl fluoride

Isomeric SMILES: C(=O)(C(C(C(C(F)(F)(F)(F)(F)(F)(F)(F)(F)(F)F

InChIKey: RUFSEXELMOQBMOF-UHFFFAOYSA-N

InChI: InChI=1S/C5F10O/c6-1(16)2(7,8)3(9,10)4(11,12)5(13,14)15

Create Date: 2005-08-08

Property Name	Property Value
Molecular Weight	266.04
XLogP3-AA	3.4
Hydrogen Bond Donor Count	0
Hydrogen Bond Acceptor Count	11
Rotatable Bond Count	3
Exact Mass	265.97894624



# Download files contain additional information...



	A	B	C	D	E	F	G	H	I	J	K	L
1	cid	cmpdnam	cmpdsyno	mw	mf	polararea	complexity	xlogp	heavycnt	hbonddor	hbondacc	rotbonds
2	67812	Perfluorov	375-62-2	266.04	C5F10O	17.1	288	3.4	16	0	11	3
3	67814	Nonafluor	375-72-4	302.09	C4F10O2S	42.5	386	3.4	17	0	12	3
4	67815	Perfluorok	375-73-5	300.1	C4HF9	M	N	O	P	Q	R	S
5	69494	Pentane, 1638-79-9		395.94	C5F11	inchi	isosmiles	inchikey	iupacnam	meshhea	annothits	annothitc
6	69939	1-Butanes	812-94-2	385.25	C9H12	InChI=1S/C(=O)(C(C	RUFSEXELV	2,2,3,3,4,4	NULL		Classificat	6 NULL
7	7										Classificat	6 NULL
8	7										Biomolecu	11 NULL
9	74										Chemical a	7 NULL
10	74										Classificat	4 NULL
11	75	EPA CPDat Chemical and Product Categories									Classificat	4 NULL
12	88	1 item										6 NULL
13	100											8 NULL
14	100											
15	104											

## 8 Use and Manufacturing

### 8.1 Uses

EPA CPDat Chemical and Product Categories

1 item

**Category**

used as a stain or water repellent

*The Chemical and Physical Properties of Perfluorinated Compounds, vol. 1*

► EPA Chemical and Physical Properties Database

### 8.2 Methods of Manufacturing

Perfluoroalkanesulfonyl fluorides are which a hydrocarbon sulfonyl fluoride ... The electrochemical yield is excellent with the increasing length of the carbon chain. Alkaline hydrolysis of perfluoroalkane acidified and distilled from concentrated sulfuric acid.

*Siegemund G et al; Fluorine Compounds, NY, NY: John Wiley & Sons. Online Posting*

► Hazardous Substances Data Bank (HSDB)

### 8.3 U.S. Production

Production volumes for non-confidential chemicals reported under the Inventory Update Rule.

Year	Production Range (pounds)
1986	No Reports
1990	No Reports
1994	10 thousand - 500 thousand
1998	No Reports
2002	10 thousand - 500 thousand

*US EPA; Non-confidential Production Volume Information Submitted by Companies for Chemicals Under the 1986-2002 Inventory Update Rule (IUR). 1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptafluoro- (1763-23-1). Available from, as of November 2, 2010: <https://www.epa.gov/oppt/iur/tools/data/2002-vol.html>*

► Hazardous Substances Data Bank (HSDB)

PubChem Compound TOC ? 49,493,641

► Agrochemical Information ? 3,045

► Associated Disorders and Diseases ? 20,847

► Biologic Description ? 2,056,521

► Biological Test Results ? 3,622,920

► Biomolecular Interactions and Pathways ? 125,253

► Chemical and Physical Properties ? 263,015

► Classification ? 1,454,824

► Drug and Medication Information ? 17,922

► Food Additives and Ingredients ? 8,414

► Identification ? 4,968

► Information Sources ? 20,271,277

► Literature ? 1,833,941

► Names and Identifiers ? 1,275,170

► Patents ? 36,351,418

► Pharmacology and Biochemistry ? 110,628

► Related Records ? 9,224,590

► Safety and Hazards ? 149,319

► Spectral Information ? 480,730

► Structures ? 9,117,635

► Toxicity ? 114,012

► Use and Manufacturing ? 115,321

Chemical Safety ? 147,023



# Outline

- Background and Motivation
- PubChem PFAS Tree
- How can this support regulation
- Live Demo
- Questions / Discussion

▼ PFAS and Fluorinated Compounds in PubChem	?	↗	20,092,587
▶ OECD PFAS definition	?	↗	6,063,764
▶ Organofluorine compounds	?	↗	19,173,213
▶ Other diverse fluorinated compounds	?		106,093
▶ PFAS and fluorinated compound collections	?	↗	1,784,338
▶ PFAS by functional class			6,954,048
▼ Regulatory PFAS collections	?		25,024
▶ Long-chain PFCAs and related substances	?		17,716
▶ PFHxS and related substances	?		649
▶ PFOA and related substances	?		23,696
▶ PFOA and related substances - exclusions	?	↗	68
▶ PFOS and related substances	?		1,301

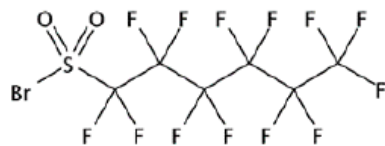
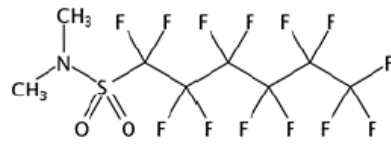
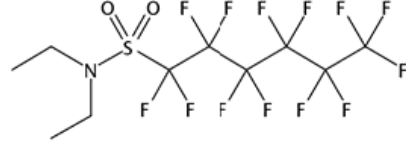


# POPRC Meets PubChem PFAS Tree ...

- Several POPRC lists available: now added to PubChem

UNEP/POPS/POPRC.17/INF/14/Rev.1

## Initial indicative list of perfluorohexane sulfonic acid (PFHxS), its salts and PFHxS-related compounds

CAS	Name	Structure
111393-39-6	1-Hexanesulfonyl bromide, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-	
1270179-82-2	1-Hexanesulfonamide, 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-N,N-dimethyl-	
1270179-93-5	1-Hexanesulfonamide, N,N-diethyl-1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluoro-	
127133-66-8	2-Propenoic acid, 2-methyl-, polymers with Bu methacrylate, lauryl methacrylate and 2-[methyl[(perfluoro-C4-8-alkyl)sulfonyl]amino]ethyl methacrylate	
129813-71-4	Sulfonamides, C4-8-alkane, perfluoro, N-methyl-N-(2-oxiranylmethyl)	



# POPRC Meets PubChem PFAS Tree ...

- Several POPRC lists available: now added to PubChem

## Initial indicative list of perfluorohexane sulfonic acid (PFHxS), its salts and PFHxS-related compounds

CAS		
111393-39-6	1-Hexanesulfonyl bromide, 1,1,1,2,2,2-hexafluoro-	
1270179-82-2	1-Hexanesulfonamide, 1,1,2,2,3,3-hexafluoro-	
1270179-93-5	1-Hexanesulfonamide, N,N-diethyl-, 1,1,2,2,3,3-hexafluoro-	
127133-66-8	2-Propenoic acid, 2-methyl-5-(perfluorohexyl)-, methyl ester and 2-[methyl[(perfluorohexyl)amino]methoxy]acrylate	
129813-71-4	Sulfonamides, C4-8-alkane, perfluorinated	

Regulatory PFAS collections ? 25,024

▶ Long-chain PFCAs and related substances ? 17,716

▶ PFHxS and related substances ? 649

▶ [Annex A] PFHxS plus its salts and PFHxS-related compounds as defined in Annex A of the Stockholm Convention ? ↗ 540

▶ [Annex A] PFHxS plus its salts and PFHxS-related compounds by annotation ? 402

▶ Compounds with a (C6F13)S(=O)(=O) moiety in PubChem by SMARTS ? 538

Initial indicative list of PFHxS plus its salts and PFHxS-related compounds ? ↗ 76

PFHxS and any branched isomers (included in PubChem) ? 2

PFHxS and any branched isomers and their salts (included in PubChem) ? 52

PFHxS and branched isomer combined substructure query in PubChem ? 186







# POPRC Meets PubChem PFAS Tree ...



- Adding regulatory collections to the PFAS Tree

## ▼ PFAS and Fluorinated Compounds in PubChem ? ↗ 20,092,587

- ▶ OECD PFAS definition ? ↗ 6,063,764
- ▶ Organofluorine compounds ? ↗ 19,173,213
- ▶ Other diverse fluorinated compounds ? 106,093
- ▶ PFAS and fluorinated compound collections ? ↗ 1,784,338
- ▶ PFAS by functional class 6,954,048

## ▼ Regulatory PFAS collections ? 25,024

- ▶ Long-chain PFCAs and related substances ? 17,716
- ▶ PFHxS and related substances ? 649
- ▶ PFOA and related substances ? 23,696
- ▶ PFOA and related substances - exclusions ? ↗ 68
- ▶ PFOS and related substances ? 1,301

## ▼ PFHxS and related substances ? 649

- ▶ [Annex A] PFHxS plus its salts and PFHxS-related compounds as defined in Annex A of the Stockholm Convention ? ↗ 540
- ▶ [EU REACH] PFHxS (linear or branched) plus its salts and related substances according to EU REACH (draft definition) ? ↗ 649
- ▶ Compounds with a (C6F13)S moiety in PubChem by SMARTS ? 649
- ▶ Compounds with a (C6F13)S(=O)(=O) moiety in PubChem by SMARTS ? 538
- ▶ Difference between Annex A and EU REACH definitions ? 109
- Compounds that transform to PFHxS (via PubChem Transformations) ?
- ▶ Initial indicative list of PFHxS plus its salts and PFHxS-related compounds ? ↗ 76
- PFHxS and any branched isomers (included in PubChem) ? 2
- PFHxS and any branched isomers and their salts (included in PubChem) ? 52
- PFHxS and branched isomer combined substructure query in PubChem ? 186



# POPRC Meets PubChem PFAS Tree ... (draft features)

- Several new developments in parallel

▼ PFAS and Fluorinated Compounds in PubChem	?	↗	20,092,587
▶ OECD PFAS definition	?	↗	6,063,764
▶ Organofluorine compounds	?	↗	19,173,213
▶ Other diverse fluorinated compounds	?		106,093
▶ PFAS and fluorinated compound collections	?	↗	1,784,338
▶ PFAS by functional class			6,954,048
▼ Regulatory PFAS collections	?		25,024
▶ Long-chain PFCAs and related substances	?		17,716
▶ PFHxS and related substances	?		649
▶ PFOA and related substances	?		23,696
▶ PFOA and related substances - exclusions	?	↗	68
▶ PFOS and related substances	?		1,301

This is the difference  
between with and  
without salts/mixtures



# POPRC Meets PubChem PFAS Tree ... (draft features)

- Several new developments in parallel

▼ PFAS and Fluorinated Compounds in PubChem	?	↗	20,092,587
▶ OECD PFAS definition	?	↗	6,063,764
▶ Organofluorine compounds	?	↗	19,173,213
▶ Other diverse fluorinated compounds	?		106,093
▶ PFAS and fluorinated compound collections	?	↗	1,784,338
▶ PFAS by functional class			6,954,048
▼ Regulatory PFAS collections	?		25,024
▶ Long-chain PFCAs and related substances	?		17,716
▶ PFHxS and related substances	?		649
▶ PFOA and related substances	?		23,696
▶ PFOA and related substances - exclusions	?	↗	68
▶ PFOS and related substances	?		1,301

This is the difference  
between with and  
without salts/mixtures

▶ PFAS by functional class	6,954,048
▼ PFAS fragment with 1 connection	6,311,331
▼ PFAS-Aliphatic	2,831,555
▶ Contains PFAS-C	2,089,733
▶ Contains PFAS-N	24,329
▶ Contains PFAS-O	516,611
▶ Contains PFAS-P	2,027
▶ Contains PFAS-S	219,017
▶ More PFAS-Element cases	3,515



# Outline

- Background and Motivation
- PubChem PFAS Tree
- How can this support regulation
- Live Demo
- Questions / Discussion

▼ PFAS and Fluorinated Compounds in PubChem	?	↗	20,092,587
▶ OECD PFAS definition	?	↗	6,063,764
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▶ PFOA and related substances - exclusions	?	↗	68
▶ PFOS and related substances	?		1,301



# Live Demo – LC-PFCAs



▼ Regulatory PFAS collections ? 25,024

▼ Long-chain PFCAs and related substances ? 17,716

▼ [Draft] Nomination of long-chain PFCAs (draft definition) ? ↗ 671

▶ [Draft] Nomination of long-chain PFCAs by annotation ? 540

Compounds related to long-chain PFCAs [WiP] ? ↗

Compounds that transform to long-chain PFCAs in PubChem

Draft indicative list of long-chain PFCAs plus their salts and related compounds

Long-chain PFCAs including any branched isomers (included in PubChem)

Long-chain PFCAs including any branched isomers and their salts (included in PubChem)

Long-chain PFCAs substructure query in PubChem ?

▶ Compounds related to long-chain PFCAs [WiP] ? ↗ 1

Compounds that transform to long-chain PFCAs in PubChem (via PubChem Transformations) ? 3

Draft indicative list of long-chain PFCAs plus their salts and related compounds ? ↗ 83

Long-chain PFCAs including any branched isomers (included in PubChem) ? 39

Long-chain PFCAs including any branched isomers and their salts (included in PubChem) ? 171

Long-chain PFCAs substructure query in PubChem ? 607

▼ [Draft] Nomination of long-chain PFCAs by annotation ? 540

[Draft] LC-PFCAs, salts and related - annotation 'Literature' ? 46

[Draft] LC-PFCAs, salts and related - annotation 'Patents' ? 477

[Draft] LC-PFCAs, salts and related - annotation 'Safety and Hazards', 'Toxicity' ? 34

[Draft] LC-PFCAs, salts and related - annotation 'Use and Manufacturing' ? 130

[Draft] LC-PFCAs, salts and related - CID date 2022 ? 4



# Live Demo – PFHxS

## ▼ Regulatory PFAS collections ? 25,024

### ▶ Long-chain PFCAs and related substances ? 17,716

### ▼ PFHxS and related substances ? 649

- ▶ [Annex A] PFHxS plus its salts and PFHxS-related compounds as defined in Annex A of the Stockholm Convention ? ↗ 540
- ▶ [EU REACH] PFHxS (linear or branched) plus its salts and related substances according to EU REACH (draft definition) ? ↗ 649
- ▶ Compounds with a (C6F13)S moiety in PubChem by SMARTS ? 649
- ▶ Compounds with a (C6F13)S(=O)(=O) moiety in PubChem by SMARTS ? 538
- ▶ Difference between Annex A and EU REACH definitions ? 109

Compounds that transform to

Initial indicative list of PFHxS

PFHxS and any branched is

PFHxS and any branched is

PFHxS and branched isome

### ▼ [Annex A] PFHxS plus its salts and PFHxS-related compounds as defined in Annex A of the Stockholm Convention ? ↗ 540

#### ▼ [Annex A] PFHxS plus its salts and PFHxS-related compounds by annotation ? 402

[Annex A] PFHxS, salts and related - annotation 'Literature' ? 15

[Annex A] PFHxS, salts and related - annotation 'Patents' ? 312

[Annex A] PFHxS, salts and related - annotation 'Safety and Hazards', 'Toxicity' ? 14

[Annex A] PFHxS, salts and related - annotation 'Use and Manufacturing' ? 108

[Annex A] PFHxS, salts and related - CID date 2022 ? 9



# Live Demo – PFHxS (II)

▼ Regulatory PFAS collections ? 25,024

▶ Long-chain PFCAs and related substances ? 17,716

▼ PFHxS and related substances ? 649

▶ [Annex A] PFHxS plus its salts and PFHxS-related compounds as defined in Annex A of the Stockholm Convention ? ↗ 540

▶ [EU REACH] PFHxS (linear or branched) plus its salts and related substances according to EU REACH (draft definition) ? ↗ 649

▶ Compounds with a (C6F13)S moiety in PubChem by SMARTS ? 649

▶ Compounds with a (C6F13)S(=O)(=O) moiety in PubChem by SMARTS ? 538

▶ Difference between Annex A and EU REACH definitions ? 109

Compounds that transform to PFHxS (via PubChem Transformations) ?

Initial indicative list of PFHxS plus its salts and PFHxS-related compounds ? ↗ 16

PFHxS and any branched isomers ▼ Difference between Annex A and EU REACH definitions ? 109

PFHxS and any branched isomers PFHxS in EU REACH but not Annex A - all ? 109

PFHxS and branched isomers PFHxS in EU REACH but not Annex A - annotation 'Use and Manufacturing' ? 5

PFHxS in EU REACH but not Annex A - annotation 'Use and Manufacturing', 'Literature' ? 11



# Live Demo – PFOA

▼ Regulatory PFAS collections ? 25,024

▶ Long-chain PFCAs and related substances ? 17,716

▶ PFHxS and related substances ? 649

▼ PFOA and related substances ? 23,696

▶ [Annex A] PFOA plus its salts and PFOA-related compounds as defined in Annex A of the Stockholm Convention [WiP] ? ↗ 737

Compounds that transform to PFOA (via PubChem Transformations) ? 7

Compounds with a linear (C7F15)C moiety in PubChem by SMARTS ? 23,362

Contains 01xC07F15-branched (PubChem PFAS Tree) ? 23

Contains 01xC07F15-linear (PubChem PFAS Tree) ? 3,290

PFOA and branched isomer combined substance

PFOA including any branched isomers (including

PFOA plus any branched isomers and their salts

Selected substances of PFOA plus its salts and

Updated indicative list of PFOA plus its salts

▶ PFOA and related substances - exclusions ?

▶ PFOS and related substances ? 1,301

▼ [Annex A] PFOA plus its salts and PFOA-related compounds by annotation ? 539

[Annex A] PFOA, salts and related - annotation 'Literature' ? 80

[Annex A] PFOA, salts and related - annotation 'Patents' ? 400

[Annex A] PFOA, salts and related - annotation 'Safety and Hazards', 'Toxicity' ? 43

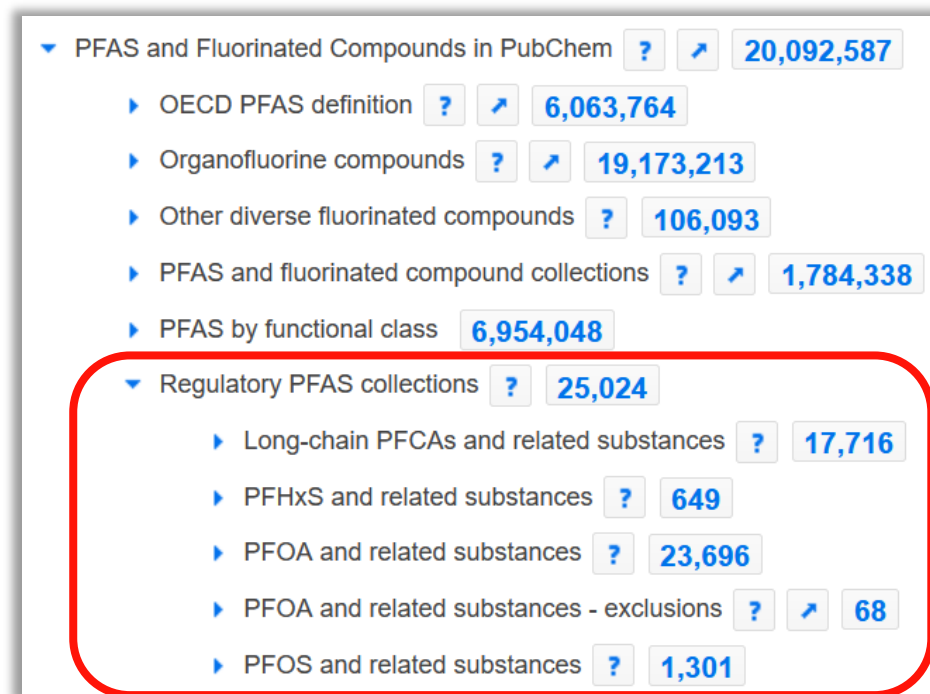
[Annex A] PFOA, salts and related - annotation 'Use and Manufacturing' ? 228

[Annex A] PFOA, salts and related - CID date 2022 ? 11



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▼ PFAS and Fluorinated Compounds in PubChem	?	↗	20,092,587
▶ OECD PFAS definition	?	↗	6,063,764
▶ Organofluorine compounds	?	↗	19,173,213
▶ Other diverse fluorinated compounds	?		106,093
▶ PFAS and fluorinated compound collections	?	↗	1,784,338
▶ PFAS by functional class			6,954,048
▼ Regulatory PFAS collections	?		25,024
▶ Long-chain PFCAs and related substances	?		17,716
▶ PFHxS and related substances	?		649
▶ PFOA and related substances	?		23,696
▶ PFOA and related substances - exclusions	?	↗	68
▶ PFOS and related substances	?		1,301



# Questions – What is “Useful”?

- How to constrain numbers - example of PFHxS

▼ Regulatory PFAS collections

?

25,024

▶ Long-chain PFCAs and related substances

?

17,716

▼ PFHxS and related substances

?

649

▶ [Annex A] PFHxS plus its salts and PFHxS-related compounds as defined in Annex A of the Stockholm Convention

?

↗

589

▶ [EU REACH] PFHxS (linear or branched) plus its salts and related substances according to EU REACH (draft definition)

?

↗

649

▶ Compounds with a (C6F13)S moiety in PubChem by SMARTS

?

649

▶ Compounds with a (C6F13)S(=O)(=O) moiety in PubChem by SMARTS

?

538

▼ Difference between Annex A and EU REACH definitions

?

109

PFHxS in EU REACH but not Annex A - all

?

109

PFHxS in EU REACH but not Annex A - annotation 'Use and Manufacturing'

?

5

PFHxS in EU REACH but not Annex A - annotation 'Use and Manufacturing', 'Literature'

?

11

Compounds that transform to PFHxS (via PubChem Transformations)

?

Initial indicative list of PFHxS plus its salts and PFHxS-related compounds

?

↗

76

PFHxS and any branched isomers (included in PubChem)

?

2

PFHxS and any branched isomers and their salts (included in PubChem)

?

52

PFHxS and branched isomer combined substructure query in PubChem

?

186

Annotation content?

Salt/mixture/ isomer breakdown?

Different definitions?

Annotation content?

Salt/mixture/  
isomer  
breakdown?



# Questions: Cases that are challenging...

- LC-PFCAs ( $C_nF_{2n+1}$  related,  $8 \leq n \leq 20$ )

▼ Long-chain PFCAs and related substances ? 17,716

- ▶ [Draft] Nomination of long-chain PFCAs (draft definition) ? 671
- ▼ Compounds related to long-chain PFCAs [WiP] ? 17,653
  - Merged  $C_nF_{2n+1}$  ( $8 \leq n \leq 20$ ) - partial query ? 14,873
  - Merged  $C_nF_{2n+1}$  ( $8 \leq n \leq 20$ ) mixtures and components - partial query ? 3,357
  - Merged  $C_nF_{2n+1}$  ( $8 \leq n \leq 20$ ) plus salts - partial query ? 16,444
  - Merged  $C_nF_{2n+1}$  ( $8 \leq n \leq 20$ ) same connectivity - partial query ? 9,574
  - Merged  $C_nF_{2n+1}$  ( $8 \leq n \leq 20$ ) same parent and connectivity - partial query ? 10,273
- Compounds that transform to long-chain PFCAs in PubChem (via PubChem Transformations) ? 3
- Draft indicative list of long-chain PFCAs plus their salts and related compounds ? ↗ 83
- Long-chain PFCAs including any branched isomers (included in PubChem) ? 39
- Long-chain PFCAs including any branched isomers and their salts (included in PubChem) ? 171
- Long-chain PFCAs substructure query in PubChem ? 607



# Questions: Cases that are challenging...

- LC-PFCAs ( $C_nF_{2n+1}$  related,  $8 \leq n \leq 20$ )

## PubChem Classification Browser

Help

Browse PubChem data using a classification of interest, or search for PubChem records annotated with the desired classification/term (e.g., MeSH: phenylpropionates, or Gene Ontology: DNA repair). [More...](#)

Select classification

PubChem: PFAS and Fluorinated Compounds in PubChem

Search selected classification by

Keyword

C08F17

Search

Clear

**Classification description (from PubChem)**

A classification tree to browse per- and polyfluoroalkyl substances (PFAS) and other fluorinated compounds in PubChem. The 'OECD PFAS definition' node contains PubChem content matching the OECD PFAS definition of saturated CF2 (Report ENV/CBC/MONO(2021)25 from 9 July 2021). The 'Organofluorine compounds' node contains organofluorine compounds in PubChem as defined in the same report. The 'Other diverse fluorinated compounds' node helps explore a wide variety of other fluorinated compounds. The 'PFAS and fluorinated compound collections' node gathers several collections of PFAS and/or fluorinated compounds from various resources.

Update: 2022-09-12 14:04:56 [More...](#)

Data type counts to display

Display zero count nodes?

View type

Page size

None

Compound

Yes

No

Tree

List

10

20

50

100

200

PubChem: PFAS and Fluorinated Compounds in PubChem Search for KEYWORD C08F17 ✕

Results 1 to 10 of 364

1 2 3 4 5 6 ... 37



# Questions: Cases that are challenging...

- LC-PFCAs ( $C_nF_{2n+1}$  related,  $8 \leq n \leq 20$ )

## PubChem Classification Browser

Browse PubChem data using a classification of interest, or search for PubChem records annotated with the desired classification/term (e.g., DNA repair). [More...](#)

Select classification

PubChem: PFAS and Fluorinated Compounds in PubChem

Search selected classification by

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Update: 2022-09-12 14:04:56 [More...](#)

Data type counts to display

Display zero count nodes?

View type

Page size

None Compound Yes No

Tree List

10 20 50 100 200

PubChem: PFAS and Fluorinated Compounds in PubChem Search for KEYWORD C08F17

Results 1 to 10 of 364

Molecule contains PFAS parts larger than CF2/CF3	?	222,342
Breakdown by isolated PFAS part count	?	222,342
Contains 01 isolated PFAS part	?	167,552
Count of molecules 01001-10000	?	34,792
Contains 01xC08F17-linear		9,120
Contains 02 isolated PFAS parts	?	38,263
Count of molecules 00001-10	?	1,531
Contains isolated branched PFAS part	?	351
Contains 01xC03F07-linear,01xC08F17-branched		1
Contains 01xC06F11-branched,01xC08F17-linear		1
Contains 01xC08F17-linear,01xC09F19-branched		1
Contains 01xCF3,01xC08F17-branched		4
Contains isolated linear PFAS part	?	976
Contains 01xC03F05-unsaturated-linear,01xC08F17-linear		1
Contains 01xC03F07-linear,01xC08F17-branched		1
Contains 01xC04F07-unsaturated-linear,01xC08F17-linear		1
Contains 01xC04F08-linear,01xC08F17-linear		5
Contains 01xC05F11-linear,01xC08F17-linear		4
Contains 01xC07F14-linear,01xC08F17-linear		3
Contains 01xC08F16-linear,01xC08F17-linear		10
Contains 01xC08F17-linear,01xC09F19-linear		4
Contains 01xC08F17-linear,01xC10F20-linear		2



# Questions: Cases that are challenging...

- LC-PFCAs ( $C_nF_{2n+1}$  related,  $8 \leq n \leq 20$ )

What about  $F \neq 2n+1$ ?  
Branched, cyclic, unsaturated?

## PubChem Classification

Browse PubChem data using a classification (e.g., DNA repair). More...

Select classification

PubChem: PFAS and Fluorinated Compounds

Classification

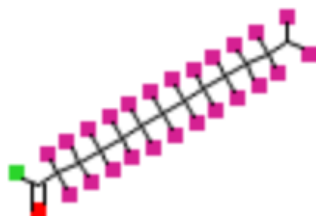
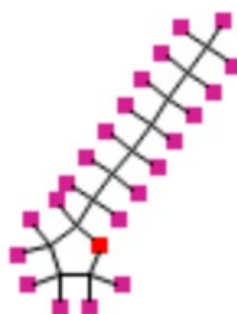
A classification  
definition  
diverse  
compounds  
Updated

Data type

Normal

PubChem

Results



Count of molecules 00101-1000 ? 8,490

- Contains isolated branched PFAS part ? 1,825
- Contains isolated cyclic PFAS part ? 1,346
- Contains isolated linear PFAS part ? 4,864

Contains 01xC03F05-linear 318

Contains 01xC04F07-linear 104

Contains 01xC05F09-linear 383

Contains 01xC08F16-linear 851

Contains 01xC09F18-linear 364

Contains 01xC09F19-linear 704

Contains 01xC10F20-linear 264

Contains 01xC11F22-linear 128

Contains 01xC11F23-linear 486

Molecule contains PFAS parts larger than CF2/CF3 ? 222,342

Breakdown by isolated PFAS part count ? 222,342

Contains 01 isolated PFAS part ? 167,552

Count of molecules 01001-10000 ? 34,792

Contains 01xC08F17-linear 9,120

Contains 02 isolated PFAS parts ? 38,263

Count of molecules 00001-10 ? 1,531

Contains isolated branched PFAS part ? 351

Contains 01xC03F07-linear,01xC08F17-branched 1

Contains 01xC06F11-branched,01xC08F17-linear 1

Contains 01xC08F17-linear,01xC09F19-branched 1

Contains 01xCF3,01xC08F17-branched 4

Contains isolated linear PFAS part ? 976

Contains 01xC03F05-unsaturated-linear,01xC08F17-linear 1

Contains 01xC03F07-linear,01xC08F17-branched 1

Contains 01xC04F07-unsaturated-linear,01xC08F17-linear 1

Contains 01xC04F08-linear,01xC08F17-linear 5

Contains 01xC05F11-linear,01xC08F17-linear 4

Contains 01xC07F14-linear,01xC08F17-linear 3

Contains 01xC08F16-linear,01xC08F17-linear 10

Contains 01xC08F17-linear,01xC09F19-linear 4

Contains 01xC08F17-linear,01xC10F20-linear 2



# Questions: Cases that are challenging - Exclusions

- (b) Compounds related to long-chain PFCAs which, in the proposal, are defined as any substance that is a precursor and **may degrade or transform to long-chain PFCAs**, where the perfluorinated alkyl moiety has the formula  $C_nF_{2n+1}$  (where  $8 \leq n \leq 20$ ) and is directly bonded to any **chemical moiety other than a fluorine, chlorine or bromine atom**

*Requires exclusions ...  
plus many strange cases...*

▼ Other diverse fluorinated compounds	?	193
▼ Contains fluorine bond to non-carbon element	?	5
▼ Count of molecules 00101-1000	?	2
▶ Contains a F-Ge bond	2	
▼ Count of molecules 10001-100000	?	3
▶ Contains a F-B bond	3	

▼ Contains non-organic element	?	193
▶ Count of molecules 00101-1000	?	19
▼ Count of molecules 01001-10000	?	97
▶ Contains Al atom	5	
▶ Contains As atom	11	
▶ Contains Ge atom	30	
▶ Contains Se atom	22	
▶ Contains Sn atom	29	
▼ Count of molecules 10001-100000	?	80
▶ Contains B atom	80	



# Questions: Cases that are challenging – Exclusions (PFOA)

- The following compounds are **not** included as PFOA-related compounds:
  - (i) C<sub>8</sub>F<sub>17</sub>-X, where X= F, Cl, Br;
  - (ii) Fluoropolymers that are covered by CF<sub>3</sub>[CF<sub>2</sub>]<sub>n</sub>-R', where R'=any group, n>16;
  - (iii) Perfluoroalkyl carboxylic and phosphonic acids (including their salts, esters, halides and anhydrides) with ≥8 perfluorinated carbons;
  - (iv) Perfluoroalkane sulfonic acids (including their salts, esters, halides and anhydrides) with ≥9 perfluorinated carbons;
  - (v) Perfluorooctane sulfonic acid (PFOS), its salts and perfluorooctane sulfonyl fluoride (PFOSF), as listed in Annex B to the Convention.



# Questions: Cases that are challenging – Exclusions (PFOA)

- PFOA

▼ PFOA and related substances - exclusions ? ↗ 68

▼ C8F17-X where X=F, Cl, Br ? ↗ 26

C8F17-X where X=Br ? ↗ 2

C8F17-X where X=Cl ? ↗ 4

C8F17-X where X=F ? ↗ 20

Fluoropolymers CF<sub>3</sub>[CF<sub>2</sub>]<sub>n</sub>-R where n>16 and R=any [WiP] ? ↗

PFCAs and PFPAs (plus salts, esters, halides and anhydrides) with 8+ perfluorocarbons [WiP] ? ↗

PFOS plus its salts and PFOSF as listed in Annex B of the Stockholm Convention ? ↗ 8

PFSAAs (plus salts, esters, halides and anhydrides) with 9+ perfluorocarbons [WiP] ? ↗

Updated indicative list of substances not covered by the PFOA listing ? ↗ 35



# Future topic: Expanding to Polymers/UVCBs

*Functionality under  
development at  
PubChem*

## Poly(vinyl chloride)

See also:  [Vinyl Chloride](#) (related).

**PubChem CID** Not available because this is not a discrete structure.

**Molecular Formula** (C<sub>2</sub>H<sub>3</sub>Cl)<sub>n</sub>

Polyvinyl chloride latex is a viscous white liquid. A 51% by mass emulsion of polyvinyl chloride in water. (NTP, 1992)

► [CAMEO Chemicals](#)

▼ S80   PFASGLUEGE   Overview of PFAS Uses	?	1,250
▼ PFAS Polymer Type	?	489
Non-polymer	?	487
Polymer	?	1
Unclear	?	1
► PFAS Structural Category	?	1,230
► PFAS Use Category	?	489
► Use Type Information Source	?	489





Recap:

# PubChem PFAS Tree



▼ PFAS and Fluorinated Compounds in PubChem	?	↗	19,721,046
▶ OECD PFAS definition	?	↗	6,213,365
▶ Organofluorine compounds	?	↗	19,567,903
▶ Other diverse fluorinated compounds	?		114,887
▶ PFAS and fluorinated compound collections	?	↗	1,788,643
▼ Regulatory PFAS collections	?		25,838
▶ Long-chain PFCAs (LC-PFCAs) and related substances	?		18,400
▶ PFHxS and related substances	?		651
▶ PFOA and related substances	?		24,474
▶ PFOA and related substances - exclusions	?	↗	68
▶ PFOS and related substances	?		1,301

*PubChem PFAS Tree enhanced  
with regulatory collections*

*Now publicly available*

*Feedback welcome!*

*Twitter updates: [@ESchymanski](https://twitter.com/ESchymanski)*



*Documentation:*

<https://pubchem.ncbi.nlm.nih.gov/classification/#hid=120>



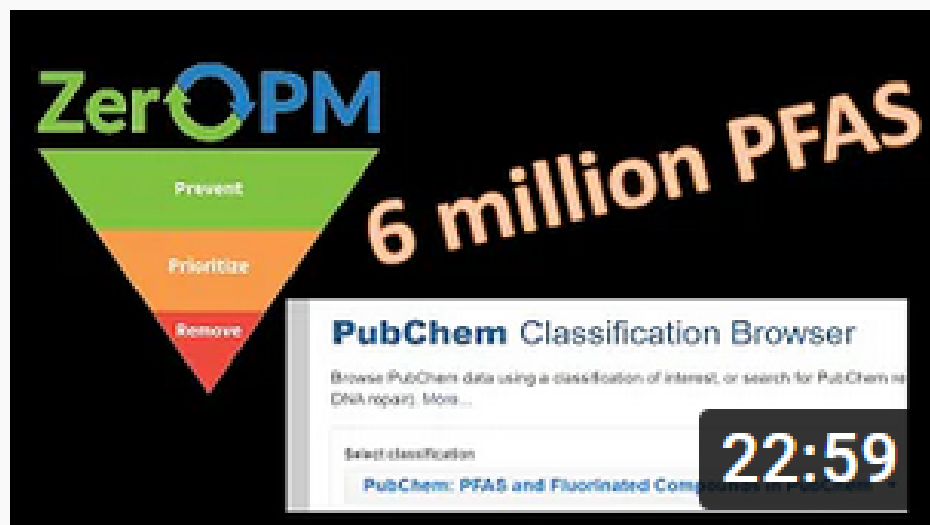
# YouTube video with more information:



▼ PFAS and Fluorinated Compounds in PubChem ? ↗ 19,405,136

▼ OECD PFAS definition ? ↗ 6,094,616

- ▶ Molecule contains isolated CF2 ? 586,112
- ▶ Molecule contains isolated CF
- ▶ Molecule contains isolated C(F)F<sub>2</sub>
- ▶ Organofluorine compounds
- ▶ Other diverse fluorinated compounds
- ▼ PFAS and Fluorinated Compounds in PubChem
- ▶ Compound is a PFAS ? 1,777,052
- ▶ Other fluorinated chemical content in PubChem ? ↗ 1,674
- NIST PFAS suspect list ? ↗ 4,948



Navigating over 6 million PFAS! A wa...

ZeroPM - H2020  
367 views •  
2 months ago



<https://pubchem.ncbi.nlm.nih.gov/classification/#hid=120>



# Acknowledgements & Questions?

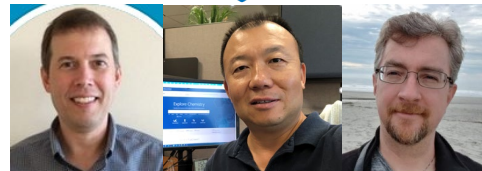
Email: [emma.schymanski@uni.lu](mailto:emma.schymanski@uni.lu)

Twitter: [@ESchymanski](https://twitter.com/ESchymanski)

Slides here:



## PubChem



NIH U.S. National Library of Medicine  
National Center for Biotechnology Information

Evan Bolton, Jeff Zhang,  
Paul Thiessen + the team  
[@EvanBolton](https://twitter.com/EvanBolton) [@pubchem](https://twitter.com/pubchem)

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Medicine (NLM), National Institutes of Health

NIH U.S. National Library of Medicine  
National Center for Biotechnology Information

PubChem

norman

MassBank  
High Quality Mass Spectral Database

UNIVERSITY OF  
COPENHAGEN

Stockholm  
University  
KEMI

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WASHINGTON

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Baudirektion  
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Gewässerschutz

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