



# Are there really 6 million PFAS in PubChem?

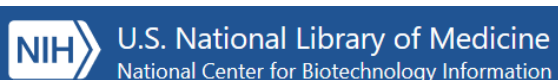


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National Library of Medicine, National Institutes of Health



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zenodo.7756622](https://doi.org/10.5281/zenodo.7756622)

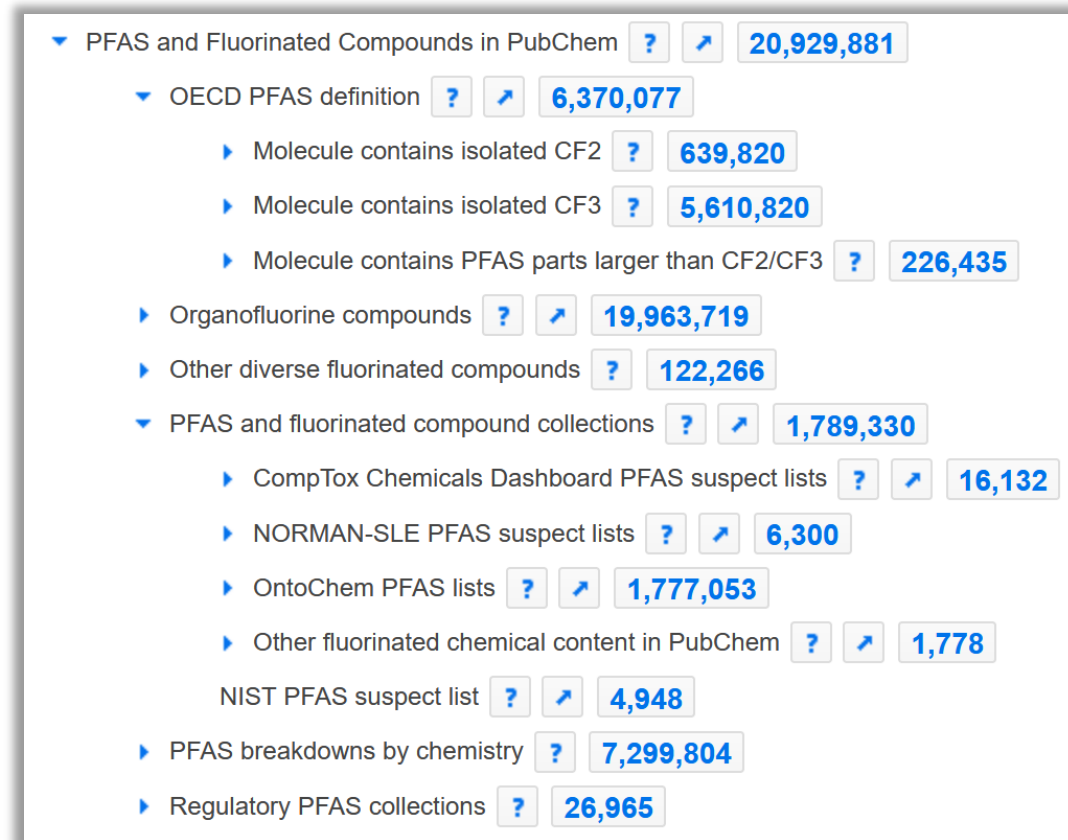


# No...it's already **7 million!**

▼ PFAS and Fluorinated Compounds in PubChem	?	↗	20,929,881
▶ OECD PFAS definition	?	↗	6,370,077
▶ Organofluorine compounds	?	↗	19,963,719
▶ Other diverse fluorinated compounds	?		122,266
▶ PFAS and fluorinated compound collections	?	↗	1,789,330
▶ PFAS breakdowns by chemistry	?		7,299,804
▶ Regulatory PFAS collections	?		26,965

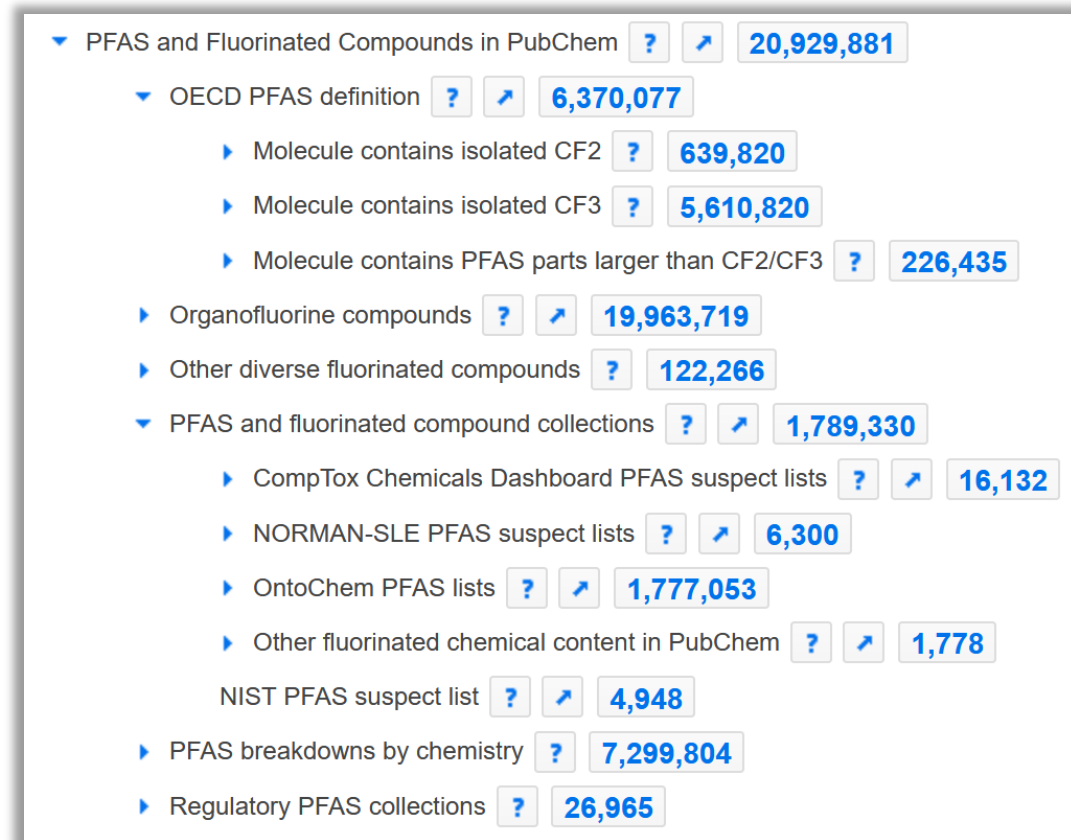
# Outline

- Background and Motivation
- PubChem PFAS Tree
  - OECD PFAS & organofluorine compounds
  - PFAS suspect lists
  - Regulatory PFAS collections
  - PFAS breakdown by chemistry
- How many PFAS are really “out there”?
- Questions / Discussion



# Outline

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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

114M Compounds 302M Substances 304M Bioactivities 35M Literature 908 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

Gene

PFOA

Ptma

PFOS

Ptpa

PFDA

Pura

## Explore Chemistry

Quickly find chemical information from authoritative sources

335-67-1

Compound

Gene

Taxonomy

335-67-1

snoRNA:Me285-C3351

Prevotella buccae ATCC 33574

335161-24-5

zinc finger protein 335

335621-00-6

CG3356

335161-19-8

CG33557

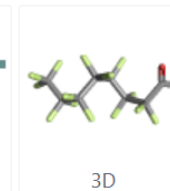
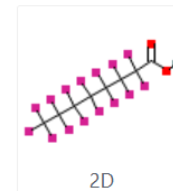
COMPOUND SUMMARY

## Perfluorooctanoic acid

PubChem CID

9554

Structure



Find Similar Structures

Chemical Safety



Corrosive



Irritant



Health Hazard

Laboratory Chemical Safety Summary (LCSS) Datasheet

Molecular Formula

$C_8HF_{15}O_2$

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

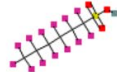
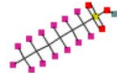
PubChem Compound TOC ? 65,945,956

- Agrochemical Information ? 3,090
- Associated Disorders and Diseases ? 29,990**
- Biologic Description ? 2,464,499
- Biological Test Results ? 4,497,660
- Chemical and Physical Properties ? 267,837
- Classification ? 22,519,643
- Drug and Medication Information ? 19,108
- Food Additives and Ingredients ? 7,330
- Identification ? 4,679
- Information Sources ? 45,543,994
- Interactions and Pathways ? 204,199
- Literature ? 2,093,924
- Names and Identifiers ? 4,974,374
- Patents ? 38,011,045
- Pharmacology and Biochemistry ? 113,370
- Related Records ? 13,106,996
- Safety and Hazards ? 171,124
- Spectral Information ? 1,535,927
- Structures ? 11,758,915
- Toxicity ? 116,629
- Use and Manufacturing ? 105,669**

## 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 sc
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 \(HSDB\)](#)

<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 Suspect List Exchange

The NORMAN Suspect List Exchange (NORMAN-SLE) was established in 2013 to facilitate the exchange of information on suspected substances. The NORMAN-SLE documents all individual collections of substances (see Source column in SusDat). NORMAN-SLE versions are available for download. Comments and contributions are welcome - please email us at [nds@norman-network.com](mailto:nds@norman-network.com). Please refer to our [documentation](#) pages for: [citation](#) instructions.

No.	Abbreviation	Description	Link
S0	SUSDAT	<b>Merged NORMAN Suspect List: SusDat</b>	<a href="#">Introduction</a>

### Antibiotic Resistance Bacteria/Genes

A database of ARBs/ARGs in environmental matrices

Mohammed Taha *et al.* (2022) DOI: [10.1186/s12302-022-00680-6](https://doi.org/10.1186/s12302-022-00680-6)

## RESEARCH

Open Access



# The NORMAN Suspect List Exchange (NORMAN-SLE): facilitating European and worldwide collaboration on suspect screening in high resolution mass spectrometry

Hiba Mohammed Taha<sup>1</sup>, Reza Aalizadeh<sup>2</sup>, Nikiforos Alygizakis<sup>3,2</sup>, Jean-Philippe Antignac<sup>4</sup>, Hans Peter H. Arp<sup>5,6</sup>, Richard Bade<sup>7</sup>, Nancy Baker<sup>8</sup>, Lidia Belova<sup>9</sup>, Lubertus Bijlsma<sup>10</sup>, Evan E. Bolton<sup>11</sup>, Werner Brack<sup>12,13</sup>, Alberto Celma<sup>10,14</sup>, Wen-Ling Chen<sup>15</sup>, Tiejun Cheng<sup>11</sup>, Parviel Chirsir<sup>1</sup>, Ľuboš Čirka<sup>16,3</sup>, Lisa A. D'Agostino<sup>17</sup>, Yannick Djoumbou Feunang<sup>18</sup>, Valeria Dulio<sup>19</sup>, Stellan Fischer<sup>20</sup>, Pablo Gago-Ferrero<sup>21</sup>, Aikaterini Galani<sup>2</sup>, Birgit Geueke<sup>22</sup>, Natalia Glowacka<sup>3</sup>, Juliane Glüge<sup>23</sup>, Ksenia Groh<sup>24</sup>, Sylvia Grosse<sup>25</sup>, Peter Haglund<sup>26</sup>, Pertti J. Hakkinen<sup>11</sup>, Sarah E. Hale<sup>5</sup>, Felix Hernandez<sup>10</sup>, Elisabeth M.-L. Janssen<sup>24</sup>, Tim Jonkers<sup>27</sup>, Karin Kiefer<sup>24</sup>, Michal Kirchner<sup>28</sup>, Jan Koschorreck<sup>29</sup>, Martin Krauss<sup>12</sup>, Jessy Krier<sup>1</sup>, Marja H. Lamoree<sup>27</sup>, Marion Letzel<sup>30</sup>, Thomas Letzel<sup>31</sup>, Qingliang Li<sup>11</sup>, James Little<sup>32</sup>, Yanna Liu<sup>33</sup>, David M. Lunderberg<sup>34,35</sup>, Jonathan W. Martin<sup>17</sup>, Andrew D. McEachran<sup>36</sup>, John A. McLean<sup>37</sup>, Christiane Meier<sup>29</sup>, Jeroen Meijer<sup>38</sup>, Frank Menger<sup>14</sup>, Carla Merino<sup>39,40</sup>, Jane Muncke<sup>22</sup>, Matthias Muschket<sup>12</sup>, Michael Neumann<sup>29</sup>, Vanessa Neveu<sup>41</sup>, Kelsey Ng<sup>3,42</sup>, Herbert Oberacher<sup>43</sup>, Jake O'Brien<sup>7</sup>, Peter Oswald<sup>3</sup>, Martina Oswaldova<sup>3</sup>, Jaqueline A. Picache<sup>37</sup>, Cristina Postigo<sup>44,14</sup>, Noelia Ramirez<sup>45,39</sup>, Thorsten Reemtsma<sup>12</sup>, Justin Renaud<sup>46</sup>, Pawel Rostkowski<sup>47</sup>, Heinz Rüdell<sup>48</sup>, Reza M. Salek<sup>41</sup>, Saer Samanipour<sup>49</sup>, Martin Scherlinger<sup>23,42</sup>, Ivo Schliebner<sup>29</sup>, Wolfgang Schulz<sup>50</sup>, Tobias Schulze<sup>12</sup>, Manfred Sengl<sup>30</sup>, Benjamin A. Shoemaker<sup>11</sup>, Kerry Sims<sup>51</sup>, Heinz Singer<sup>24</sup>, Randolph R. Singh<sup>1,52</sup>, Mark Sumarah<sup>46</sup>, Paul A. Thiessen<sup>11</sup>, Kevin V. Thomas<sup>7</sup>, Sonia Torres<sup>39</sup>, Xenia Trier<sup>53</sup>, Annemarie P. van Wezel<sup>54</sup>, Roel C. H. Vermeulen<sup>38</sup>, Jelle J. Vlaanderen<sup>38</sup>, Peter C. von der Ohe<sup>29</sup>, Zhanyun Wang<sup>55</sup>, Antony J. Williams<sup>56</sup>, Egon L. Willighagen<sup>57</sup>, David S. Wishart<sup>58</sup>, Jian Zhang<sup>11</sup>, Nikolaos S. Thomaidis<sup>2</sup>, Juliane Hollender<sup>23,24</sup>, Jaroslav Slobodnik<sup>3</sup> and Emma L. Schymanski<sup>1</sup>



### SEARCH All Databases

Searching for individual substance or group(s) of substances

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



### 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



# NORMAN Suspect List Exchange 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.

<b>Organization</b>	NORMAN Network (c/o UniLu)
<b>Category</b>	Research and Development
<b>URL</b>	<a href="https://www.norman-network.com/nds/SLE/">https://www.norman-network.com/nds/SLE/</a>
<b>License Note</b>	Data: CC-BY 4.0; Code (hosted by ECI, LCSB): Artistic-2.0
<b>License URL</b>	<a href="https://creativecommons.org/licenses/by/4.0/">https://creativecommons.org/licenses/by/4.0/</a>
<b>Contact Name</b>	Emma Schymanski
<b>Address</b>	6 avenue du Swing, Belvaux, Luxembourg, 4367
<b>Data Source ID</b>	23819
<b>Data in PubChem</b>	117,553 Live Substances 20,587 Annotations 1 Classification
<b>Last Updated</b>	2023/03/15

NORMAN Suspect List Exchange Classification ? ↗ 114,059

- ▶ S13 | EUCOSMETICS | Combined Inventory of Ingredients Employed in Cosmetic Products (2000) and Revised Inventory (2006) ? 3,766
- ▶ S25 | OECDPFAS | List of PFAS from the OECD ? 3,678
- ▶ S36 | UBAPMT | ...
- ▶ S47 | ECHAPLA | ...
- ▶ S50 | CCSCOMP | ...
- ▶ S60 | SWISSPES | ...
- ▶ S61 | UJICCSLIE | ...
- ▶ S66 | EAWAGTP | ...
- ▶ S68 | HSDBTPS | ...
- ▶ S69 | LUXPEST | ...
- ▶ S72 | NTUPHTW | ...
- ▶ S75 | CyanoMett | ...
- ▶ S77 | FCCDB | ...
- ▶ S79 | UACCSCE | ...
- ▶ S80 | PFASGLUEGE | Overview of PFAS Uses ? 1,251
- ▶ S00 | SUSDAT | Merged NORMAN Suspect List: SusDat ? 98,145
- ▶ S01 | MASSBANK | NORMAN Compounds in MassBank EU ? 7,117
- ▶ S02 | STOFFIDENT | HSWT/LfU STOFF-IDENT Database of Water-Relevant Substances ? 11,239
- ▶ S03 | NORMANCT15 | NORMAN Collaborative Trial Targets and Suspects ? 624
- ▶ S04 | UJIBADE | Target List from UJI used in Bade et al 2015 ? 541

S09 | PFASTRIER | PFAS Suspect List of fluorinated substances from X. Trier and colleagues ? 474

S14 | KEMIPFAS | PFAS Highly Fluorinated Substances List from KEMI ? 1,338

S25 | OECDPFAS | List of PFAS from the OECD ? 3,645

S46 | PFASNTREV19 | List of PFAS reported in Non-Target HRMS Studies from Liu et al 2019 ? 680

S80 | PFASGLUEGE | Overview of PFAS Uses ? 988

S89 | PRORISKPFAS | List of PFAS Compiled from NORMAN SusDat ? 4,269

S90 | ZEROPMBOX1 | ZeroPM Box 1 Substances ? 38

S95 | PFASANEXCH | PFAS List from the NORMAN PFAS Analytical Exchange Activity ? 93

S96 | ECIPFAS | Updatable List to add PFAS Structures to Public Resources from ECI (UniLu) ? 257

S100 | PFASREACH | List of PFAS identified in REACH 2019 ? 432

S102 | PARCPFAS | List of PFAS from PARC WP4 ? 190

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

## Environmental Science Processes & Impacts



PAPER

View Article Online  
View Journal | View Issue

Check for updates

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>id</sup>\*<sup>a</sup> Martin Scheringer,<sup>id</sup><sup>a</sup> Ian T. Cousins,<sup>id</sup><sup>b</sup> Jamie C. DeWitt,<sup>c</sup> Gretta Goldenman,<sup>d</sup> Dorte Herzke,<sup>id</sup><sup>ef</sup> Rainer Lohmann,<sup>id</sup><sup>g</sup> Carla A. Ng,<sup>id</sup><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>





# FAIRifying PFAS – Bugsel *et al.* (2022) – new PFAS & data

Analytical and Bioanalytical Chemistry (2022) 414:1217–1225  
<https://doi.org/10.1007/s00216-021-03463-9>

RESEARCH PAPER



## LC-HRMS screening of per- and polyfluorinated alkyl substances (PFAS) in impregnated paper samples and contaminated soils

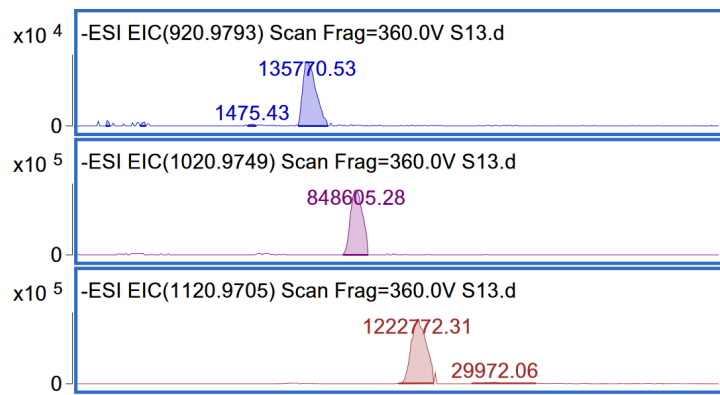
Boris Bugsel<sup>1</sup> · Rebecca Bauer<sup>1</sup> · Florian Herrmann<sup>2</sup> · Martin E. Maier<sup>2</sup> · Christian Zwiener<sup>1</sup>

Received: 9 April 2021 / Revised: 1 June 2021 / Accepted: 8 June 2021 / Published online: 8 July 2021  
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### Abstract

High per- and polyfluorinated alkyl substance (PFAS) concentrations have been detected in agricultural soils in Southwest Germany. Discharges of PFAS-contaminated paper sludge and compost are suspected to be the cause of the contamination. Perfluorinated carboxylic acids (PFCAs) have been detected also in groundwater, drinking water, and plants in this area. Recently, previously unknown compounds have been identified by high-resolution mass spectrometry (HRMS). Major contaminants were polyfluorinated dialkylated phosphate esters (diPAPs) and N-ethyl perfluorooctane sulfonamide ethanol-based phosphate diester (diSAmPAP). In this study, HRMS screening for PFAS was applied to 14 soil samples from the contaminated area and 14 impregnated paper samples which were from a similar period than the contamination. The paper samples were characterized by diPAPs (from 4:2/6:2 to 12:2/12:2), fluorotelomer mercapto alkyl phosphates (FTMAPs; 6:2/6:2 to 10:2/10:2), and diSAmPAP. In soil samples, diPAPs and their transformation products (TPs) were the major contaminants, but also FTMAPs, diSAmPAP, and their TPs occurred. The distribution patterns of the carbon chain lengths of the precursor PFAS in soil samples were shown to resemble those in paper samples. This supports the hypothesis that paper sludge is a major source of contamination. The presence of major degradation products like PFCAs, FTSA, or PFOS and their distribution of carbon chain lengths indicate the activity of biotic or abiotic degradation processes and selective leaching processes from the upper soil horizons.

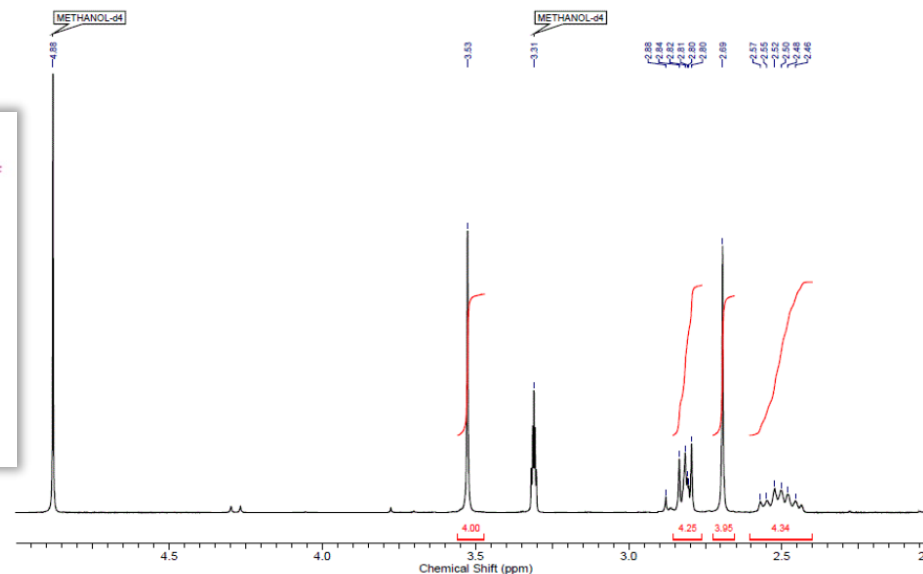
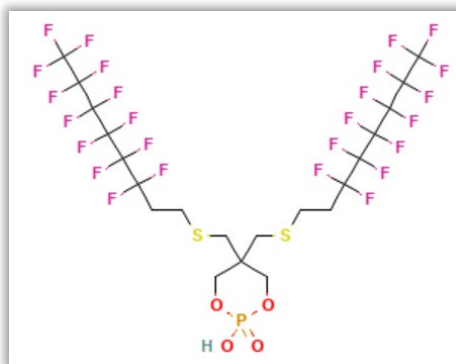
**Fig. 2** Extracted ion chromatograms for four FTMAPs in soil sample S13 (5-ppm window). 6:2/6:2 FTMAP (m/z 920.9812) was identified with the synthesized standard; further FTMAP homologues are characterized by the repeating unit C<sub>2</sub>F<sub>4</sub> (Δ m/z 99.9936) and a systematic retention time shift



## PubChem 6:2 FTMAP (Compound)

### Reference for Source

B Bugsel, R Bauer, F Herrmann, ME Maier, C Zwiener (2022) Analytical and Bioanalytical Chemistry, 414, 1217-1225 [doi:10.1007/s00216-021-03463-9](https://doi.org/10.1007/s00216-021-03463-9)



### Reference for Dataset

S74 | REFTPS | Transformation Products and Reactions from Literature  
[doi:10.5281/zenodo.4318838](https://doi.org/10.5281/zenodo.4318838)

► NORMAN Suspect List Exchange



# Motivation: Revised PFAS Definition in OECD 2021 Monograph



Organisation for Economic Co-operation and Development

ENV/CBC/MONO(2021)25

Unclassified

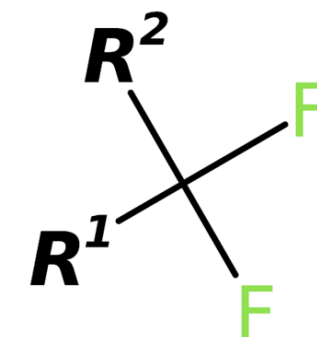
English - Or. English

9 July 2021

ENVIRONMENT DIRECTORATE  
CHEMICALS AND BIOTECHNOLOGY COMMITTEE

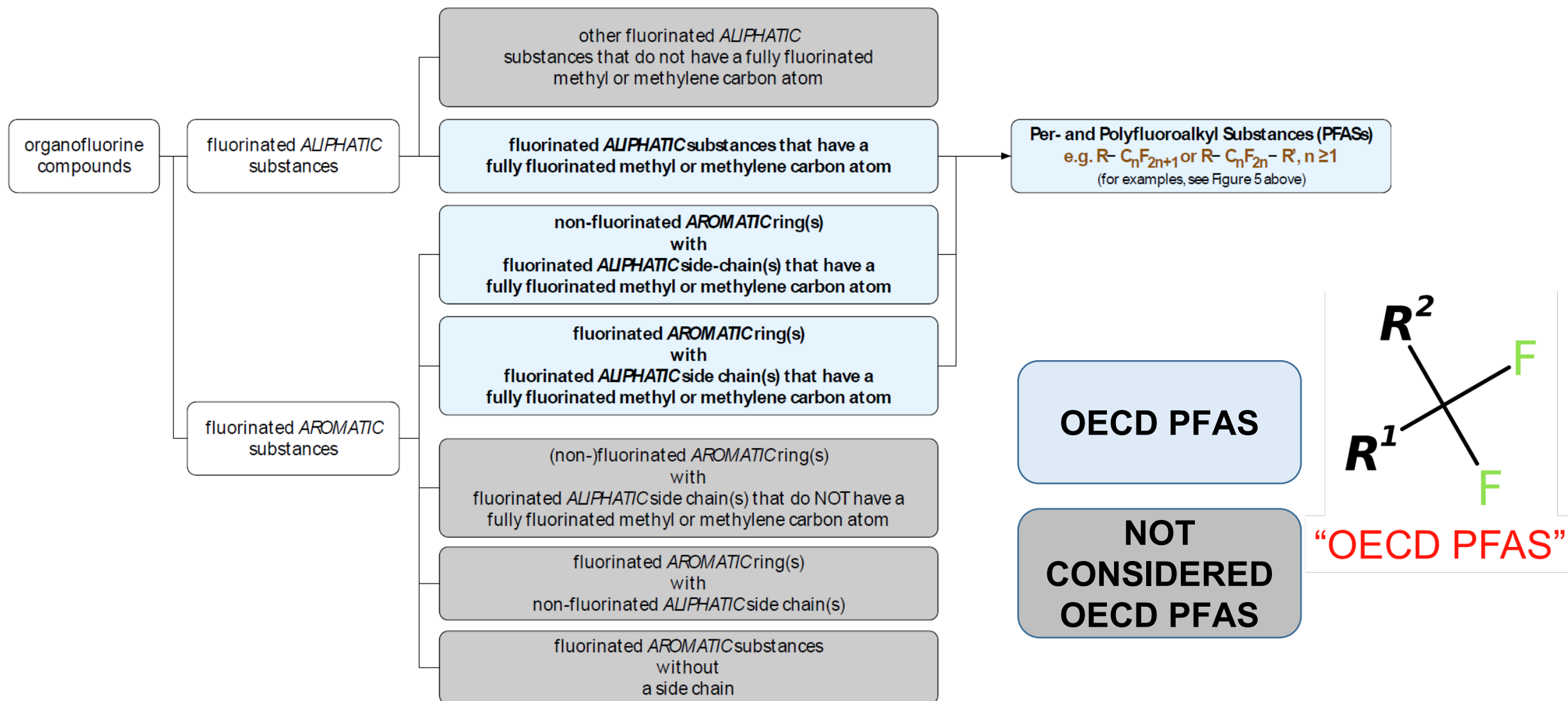
Reconciling Terminology of the Universe of Per- and Polyfluoroalkyl Substances:  
Recommendations and Practical Guidance

Series on Risk Management  
No.61



“OECD PFAS”

# 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

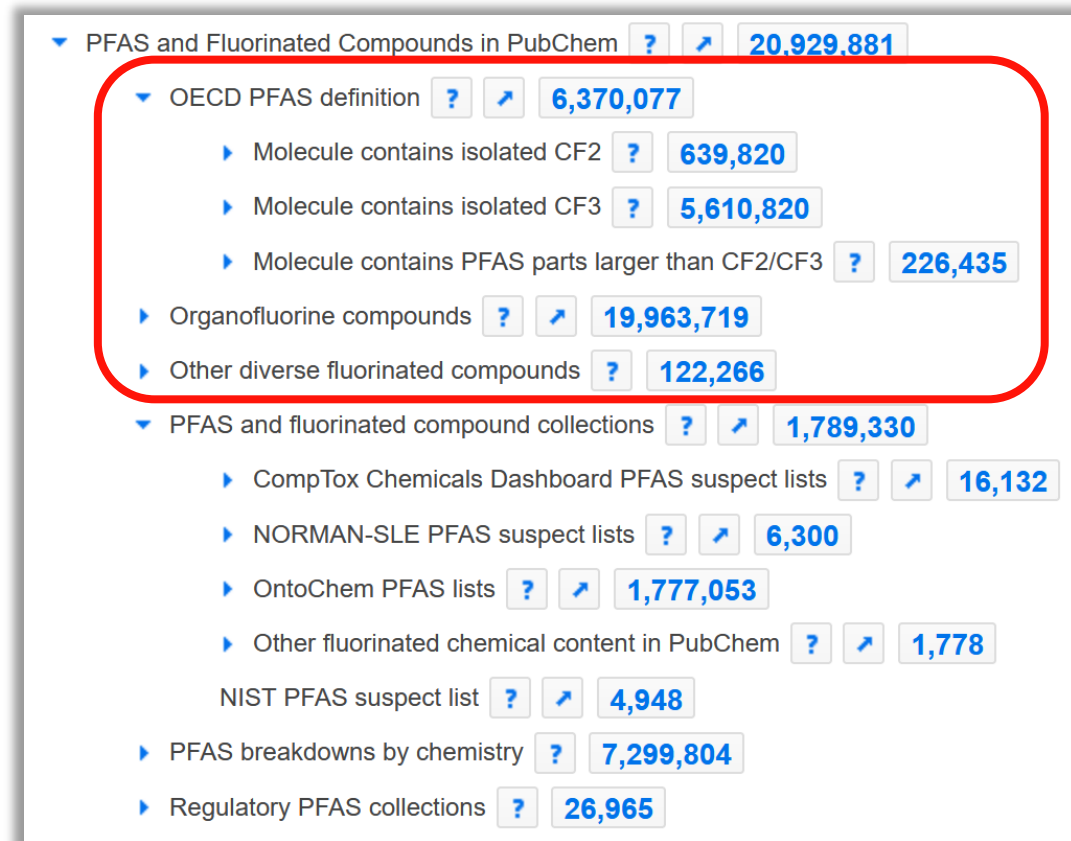
Draw Structure Upload ID List Browse Data Periodic Table

114M Compounds 302M Substances 304M Bioactivities 35M Literature 908 Data Sources

See More Statistics > Explore Data Sources >

# Outline

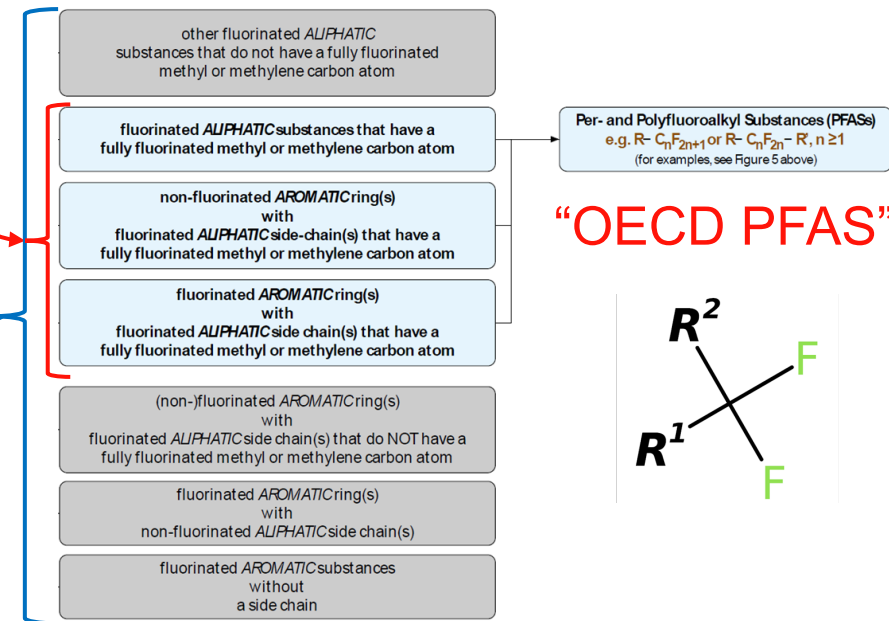
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- How many PFAS are really “out there”?
- Questions / Discussion



# The PubChem PFAS Tree



- PFAS and Fluorinated Compounds in PubChem ? ↗ 20,929,881
  - OECD PFAS definition ? ↗ 6,370,077
    - Molecule contains isolated CF<sub>2</sub> ? 639,820
    - Molecule contains isolated CF<sub>3</sub> ? 5,610,820
    - Molecule contains PFAS parts larger than CF<sub>2</sub>/CF<sub>3</sub> ? 226,435
  - Organofluorine compounds ? ↗ 19,963,719
    - Fluorinated aliphatic substances ? 880,258
    - Fluorinated aromatic substances ? 19,012,193
    - Other fluorinated substances ? 95,325
  - Other diverse fluorinated compounds ? 122,266
    - Contains fluorine bond to non-carbon element ? 27,786
    - Contains non-organic element ? 121,181
  - PFAS and fluorinated compound collections ? ↗ 1,789,330



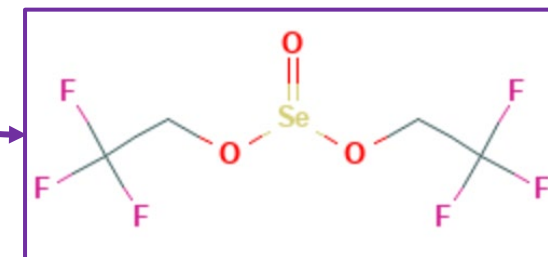
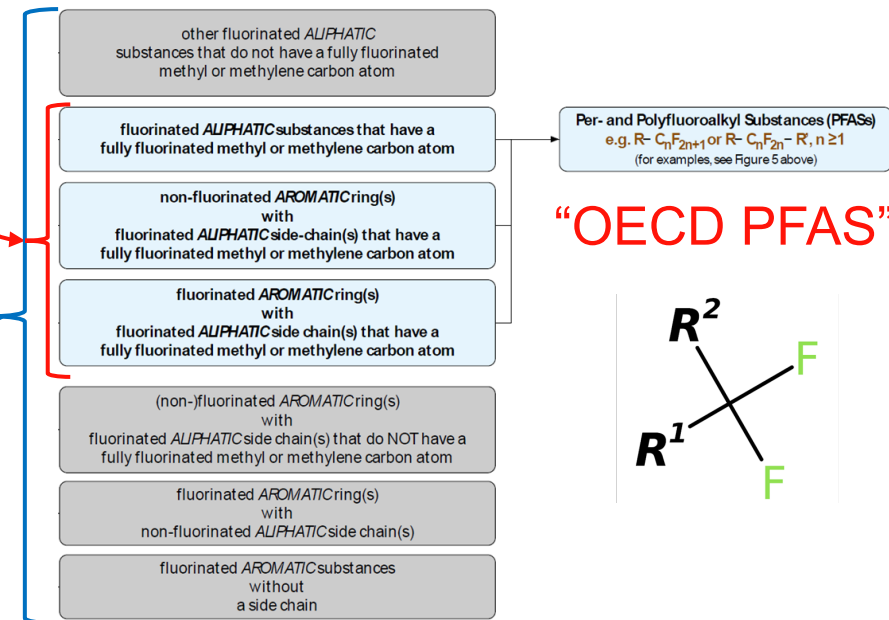
OECD Monograph [ENV/CBC/MONO\(2021\)25](#) (9 July 2021)



# The PubChem PFAS Tree



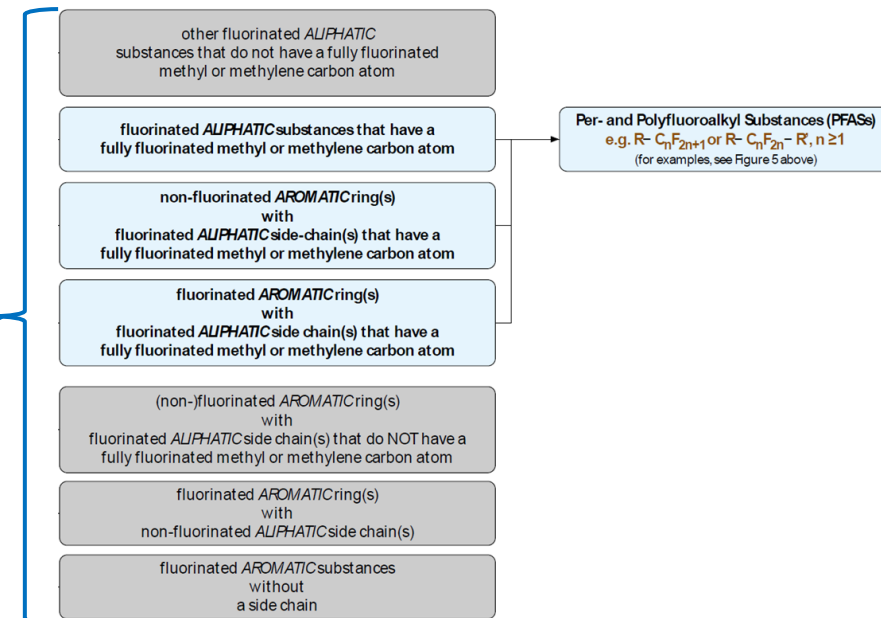
- ▼ PFAS and Fluorinated Compounds in PubChem ? ↗ **20,929,881**
  - ▼ OECD PFAS definition ? ↗ **6,370,077**
    - ▶ Molecule contains isolated CF<sub>2</sub> ? **639,820**
    - ▶ Molecule contains isolated CF<sub>3</sub> ? **5,610,820**
    - ▶ Molecule contains PFAS parts larger than CF<sub>2</sub>/CF<sub>3</sub> ? **226,435**
  - ▼ Organofluorine compounds ? ↗ **19,963,719**
    - ▶ Fluorinated aliphatic substances ? **880,258**
    - ▶ Fluorinated aromatic substances ? **19,012,193**
    - ▶ Other fluorinated substances ? **95,325**
  - ▼ Other diverse fluorinated compounds ? **122,266**
    - ▶ Contains fluorine bond to non-carbon element ? **27,786**
    - ▶ Contains non-organic element ? **121,181**
  - ▶ PFAS and fluorinated compound collections ? ↗ **1,789,330**



# The PubChem PFAS Tree - Organofluorine



- ▼ PFAS and Fluorinated Compounds in PubChem ? ↗ 20,929,881
  - ▼ OECD PFAS definition ? ↗ 6,370,077
    - ▶ Molecule contains isolated CF<sub>2</sub> ? 639,820
    - ▶ Molecule contains isolated CF<sub>3</sub> ? 5,610,820
    - ▶ Molecule contains PFAS parts larger than CF<sub>2</sub>/CF<sub>3</sub> ? 226,435
  - ▼ Organofluorine compounds ? ↗ 19,963,719
    - ▶ Fluorinated aliphatic substances ? 880,258
    - ▶ Fluorinated aromatic substances ? 19,012,193
    - ▶ Other fluorinated substances ? 95,325
  - ▼ Other diverse fluorinated compounds ? 122,266
    - ▶ Contains fluorine bond to non-carbon element ? 27,786
    - ▶ Contains non-organic element ? 121,181
  - ▶ PFAS and fluorinated compound collections ? ↗ 1,789,330



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# >19 M Organofluorine compounds in PubChem

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



▼ Organofluorine compounds ? ↗ 19,963,719

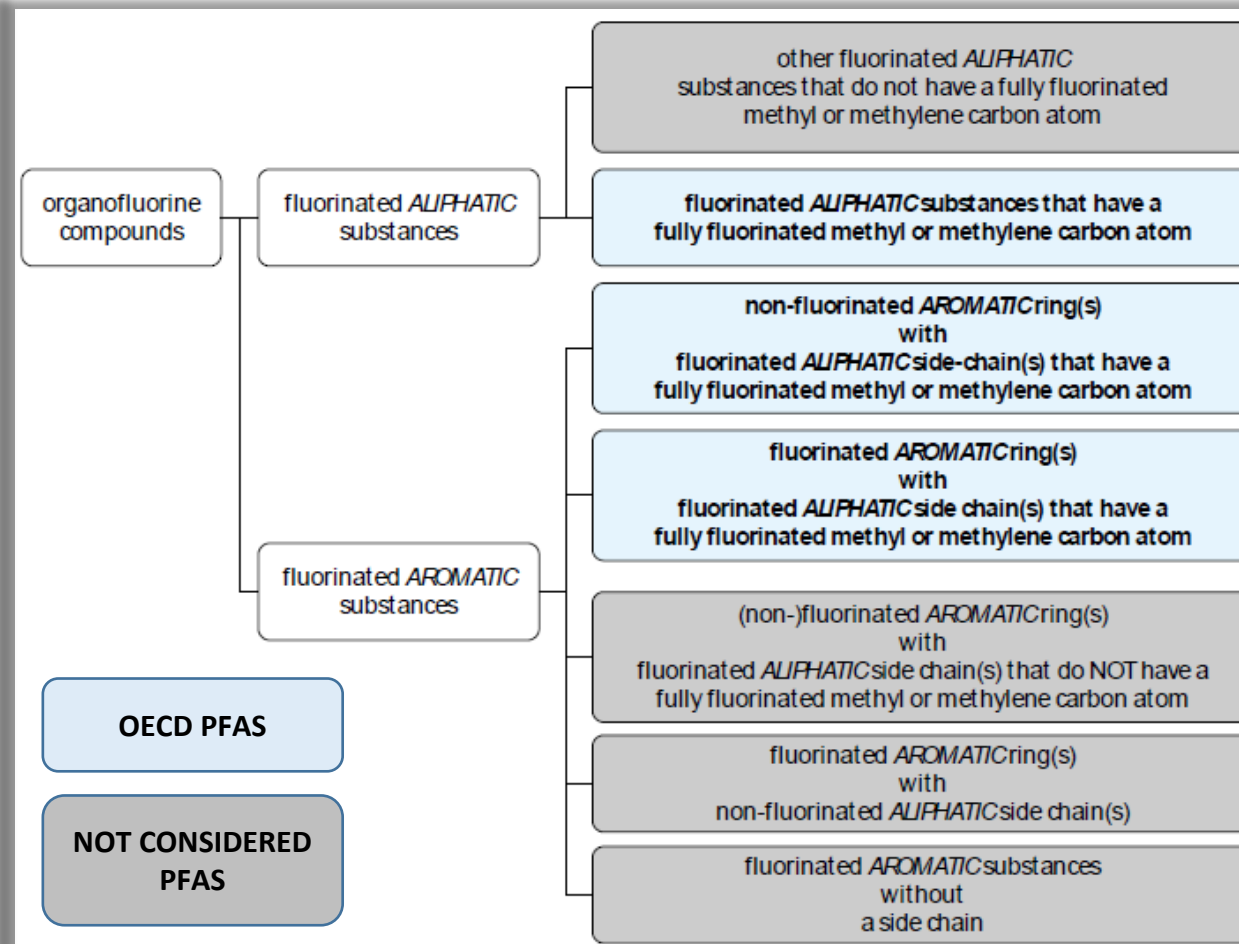
▼ Fluorinated aliphatic substances ? 880,258

- ▶ Fluorinated aliphatic substances that have a fully fluorinated methyl or methylene carbon atom ? 589,226
- ▶ Other fluorinated aliphatic substances that do NOT have a fully fluorinated methyl or methylene carbon atom ? 291,032

▼ Fluorinated aromatic substances ? 19,012,193

- ▶ (Non-)Fluorinated aromatic ring(s) with fluorinated aliphatic side chain(s) that do NOT have a fully fluorinated methyl or methylene carbon atom ? 1,507,637
- ▶ Fluorinated aromatic ring(s) with fluorinated aliphatic side chain(s) that have a fully fluorinated methyl or methylene carbon atom ? 870,933
- ▶ Fluorinated aromatic ring(s) with non-fluorinated aliphatic side chain(s) ? 11,688,175
- ▶ Fluorinated aromatic substances without a side chain ? 35,529
- ▶ Non-fluorinated aromatic ring(s) with fluorinated aliphatic side chain(s) that have fully fluorinated methyl or methylene carbon atom ? 4,909,919

▶ Other fluorinated substances ? 95,325

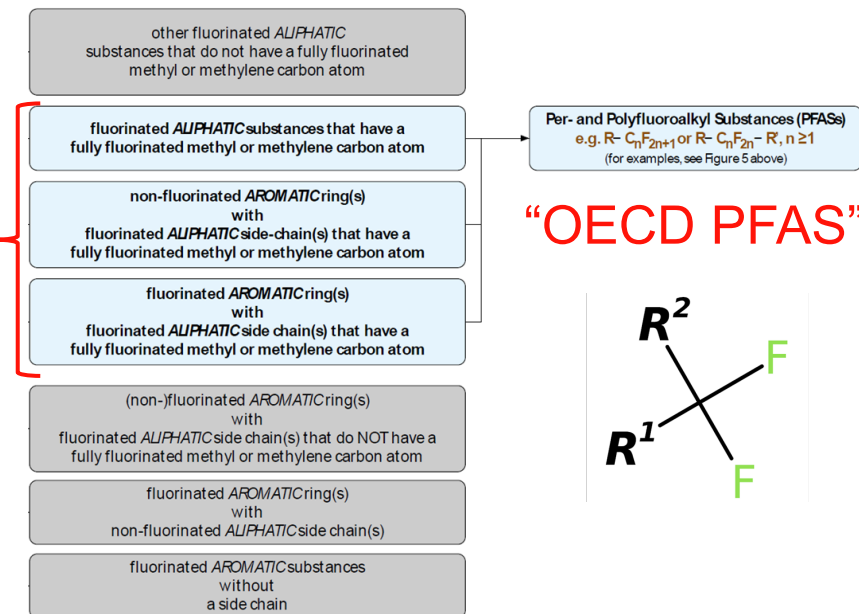




# The PubChem PFAS Tree – OECD PFAS



- ▼ PFAS and Fluorinated Compounds in PubChem ? ↗ 20,929,881
  - ▼ OECD PFAS definition ? ↗ 6,370,077
    - ▶ Molecule contains isolated CF<sub>2</sub> ? 639,820
    - ▶ Molecule contains isolated CF<sub>3</sub> ? 5,610,820
    - ▶ Molecule contains PFAS parts larger than CF<sub>2</sub>/CF<sub>3</sub> ? 226,435
  - ▼ Organofluorine compounds ? ↗ 19,963,719
    - ▶ Fluorinated aliphatic substances ? 880,258
    - ▶ Fluorinated aromatic substances ? 19,012,193
    - ▶ Other fluorinated substances ? 95,325
  - ▼ Other diverse fluorinated compounds ? 122,266
    - ▶ Contains fluorine bond to non-carbon element ? 27,786
    - ▶ Contains non-organic element ? 121,181
  - ▶ PFAS and fluorinated compound collections ? ↗ 1,789,330



OECD Monograph [ENV/CBC/MONO\(2021\)25](#) (9 July 2021)

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



▼ PFAS and Fluorinated Compounds in PubChem ? ↗ 20,929,881

▼ OECD PFAS definition ? ↗ 6,370,077

▼ Molecule contains isolated CF2 ? 639,820

▶ Contains CF2 and larger PFAS parts ? 8,941

▶ Contains only isolated CF2 ? 559,183

▶ Contains only isolated CF2/CF3 ? 71,696

▼ Molecule contains isolated CF3 ? 5,610,820

▶ Contains CF3 and larger PFAS parts ? 26,361

▶ Contains only isolated CF2/CF3 ? 71,696

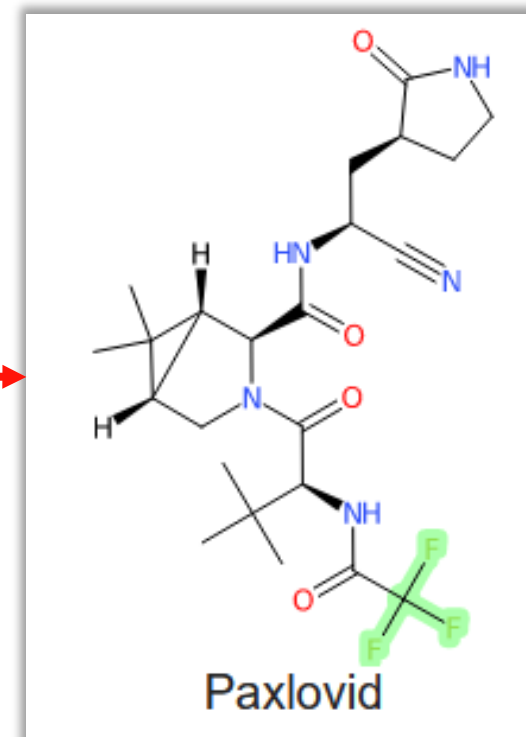
▶ Contains only isolated CF3 ? 5,512,763

▼ Molecule contains PFAS parts larger than CF2/CF3 ? 226,435

▶ Breakdown by isolated PFAS part count ? 226,435

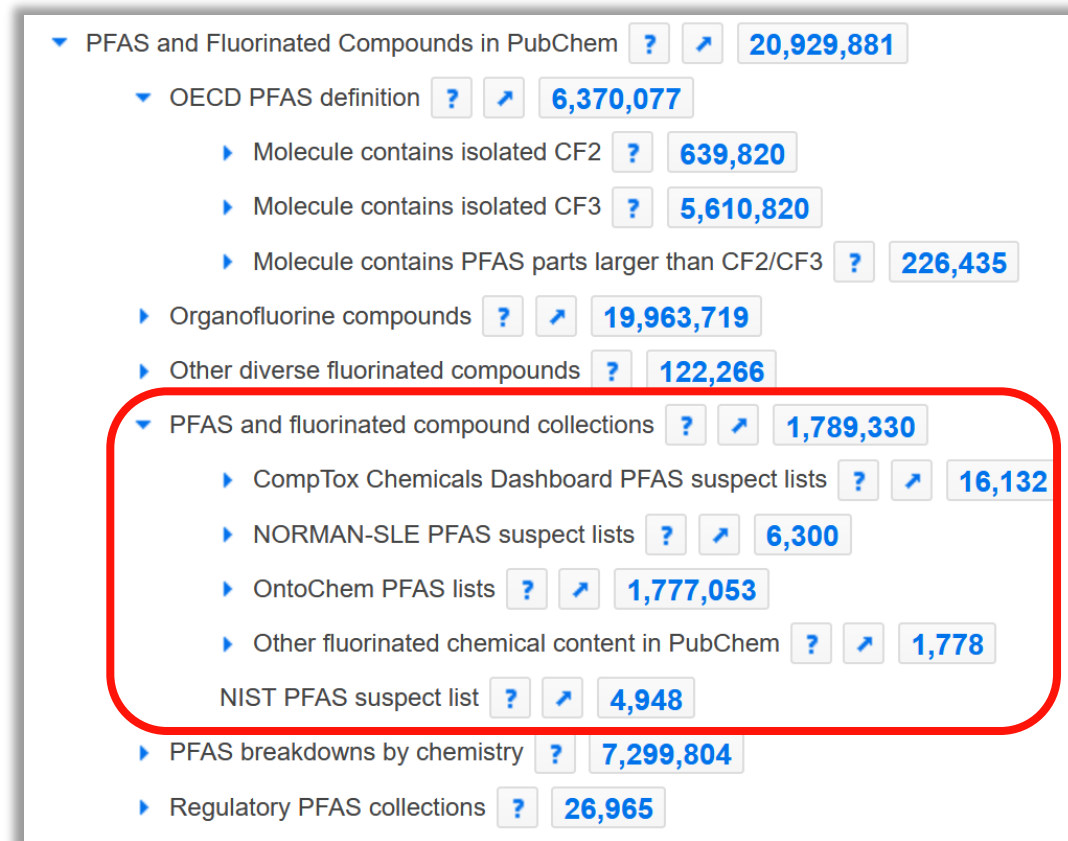
▶ Breakdown by isolated PFAS part type ? 226,435

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



# Outline

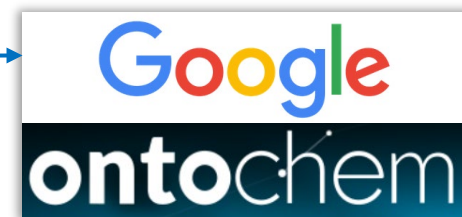
- Background and Motivation
- PubChem PFAS Tree
  - OECD PFAS & organofluorine compounds
  - PFAS suspect lists
  - Regulatory PFAS collections
  - PFAS breakdown by chemistry
- How many PFAS are really “out there”?
- Questions / Discussion



# The PubChem PFAS Tree – Collection of Suspect Lists



- PFAS and Fluorinated Compounds in PubChem **20,929,881**
  - OECD PFAS definition **6,370,077**
  - Organofluorine compounds **19,963,719**
  - Other diverse fluorinated compounds **122,266**
  - PFAS and fluorinated compound collections **1,789,330****
    - CompTox Chemicals Dashboard PFAS suspect lists **16,132**
    - NORMAN-SLE PFAS suspect lists **6,300**
    - OntoChem PFAS lists **1,777,053**
    - Other fluorinated chemical content in PubChem **1,778**
    - NIST PFAS suspect list **4,948**
  - PFAS breakdowns by chemistry **7,299,804**
  - Regulatory PFAS collections **26,965**





# Many different PFAS lists in the tree ...



PFAS and fluorinated compound collections **1,789,330**

- CompTox Chemicals Dashboard PFAS suspect lists **16,132**
- NORMAN-SLE PFAS suspect lists **6,300****
- S09 | PFASTRIER | PFAS Suspect List of fluorinated substances from X. Trier and colleagues **468**
- S14 | KEMIPFAS | PFAS Highly Fluorinated Substances List from KEMI **1,344**
- S25 | OECDPFAS | List of PFAS from the OECD **3,692****
- S46 | PFASTREVIEW19 | List of PFAS reported in Non-Target HRMS Studies from Liu et al 2019 **680**
- S80 | PFASGLUEGE | Overview of PFAS Uses **1,250****
- S89 | PRORISKPFAS | List of PFAS Compiled from NORMAN SusDat **4,240**
- S92 | FLUOROPHARMA | List of 340 ATC classified fluoro-pharmaceuticals **290**
- S94 | FLUOROPEST | List of 423 FRAC/HRAC/IRAC classified fluoro-agrochemicals **318**
- S95 | PFSANEXCH | PFAS List from the NORMAN PFAS Analytical Exchange Activity **94**
- S96 | ECIPFAS | Updateable List to add PFAS Structures to Public Resources from ECI (UniLu) **257**
- S100 | PFSAREACH | List of PFAS identified in REACH 2019 **429**

OntoChem PFAS lists **1,777,053**

Other fluorinated chemical content in PubChem **1,778**

**NIST PFAS suspect list **4,948****



## The NORMAN Suspect List Exchange (NORMAN-SLE): facilitating European and worldwide collaboration on suspect screening in high resolution mass spectrometry

Hiba Mohammed Taha<sup>1</sup>, Reza Aalizadeh<sup>2</sup>, Nikiforos Alygizakis<sup>3,2</sup>, Jean-Philippe Antignac<sup>4</sup>, Hans Peter H. Arp<sup>5,6</sup>, Richard Bade<sup>7</sup>, Nancy Baker<sup>8</sup>, Lidia Belova<sup>9</sup>, Lubertus Bijlsma<sup>10</sup>, Evan E. Bolton<sup>11</sup>, Werner Brack<sup>12,13</sup>, Alberto Celma<sup>10,14</sup>, Wen-Ling Chen<sup>15</sup>, Tiejun Cheng<sup>11</sup>, Parviel Chisir<sup>1</sup>, Luboš Cirka<sup>16,3</sup>, Lisa A. D'Agostino<sup>17</sup>, Yannick Djoumbou Feunang<sup>18</sup>, Valeria Dulio<sup>19</sup>, Stellan Fischer<sup>20</sup>, Pablo Gago-Ferrero<sup>21</sup>, Aikaterini Galani<sup>2</sup>, Birgit Geueke<sup>22</sup>, Natalia Glowacka<sup>3</sup>, Juliane Glüge<sup>23</sup>, Ksenia Groh<sup>24</sup>, Sylvia Grosse<sup>25</sup>, Peter Haglund<sup>26</sup>, Pertti J. Hakkinen<sup>11</sup>, Sarah E. Hale<sup>5</sup>, Felix Hernandez<sup>10</sup>, Elisabeth M.-L. Janssen<sup>24</sup>, Tim Jonkers<sup>27</sup>, Karin Kiefer<sup>24</sup>, Michal Kirchner<sup>28</sup>, Jan Koschorreck<sup>29</sup>, Martin Krauss<sup>12</sup>, Jessy Krier<sup>1</sup>, Marja H. Lamoree<sup>27</sup>, Marion Letzel<sup>30</sup>, Thomas Letzel<sup>31</sup>, Qingliang Li<sup>11</sup>, James Little<sup>32</sup>, Yanna Liu<sup>33</sup>, David M. Lunderberg<sup>34,35</sup>, Jonathan W. Martin<sup>17</sup>, Andrew D. McEachran<sup>36</sup>, John A. McLean<sup>37</sup>, Christiane Meier<sup>29</sup>, Jeroen Meijer<sup>38</sup>, Frank Menger<sup>14</sup>, Carla Merino<sup>39,40</sup>, Jane Muncke<sup>22</sup>, Matthias Muschket<sup>12</sup>, Michael Neumann<sup>29</sup>, Vanessa Neveu<sup>41</sup>, Kelsey Ng<sup>3,42</sup>, Herbert Oberacher<sup>43</sup>, Jake O'Brien<sup>44</sup>, Peter Oswald<sup>3</sup>, Martina Oswaldova<sup>3</sup>, Jaqueline A. Picache<sup>37</sup>, Cristina Postigo<sup>44,44</sup>, Noelia Ramirez<sup>45,39</sup>, Thorsten Reemtsma<sup>12</sup>, Justin Renaud<sup>46</sup>, Pawel Rostkowski<sup>47</sup>, Heinz Rüdell<sup>48</sup>, Reza M. Salek<sup>41</sup>, Saer Samanipour<sup>49</sup>, Martin Scheringer<sup>23,42</sup>, Ivo Schliebner<sup>29</sup>, Wolfgang Schulz<sup>50</sup>, Tobias Schulze<sup>12</sup>, Manfred Sengler<sup>30</sup>, Benjamin A. Shoemaker<sup>11</sup>, Kerry Sims<sup>51</sup>, Heinz Singer<sup>24</sup>, Randolph R. Singh<sup>1,52</sup>, Mark Sumarah<sup>16</sup>, Paul A. Thiessen<sup>11</sup>, Kevin V. Thomas<sup>7</sup>, Sonia Torres<sup>39</sup>, Xenia Trier<sup>53</sup>, Annemarie P. van Wezel<sup>54</sup>, Roel C. H. Vermeulen<sup>38</sup>, Jelle J. Vlaanderen<sup>38</sup>, Peter C. von der Ohe<sup>29</sup>, Zhanyun Wang<sup>55</sup>, Antony J. Williams<sup>56</sup>, Egon L. Willighagen<sup>57</sup>, David S. Wishart<sup>58</sup>, Jian Zhang<sup>11</sup>, Nikolaos S. Thomaidis<sup>2</sup>, Juliane Hollender<sup>23,24</sup>, Jaroslav Slobodnik<sup>3</sup> and Emma L. Schymanski<sup>1</sup>

Mohammed Taha *et al.* (2022)  
DOI: [10.1186/s12302-022-00680-6](https://doi.org/10.1186/s12302-022-00680-6)



<https://www.nist.gov/people/benjamin-place>

1,232 new CIDs!

# Many different PFAS lists in the tree ...



▼ **OntoChem PFAS lists** ? ↗ **1,777,053**

- OntoChem PFAS from CORE - Definition A ? ↗ **26,805**
- OntoChem PFAS from CORE - Definition B ? ↗ **4,114**
- OntoChem PFAS from CORE - Definition C ? ↗ **3,432**
- OntoChem PFAS from Google Patents - Definition A ? ↗ **1,762,972**
- OntoChem PFAS from Google Patents - Definition B ? ↗ **73,749**
- OntoChem PFAS from Google Patents - Definition C ? ↗ **33,649**

▼ **Other fluorinated chemical content in PubChem** ? ↗ **1,778**

- ▼ **MeSH: Fluorinated Hydrocarbons** ? ↗ **418**
  - MeSH: Chlorofluorocarbons ? ↗ **39**
  - MeSH: Fluoroacetates ? ↗ **30**
  - MeSH: Fluorobenzenes ? ↗ **104**
  - MeSH: Fluorocarbons ? ↗ **121**
- CAMEO Chemicals: Fluorinated Organic Compounds ? ↗ **120**
- ChEBI: Organofluorine Compound ? ↗ **1,372**



# PFAS in:	Definition A	Definition B	Definition C
CORE Documents	27,958	4,139	3,457
Google Patents	1,783,651	75,108	34,197
<b>Total</b>	<b>1,797,831</b>	<b>77,441</b>	<b>36,788</b>



Barnabas *et al.* (2022) *Digital Discovery*.  
 DOI: [10.1039/D2DD00019A](https://doi.org/10.1039/D2DD00019A)  
 More info: DOI: [10.5281/zenodo.7185579](https://doi.org/10.5281/zenodo.7185579)

# Many different PFAS lists in the tree ... 42 from the EPA!



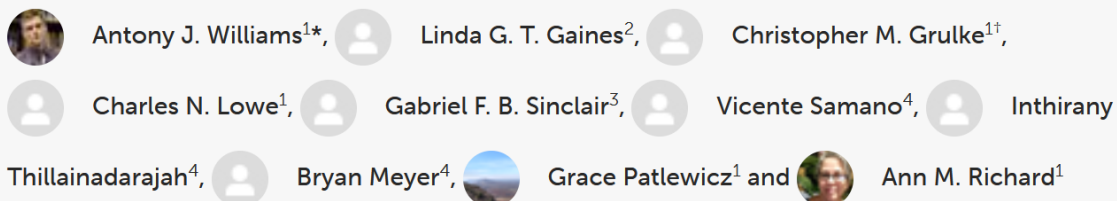
CompTox Chemicals Dashboard

CompTox Chemicals Dashboard PFAS suspect lists **16,132**

- [CCL5PFAS] WATER|EPA: Chemical Contaminants - CCL 5 PFAS subset **10,218**
- [EPAPFAS75S1] PFAS|EPA: List of 75 Test Samples (Set 1) **74**
- [EPAPFAS75S2] PFAS|EPA: List of 75 Test Samples (Set 2) **76**
- [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 **427**
- [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**

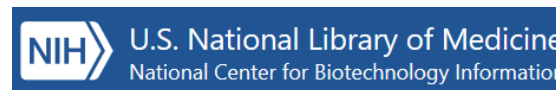
- [PFASINVITRO] PFAS|EPA: List of chemicals tested in in vitro methods 2019-2020 **182**
- [PFASKEMI] PFAS: List from the Swedish Chemicals Agency (KEMI) Report **1,499**
- [PFASLCMSGCMS] PFAS: Collection of GC-MS and LC-MS standards: Food Contact Materials **38**
- [PFASMASTER] PFAS Master List of PFAS Substances (Version 2) **10,740**
- [PFASMASTERLISTV2] PFAS: V2 PFAS Master List of PFAS Substances **6,872**
- [PFASNORDIC] PFAS: Nordic PFAS Report 2019 **202**
- [PFASNTREV19] PFAS: PFAS in Non-Target HRMS Studies (Liu et al 2019) **127**
- [PFASOECD] PFAS: Listed in OECD Global Database **3,722**
- [PFASOECDNA] NORMAN: List of PFAS from the OECD Curated by Nikiforos Alygizakis **3,203**
- [PFASPACKAGING] PFAS|EPA PFAS Substances in Pesticide Packaging **8**
- [PFASSTRUCT] Navigation Panel to PFAS Structure Lists **14,701**
- [PFASSTRUCTV1] PFAS|EPA: PFAS structures in DSSTox (update March 2018) **4,333**
- [PFASSTRUCTV2] PFAS|EPA: PFAS structures in DSSTox (update November 2019) **6,614**
- [PFASSTRUCTV3] PFAS|EPA: PFAS structures in DSSTox (update August 2020) **8,121**
- [PFASSTRUCTV4] PFAS|EPA: PFAS structures in DSSTox (update August 2021) **10,739**
- [PFASSTRUCTV5] PFAS|EPA: PFAS structures in DSSTox (update August 2022) **14,701**
- [PFASTDB] WATER|PFAS: PFAS Chemicals contained in the EPA Drinking Water Treatability Database **38**
- [PFASSTOXDB] PFAS: PFAS-Tox Database **43**
- [PFASTRI] PFAS: PFAS to the Toxics Release Inventory (TRI) Program by the National Defense Authorization Act **98**
- [PFASTRIER] PFAS Community-Compiled List (Trier et al. 2015) **592**
- [PRORISKPFAS] NORMAN|List of PFAS Compiled from NORMAN-SusDat **3,360**

## Assembly and Curation of Lists of Per- and Polyfluoroalkyl Substances (PFAS) to Support Environmental Science Research



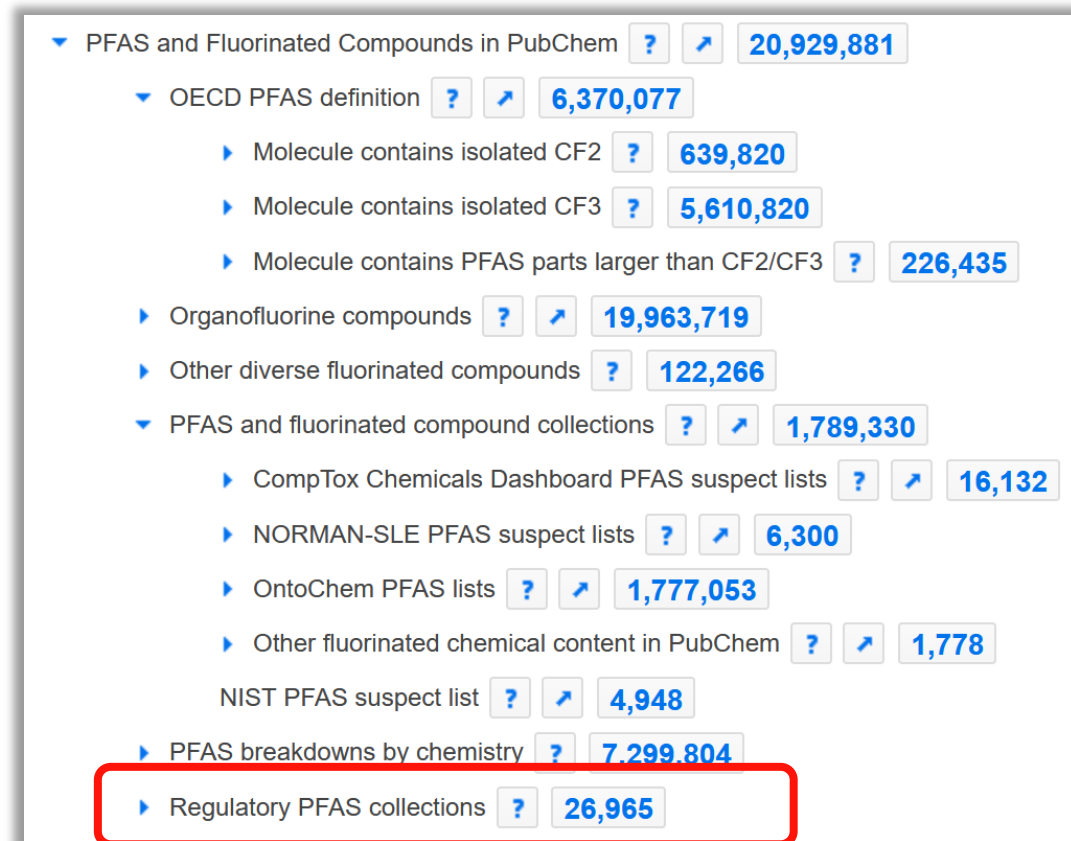
Williams *et al.* (2022) DOI: [10.3389/fenvs.2022.850019](https://doi.org/10.3389/fenvs.2022.850019)

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



# Outline

- Background and Motivation
- PubChem PFAS Tree
  - OECD PFAS & organofluorine compounds
  - PFAS suspect lists
  - Regulatory PFAS collections
  - PFAS breakdown by chemistry
- How many PFAS are really “out there”?
- Questions / Discussion





# POPRC Meets PubChem PFAS Tree ...



- Adding regulatory collections to the PFAS Tree

POPRC slides available at  
DOI: [10.5281/zenodo.7118551](https://doi.org/10.5281/zenodo.7118551)

- ▼ PFAS and Fluorinated Compounds in PubChem ? ↗ 20,929,881
  - ▶ OECD PFAS definition ? ↗ 6,370,077
  - ▶ Organofluorine compounds ? ↗ 19,963,719
  - ▶ Other diverse fluorinated compounds ? 122,266
  - ▶ PFAS and fluorinated compound collections ? ↗ 1,789,330
  - ▶ PFAS breakdowns by chemistry ? 7,299,804
  - ▼ Regulatory PFAS collections ? 26,965
    - ▶ Long-chain PFCAs (LC-PFCAs) and related substances ? 18.4
    - ▶ PFHxS and related substances ? 719
    - ▶ PFOA and related substances ? 25,565
    - ▶ PFOA and related substances - exclusions ? ↗ 68
    - ▶ PFOS and related substances ? 1,308

- ▼ PFHxS and related substances ? 719
  - ▶ [Annex A] PFHxS plus its salts and PFHxS-related compounds as defined in Annex A of the Stockholm Convention ? ↗ 607
  - ▶ [EU REACH] PFHxS (linear or branched) plus its salts and related substances according to EU REACH (draft definition) ? ↗ 719
  - ▶ Compounds with a (C6F13)S moiety in PubChem by SMARTS ? 719
  - ▶ Compounds with a (C6F13)S(=O)(=O) moiety in PubChem by SMARTS ? 605
  - ▶ Difference between Annex A and EU REACH definitions ? 112
  - 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) ? 5
    - ▶ PFHxS and any branched isomers and their salts (included in PubChem) ? 62
    - ▶ PFHxS and branched isomer combined substructure query in PubChem ? 212

Thanks to Andreas  
Buser, FOEN, CH

- Several Stockholm Convention lists available: now in 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)	

- Several Stockholm Convention lists available: now in PubChem

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

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

CAS	111393-39-6	1-Hexanesulfonyl
CAS	111393-39-6	1-Hexanesulfonyl
PFOA	335-67-	
	1270179-82-2	1-Hexanesulfonam
	45285-	
PFOA	1270179-93-5	1-Hexanesulfonam
	90480-	
	188210	
	188210	2-Propenoic acid, methacrylate and methacrylate
	188210	
	188210	
	129813-71-4	Sulfonamides, C4-

Regulatory PFAS collections	?	26,965	
▶ Long-chain PFCAs (LC-PFCAs) and related substances	?	18,427	
▶ PFHxS and related substances	?	719	
▶ [Annex A] PFHxS plus its salts and PFHxS-related compounds as defined in Annex A of the Stockholm Convention	?	↗	607
▶ [Annex A] PFHxS plus its salts and PFHxS-related compounds by annotation	?	470	
▶ Compounds with a (C6F13)S(=O)(=O) moiety in PubChem by SMARTS	?	605	
Initial indicative list of PFHxS plus its salts and PFHxS-related compounds	?	↗	76
PFHxS and any branched isomers (included in PubChem)	?	5	
PFHxS and any branched isomers and their salts (included in PubChem)	?	62	
PFHxS and branched isomer combined substructure query in PubChem	?	212	

- Several Stockholm Convention lists available: now in PubChem

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

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

SEARCH FOR

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

Treating this as a previously computed list of identifiers.

Compounds

76 results

SORT BY Relevance

Download

**Caveat: no polymer support at the moment**



Perfluorohexanesulfonic Acid; 355-46-4; 1,1,2,2,3,3,4,4,5,5,6,6,6-Tridecafluorohexane-1-sulfonic Acid; Perfluorohexane-1-sulphonic Acid; PFHxS;

Compound CID: 67734

MF: C<sub>6</sub>HF<sub>13</sub>O<sub>3</sub>S MW: 400.12g/mol

IUPAC Name: 1,1,2,2,3,3,4,4,5,5,6,6,6-tridecafluorohexane-1-sulfonic acid

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

InChIKey: QZHDEAJFRJCDMF-UHFFFAOYSA-N

InChI: InChI=1S/C6HF13O3S

/c7-1(8,3(11,12)5(15,16)17)2(9,10)4(13,14)6(18,19)23(20,21)22/h(H,20,21,22)

Create Date: 2005-08-08

ACTIONS ON RESULTS WITH ID TYPE:

Compounds

Push to Entrez

Save for Later

Linked Data Sets

ned in Annex A of the

by annotation ? 470

SMARTS ? 605

Compounds ? 76

Chem) ? 62

Chem ? 212

# Example: PFHxS in Stockholm Convention vs EU REACH

- ▼ Regulatory PFAS collections ? 26,965
  - ▶ Long-chain PFCAs (LC-PFCAs) and related substances ? 18,427
  - ▼ PFHxS and related substances ? 719
    - ▶ [Annex A] PFHxS plus its salts and PFHxS-related compounds as defined in Annex A of the Stockholm Convention ? ↗ 607
    - ▶ [EU REACH] PFHxS (linear or branched) plus its salts and related substances according to EU REACH (draft definition) ? ↗ 719
    - ▶ Compound
    - ▶ Compound
    - ▶ Difference
    - ▼ [Annex A] PFHxS plus its salts and PFHxS-related compounds as defined in Annex A of the Stockholm Convention ? ↗ 607
      - ▶ [Annex A] PFHxS plus its salts and PFHxS-related compounds by annotation ? 470
      - ▶ Compounds with a (C6F13)S(=O)(=O) moiety in PubChem by SMARTS ? 605
      - ▶ Initial indicative list of PFHxS plus its salts and PFHxS-related compounds ? ↗ 76
      - ▶ PFHxS and any branched isomers (included in PubChem) ? 5
      - ▶ PFHxS and any branched isomers and their salts (included in PubChem) ? 62
      - ▶ PFHxS and branched isomer combined substructure query in PubChem ? 212
    - ▶ PFHxS and branched isomer combined substructure query in PubChem ? 212



# Example: PFHxS in Stockholm Convention vs EU REACH

- Regulatory PFAS collections **?** **26,965**
  - Long-chain PFCAs (LC-PFCAs) and related substances **?** **18,427**
  - PFHxS and related substances **?** **719**
    - [Annex A] PFHxS plus its salts and PFHxS-related compounds as defined in Annex A of the Stockholm Convention **?** **↗** **607**
    - [EU REACH] PFHxS (linear or branched) plus its salts and related substances according to EU REACH (draft definition) **?** **↗** **719**
    - Compounds with a (C6F13)S(=O)(=O) moiety in PubChem by SMARTS **?** **605**
    - [Annex A] PFHxS plus its salts and PFHxS-related compounds as defined in Annex A of the Stockholm Convention **?** **↗** **607**
      - [Annex A] PFHxS plus its salts and PFHxS-related compounds by annotation **?** **470**
      - Compounds with a (C6F13)S(=O)(=O) moiety in PubChem by SMARTS **?** **605**
      - Initial indicative list of PFHxS plus its salts and PFHxS-related compounds **?** **↗** **76**
    - [EU REACH] PFHxS (linear or branched) plus its salts and related substances according to EU REACH (draft definition) **?** **↗** **719**
      - [EU REACH] PFHxS plus its salts and PFHxS-related compounds (draft definition) by annotation **?** **523**
      - Compounds with a (C6F13)S moiety in PubChem by SMARTS **?** **719**
      - 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) **?** **5**
      - PFHxS and any branched isomers and their salts (included in PubChem) **?** **62**
      - PFHxS and branched isomer combined substructure query in PubChem **?** **212**

# Example: PFHxS in Stockholm Convention vs EU REACH

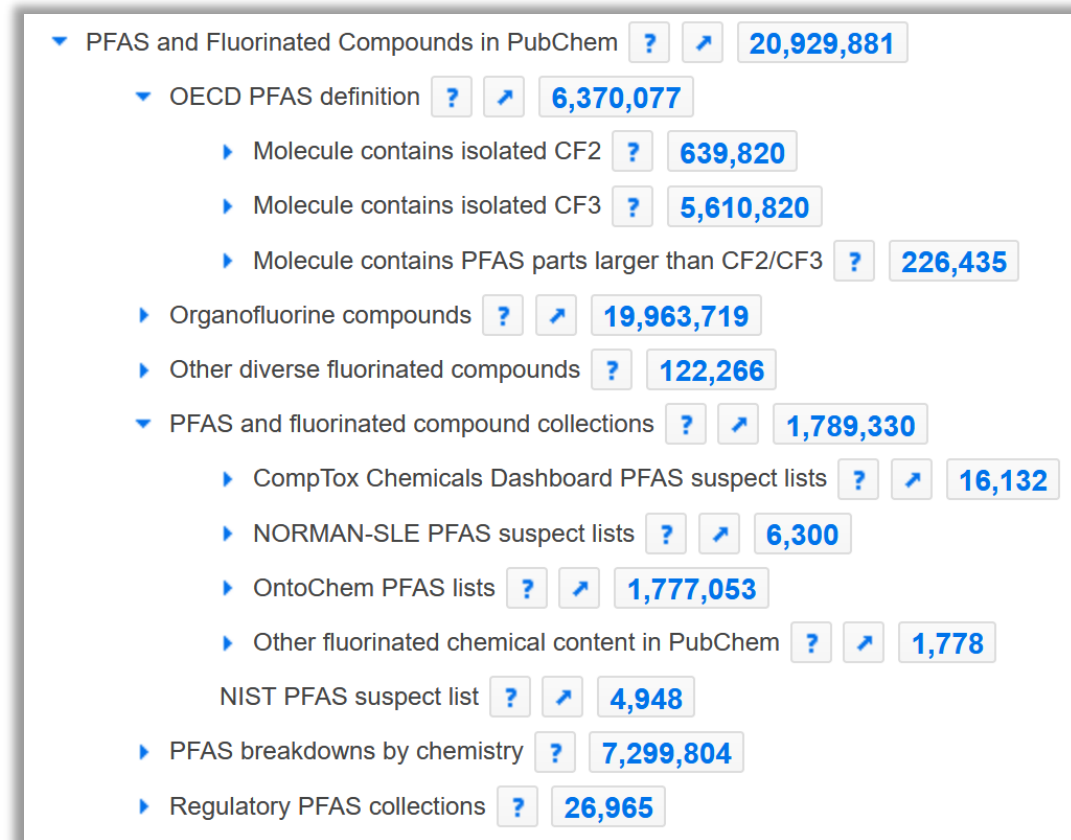
- ▼ Regulatory PFAS collections ? 26,965
  - ▶ Long-chain PFCAs (LC-PFCAs) and related substances ? 18,427
  - ▼ PFHxS and related substances ? 719
    - ▶ [Annex A] PFHxS plus its salts and PFHxS-related compounds as defined in Annex A of the Stockholm Convention ? ↗ 607
    - ▶ [EU REACH] PFHxS (linear or branched) plus its salts and related substances according to EU REACH (draft definition) ? ↗ 719
    - ▶ Compounds with a (C6F13)S moiety in PubChem by SMARTS ? 719
    - ▶ Compounds with a (C6F13)S(=O)(=O) moiety in PubChem by SMARTS ? 605
    - ▶ Difference between Annex A and EU REACH definitions ? 112
    - Compounds that transform to PFHxS (via PubChem Transformations) ?

More on this annotation content later ...

- ▼ Difference between Annex A and EU REACH definitions ? 112
  - PFHxS in EU REACH but not Annex A - all ? 112
    - PFHxS in EU REACH but not Annex A - annotation 'Literature', 'Use', 'Safety', 'Toxicity' ? 14
    - 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' ? 14

# Outline

- Background and Motivation
- PubChem PFAS Tree
  - OECD PFAS & organofluorine compounds
  - PFAS suspect lists
  - Regulatory PFAS collections
  - PFAS breakdown by chemistry
- How many PFAS are really “out there”?
- Questions / Discussion





# PFAS Breakdown by Chemistry



▼ PFAS and Fluorinated Compounds in PubChem ? ↗ 20,929,881

▼ OECD PFAS definition ? ↗ 6,370,077

▶ Molecule contains isolated CF2 ? 639,820

▶ Molecule contains isolated CF3 ? 5,610,820

▶ Molecule contains PFAS parts larger than CF2/CF3 ? 226,435

▶ Organofluorine compounds ? ↗ 19,963,719

▶ Other diverse fluorinated compounds ? 122,266

▶ PFAS and fluorinated compound collections ? ↗ 1,789,330

▼ PFAS breakdowns by chemistry ? 7,299,804

▶ Breakdown by PFAS composition ? 7,299,804

▶ Breakdown by PFAS functional groups ? 7,299,804

▶ Breakdown by PFAS part connectivity degree ? 7,299,804

▶ Breakdown by PFAS part formulas ? 7,299,804

▶ Regulatory PFAS collections ? 26,965

This is the difference between with and without salts/mixtures

# PFAS Breakdown by Chemistry



▼ PFAS breakdowns by chemistry ? **7,299,804**

▼ Breakdown by PFAS composition ? **7,299,804**

▼ Neutral ? **6,300,816**

▶ Breakdown by PFAS functional groups ? **6,300,816**

▶ Breakdown by PFAS part connectivity degree ? **6,300,816**

▶ Breakdown by PFAS part formulas ? **6,300,816**

▼ Salt/Mixture ? **999,000**

▶ Breakdown by PFAS functional groups ? **999,000**

▶ Breakdown by PFAS part connectivity degree ? **999,000**

▶ Breakdown by PFAS part formulas ? **999,000**

# PFAS Breakdown by Chemistry

## Breakdown by PFAS part connectivity degree ? 7,299,804

### PFAS parts with 1 connection ? 6,590,700

- ▶ PFAS-Aliphatic ? 2,965,669
- ▶ PFAS-Aromatic ? 3,745,003

PFAS-Cl 10

### PFAS parts with 2+ connections ? 824,575

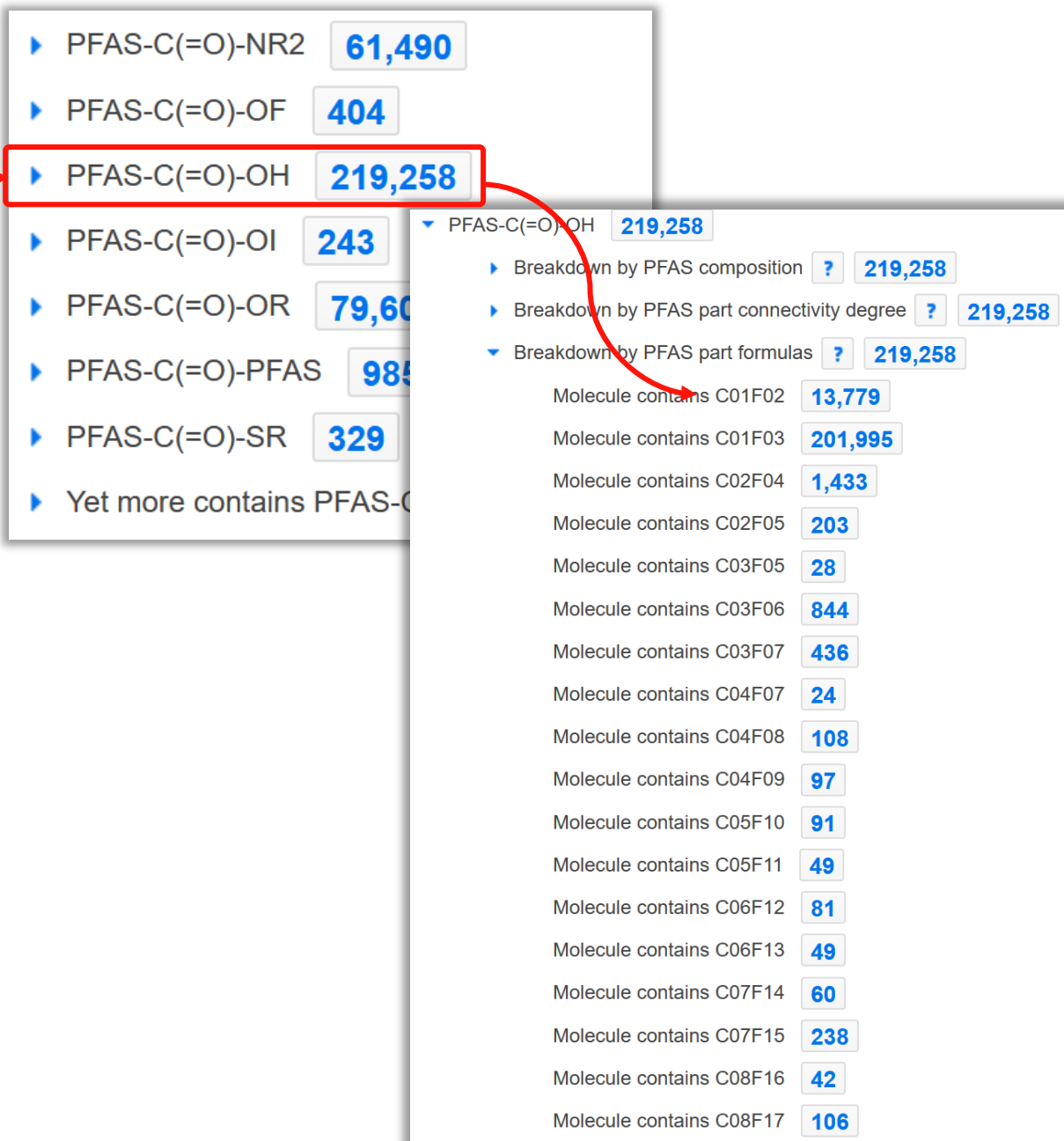
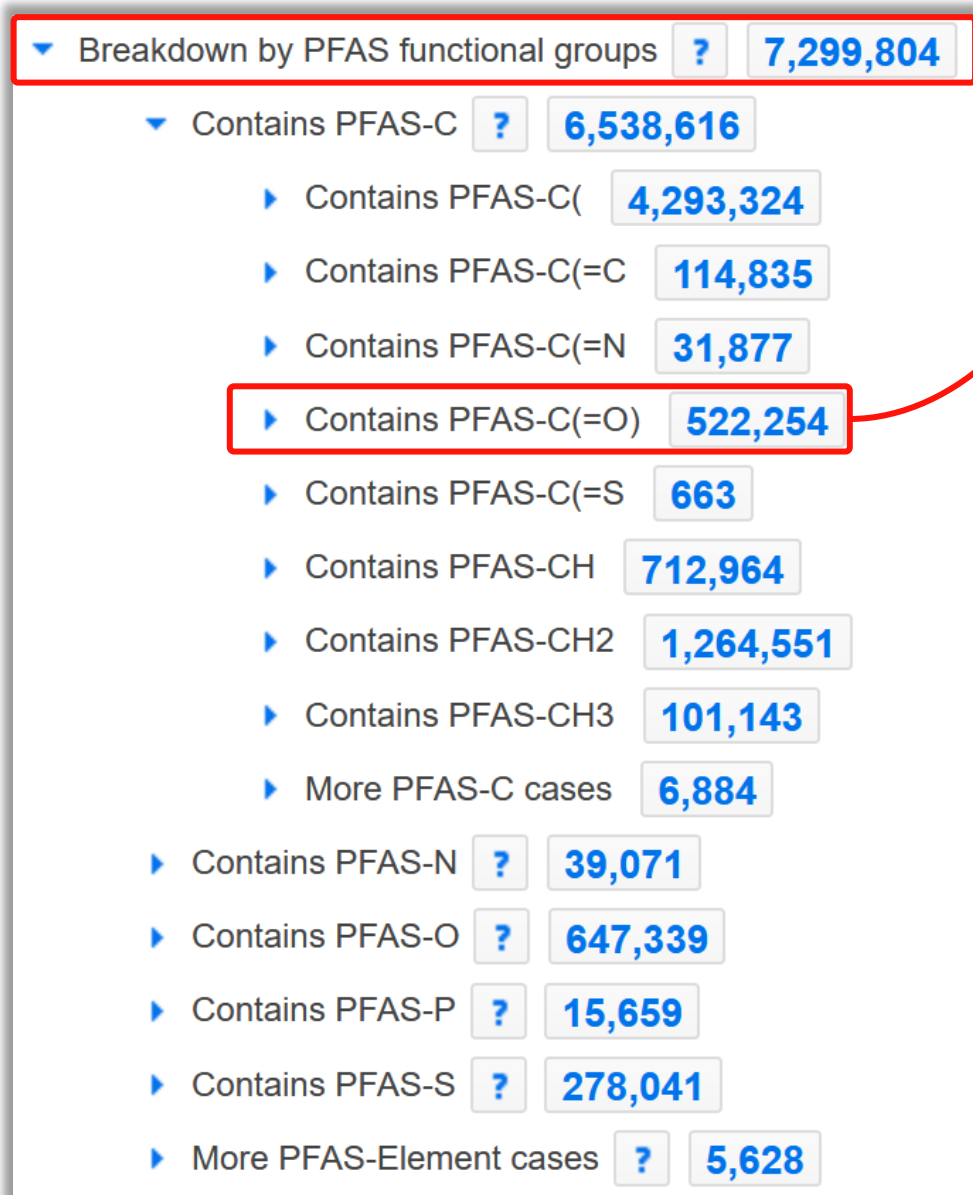
- ▶ (PFAS-Aliphatic)2 69,803
- ▶ (PFAS-Aliphatic)2, PFAS-Aromatic 42
- ▶ (PFAS-Aliphatic)3 2,041
- ▶ (PFAS-Aliphatic)4 624
- ▶ (PFAS-Aliphatic)5 132

## Breakdown by PFAS part formulas ? 7,299,804

- ▶ Molecule contains C01F02 758,055
- ▶ Molecule contains C01F03 6,421,486
- ▶ Molecule contains C02F04 41,318
- ▶ Molecule contains C02F05 65,973
- ▶ Molecule contains C03F05 1,723
- ▶ Molecule contains C03F06 26,526
- ▶ Molecule contains C03F07 50,205
- ▶ Molecule contains C04F06 783
- ▶ Molecule contains C04F07 848
- ▶ Molecule contains C04F08 6,586
- ▶ Molecule contains C04F09 23,063
- ▶ Molecule contains C05F09 1,217

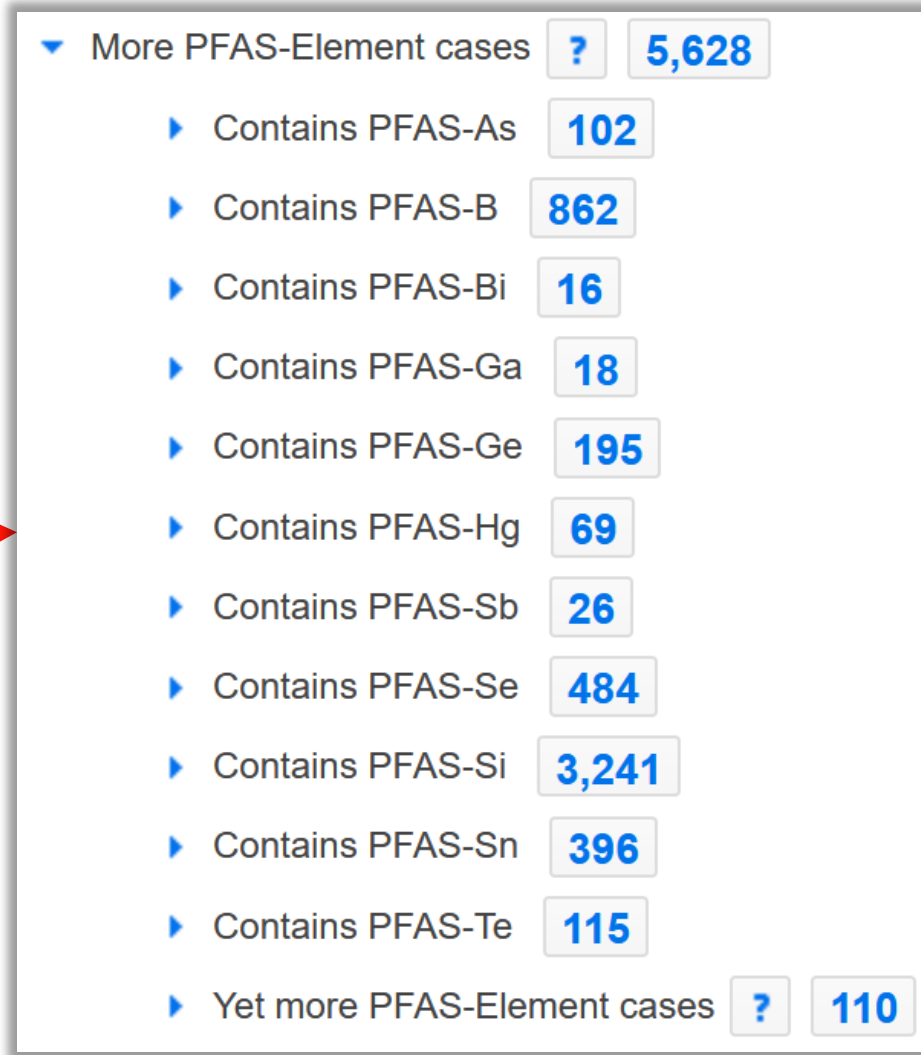
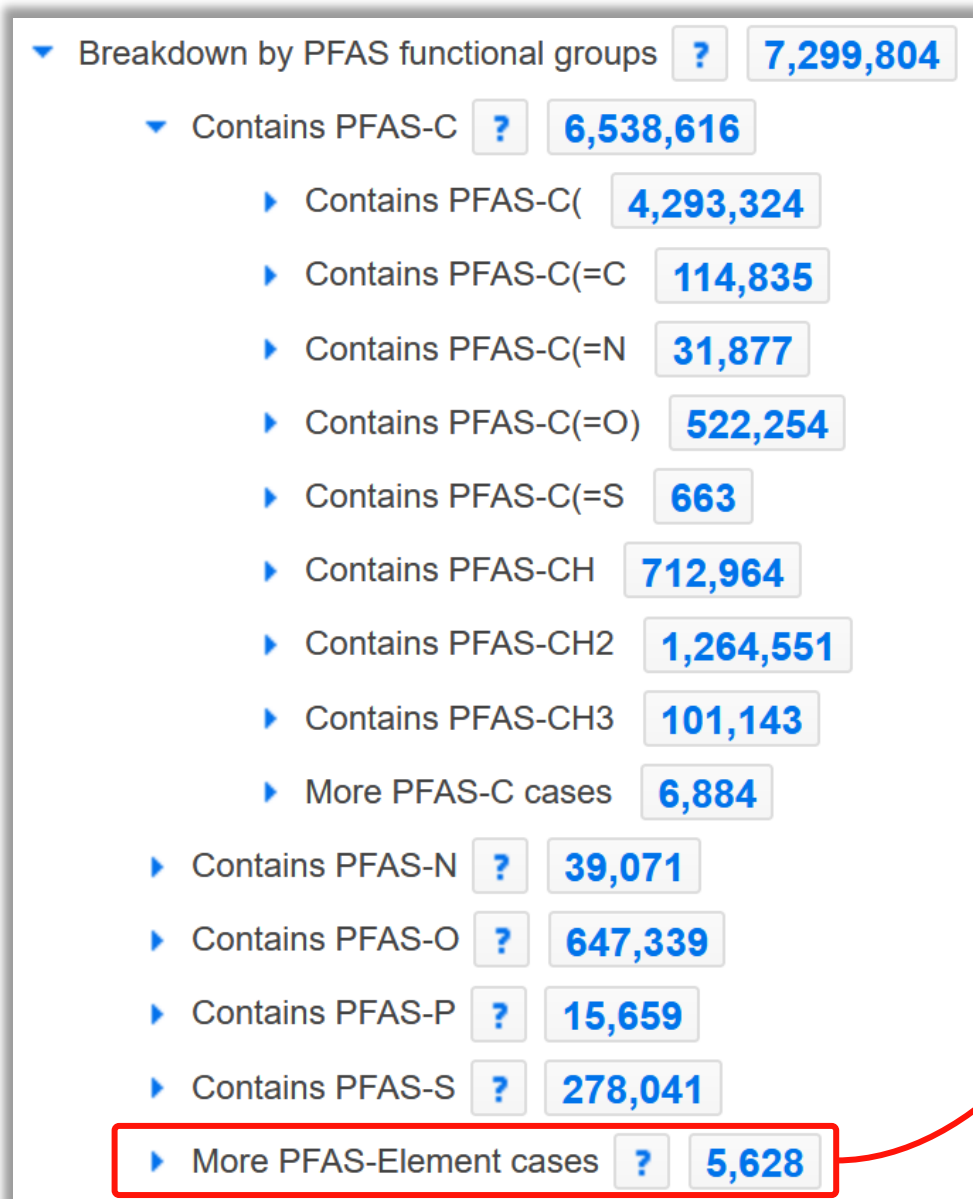
This section gets very complicated...

# PFAS Breakdown by Chemistry



# PFAS Breakdown by Chemistry

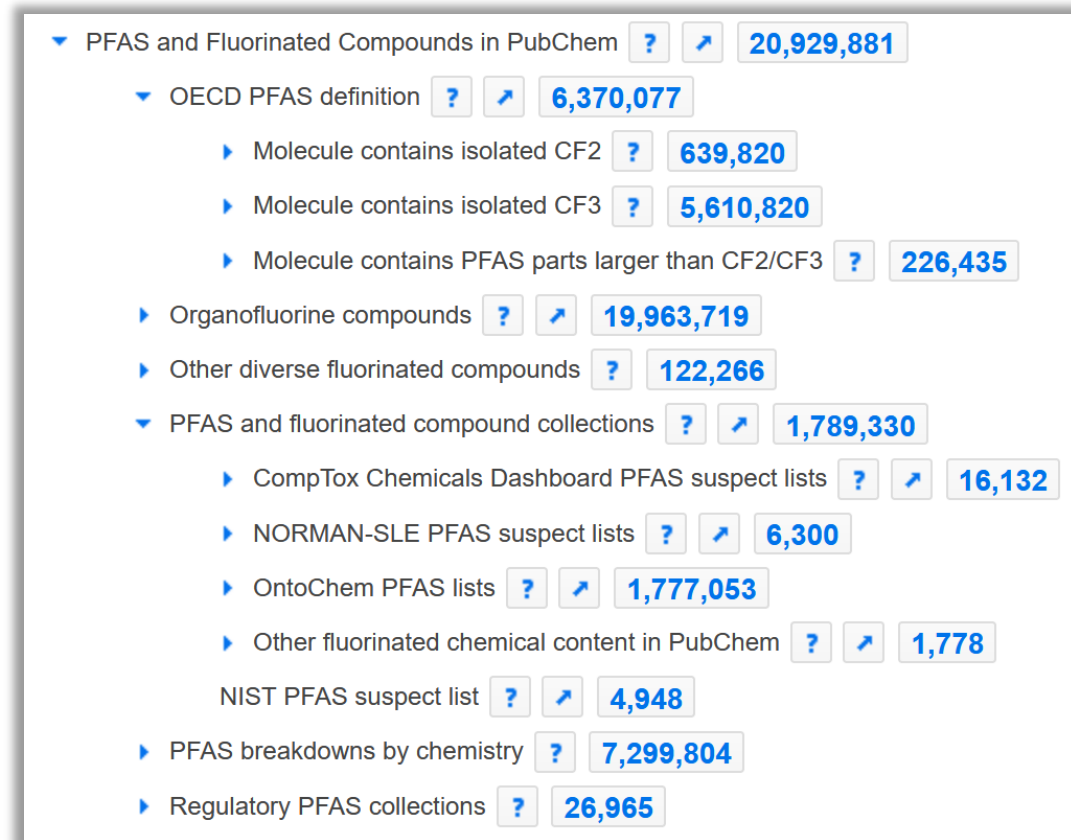
There are lots of strange things...





# Outline

- Background and Motivation
- PubChem PFAS Tree
  - OECD PFAS & organofluorine compounds
  - PFAS suspect lists
  - Regulatory PFAS collections
  - PFAS breakdown by chemistry
- How many PFAS are really “out there”?
- Questions / Discussion



# Outline

- Background and Motivation
- PubChem PFAS Tree
- How many PFAS are really “out there”?
  - Documentation & PubChem download files
  - PFHxS – who contributed new CIDs?
  - Advanced search: Larger PFAS Parts in MassBank
  - Advanced search: How many PFAS Agrochemicals are there?
  - Larger PFAS Parts database in MetFrag (very brief!)
  - Functionality under development: Polymer / UVCB handling
- Questions / Discussion



# How many PFAS are really “out there”? Example of PFHxS

## ▼ PFHxS and related substances ? 719

▶ [Annex A] PFHxS plus its salts and PFHxS-related compounds as defined in Annex A of the Stockholm Convention ? ↗ 607

▶ [EU REACH] PFHxS (linear or branched) plus its salts and related substances according to EU REACH (draft definition) ? ↗ 719

▶ Compounds with a (C6F13)S moiety in PubChem by SMARTS ? 719

Different definitions

▶ Compounds with a (C6F13)S(=O)(=O) moiety in PubChem by SMARTS ? 605

## ▼ Difference between Annex A and EU REACH definitions ? 112

PFHxS in EU REACH but not Annex A - all ? 112

PFHxS in EU REACH but not Annex A - annotation 'Literature', 'Use', 'Safety', 'Toxicity' ? 14

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' ? 14

Annotation content  
to add context?

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) ? 5

PFHxS and any branched isomers and their salts (included in PubChem) ? 62

PFHxS and branched isomer combined substructure query in PubChem ? 212

Salt/mixture/isomer  
considerations...

# Browse the PubChem PFAS Tree to find more info!

PFAS and Fluorinated Compounds in PubChem **20,929,881**

- OECD PFAS definition **6,370,077**
  - Molecule contains isolated CF2 **639,820**
  - Molecules in this category contain at least one PFAS part larger than CF2/CF3 but may also contain isolated CF2/CF3 parts
  - Molecule contains PFAS parts larger than CF2/CF3 **226,435****
  - Breakdown by isolated PFAS part count **226,435**
    - Contains 01 isolated PFAS part **170,967**
      - Count of molecules 00001-10 **861**
      - Count of molecules 00011-100 **3,375**
      - Count of molecules 00101-1000 **8,845**
      - Count of molecules 01001-10000 **35,347**
      - Count of molecules 10001-100000 **122,539**
        - Contains 01xC02F04-linear **18,172**
        - Contains 01xC02F05-linear **46,121**
        - Contains 01xC03F06-linear **13,187**
        - Contains 01xC03F07-linear **33,155**
        - Contains 01xC04F09-linear **11,904**
    - Contains 02 isolated PFAS parts **38,811**
    - Contains 03 isolated PFAS parts **10,254**
    - Contains 04 isolated PFAS parts **3,867**
    - Contains 05 isolated PFAS parts **877**

There is extensive documentation...



## PFAS and Fluorinated Compounds in PubChem Tree

Emma L. Schymanski<sup>1\*</sup>, Parviel Chirsir<sup>1</sup>, Todor Kondic<sup>1</sup>,  
Paul A. Thiessen<sup>2</sup>, Jian Zhang<sup>2</sup> and Evan E. Bolton<sup>2\*</sup>

21 March 2023

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<sup>2</sup> National Center for Biotechnology Information (NCBI), National Library of Medicine (NLM), National Institutes of Health (NIH), Bethesda, MD, 20894, USA. \*EEB: evan.bolton@nih.gov. ORCIDs: PAT: 0000-0002-1992-2086, JZ: 0000-0002-6192-4632, EEB: 0000-0002-5959-6190.

### Preamble

This document describes the "PFAS and Fluorinated Compounds in PubChem Tree" (hereafter "PubChem PFAS Tree") in PubChem [1], developed jointly between PubChem (NCBI/NLM/NIH) and the Environmental Cheminformatics group (ECI) at the LCSB, University of Luxembourg, in consultation with several community representatives (see Contributions and Acknowledgements). The PubChem PFAS Tree (see Figure 1 and Contents listing) includes all compounds in PubChem satisfying various definitions, as explained later in this document. Note that each compound in PubChem has a PubChem Compound Identifier (CID), and the blue numbers next to each node header reflects the number of compounds (i.e. CIDs) in that node.

Section	Navigation	PDF Page
PubChem PFAS Tree Nodes	Go to heading	2
- OECD PFAS Definition	Go to heading	2
- Organofluorine Compounds	Go to heading	5
- Other Diverse Fluorinated Compounds	Go to heading	6
- PFAS and Fluorinated Compound Collections	Go to heading	7
- Regulatory PFAS Collections	Go to heading	7
- PFAS Breakdowns by Chemistry	Go to heading	9
Navigating the PubChem PFAS Tree	Go to heading	9
- Search via PubChem Search	Go to heading	10
- Interactions via Entrez	Go to heading	11
- Interactions via PUG REST	Go to heading	14
Further Details	Go to heading	14
Statements and References	Go to heading	15

# Browse the PubChem PFAS Tree to find more info!



- PFAS and Fluorinated Compounds in PubChem ? ↗ 20,929,881
  - OECD PFAS definition ? ↗ 6,370,077
    - Molecule contains isolated CF2 ? 639,820
    - Molecule contains isolated CF3 ? 5,610,820
    - Molecule contains PFAS parts larger than CF2/CF3 ? 226,435**
      - Breakdown by isolated PFAS part count ? 226,435
        - Contains 01 isolated PFAS part ? 170,967
          - Count of molecules 00001-10 ? 861
          - Count of molecules 00011-100 ? 3,375
          - Count of molecules 00101-1000 ? 8,845
          - Count of molecules 01001-10000 ? 35,347
          - Count of molecules 10001-100000 ? 122,539
            - Contains 01xC02F04-linear 18,172
            - Contains 01xC02F05-linear 46,121
            - Contains 01xC03F06-linear 13,187
            - Contains 01xC03F07-linear 33,155
            - Contains 01xC04F09-linear 11,904**
          - Contains 02 isolated PFAS parts ? 38,811
          - Contains 03 isolated PFAS parts ? 10,254
        - Molecules in this category contain 5 isolated PFAS parts
        - Contains 05 isolated PFAS parts ? 877

SEARCH FOR

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

Treating this as a previously computed list of identifiers.

Compounds

11,904 results ≡ Filters SORT BY Relevance ↓ Download ↓

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  
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

[Summary](#) [Similar Structures Search](#) [Related Records](#)

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



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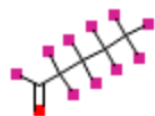


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1	cid	cmpdnam	cmpdsyno	mw	mf	polararea	complexity	xlogp	heavycnt	hbonddor	hbondacc	rotbonds						
2	67812	Perfluorov	375-62-2	266.04	C5F10O	17.1	288	3.4	16	0	11	3						
3	67814	Nonafluor	375-72-4	302.09	C4F10O2S	42.5	386	3.4	17	0	12	3						
4	67815	Perfluorok	375-73-5	300.1	C4HF9	M	N	O	P	Q	R	S	T	U	V	W	X	
5	69494	Pentane,	1638-79-9	395.94	C5F11	inchi	isosmiles	inchikey	iupacnam	meshheac	annothits	annothitcraids	cidcdate	sidsrcnam	depcatg	annotation		
6	69939	1-Butanes	812-94-2	385.25	C9H12	InChI=1S/C(=O)(C(C	RUFSEXELM	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 PH	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	PGYZCBT	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/C(=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	CXHFVFP	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(=	DYMLQJJA	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						
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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	RUFSEXELM	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 PH	Chemical	\	NULL	
10	74887	1,1,1,2,2,2	2043-55-2	272.09	C6H4F	InChI=1S/CN(CCCFC	ZDKOOLGI	1,1,2,2,3,3	NULL	Classificat	4	NULL	20050808	AAA Cher	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<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)  
 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

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	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	C4HF9O3S	62.8	387	2.3	17	1	12	3
5	69494	Pentane,	1638-79-9	395.94	C5F11I	0	289	4.8	17	0	11	3
6	69939	1-Butanes	812-94-2	385.25	C9H12F9N	66	497	2.8	23	1	13	8
7	73893	2-Propenc	1492-87-1	439.3	C12H14F9	72.1	640	3.9	27	0		
8	74534	3,3,4,4,5,5	1799-84-4	332.16	C10H9F9O	26.3	411	4.6	21	0		
9	74883	1-Hexanol	2043-47-2	264.09	C6H5F9O	20.2	243	3	16	1		
10	74887	1,1,1,2,2,2	2043-55-2	272.09	C6H4F9O	0	243	4.8	16	0		



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<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: 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	RUFSEXELM	2,2,3,3,4,4	NULL	NULL	Classificat	6	NULL
7	74										Classificat	6	NULL
8	74										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										Classificat	6	NULL
13	100										Classificat	8	NULL
14	101												
15	104												

## 8 Use and Manufacturing

### 8.1 Uses

EPA CPDat Chemical and Product Categories

1 item

#### Category

used as a stain or water

*The Chemical and Physical Scientific Data, volume*

► EPA Chemical and Product Categories

### 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. /Perfluoroalkanesulfonic Acids/

*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 ? 65,945,956
  - Agrochemical Information ? 3,090
  - Associated Disorders and Diseases ? 29,990
  - Biologic Description ? 2,464,499
  - Biological Test Results ? 4,497,660
  - Chemical and Physical Properties ? 267,837
  - Classification ? 22,519,643
  - Drug and Medication Information ? 19,108
  - Food Additives and Ingredients ? 7,330
  - Identification ? 4,679
  - Information Sources ? 45,543,994
  - Interactions and Pathways ? 204,199
  - Literature ? 2,093,924
  - Names and Identifiers ? 4,974,374
  - Patents ? 38,011,045
  - Pharmacology and Biochemistry ? 113,370
  - Related Records ? 13,106,996
  - Safety and Hazards ? 171,124
  - Spectral Information ? 1,535,927
  - Structures ? 11,758,915
  - Toxicity ? 116,629
  - Use and Manufacturing ? 105,669

# Example of PFHxS – who contributed newest CIDs?

- ▼ PFHxS and related substances ? 719
  - ▼ [Annex A] PFHxS plus its salts and PFHxS-related compounds as defined in Annex A of the Stockholm Convention ? ↗ 607
    - ▼ [Annex A] PFHxS plus its salts and PFHxS-related compounds by annotation ? 470
      - [Annex A] PFHxS, salts and related - annotation 'Literature' ? 15
      - [Annex A] PFHxS, salts and related - annotation 'Literature', 'Use', 'Safety', 'Toxicity' ? 138
      - [Annex A] PFHxS, salts and related - annotation 'Patents' ? 312
      - [Annex A] PFHxS, salts and related - annotation 'Safety and Hazards', 'Toxicity' ? 43
      - [Annex A] PFHxS, salts and related - annotation 'Use and Manufacturing' ? 108
      - [Annex A] PFHxS, salts and related - CID date 2022 or 2023 ? 76
    - ▶ Compounds with a (C6F13)S(=O)(=O) moiety in PubChem by SMARTS ? 605
    - Initial indicative list of PFHxS plus its salts and PFHxS-related compounds ? ↗ 76
    - PFHxS and any branched isomers (included in PubChem) ? 5
    - PFHxS and any branched isomers and their salts (included in PubChem) ? 62
    - PFHxS and branched isomer combined substructure query in PubChem ? 212



Who/where did these come from?





# Advanced Search Building: Large PFAS Parts in MassBank (I)

▼ OECD PFAS definition ? ↗ 6,370,077

- ▶ Molecule contains isolated CF2 ? 639,820
- ▶ Molecule contains isolated CF3 ? 5,610,820
- ▶ Molecule contains PFAS parts larger than CF2/CF3 ? 226,435



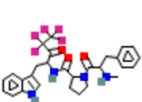
SEARCH FOR

PubChem: Molecule contains PFAS parts larger than CF2/CF3 × 🔍

Treating this as a previously computed list of identifiers.

Compounds

226,435 results Filters SORT BY Relevance Download

 **N-[1-(1H-Indole-3-ylmethyl)-2-oxo-3,3,4,4,4-pentafluorobutyl]-1-[1-oxo-2-(methylamino)-3-phenylpropyl]-2-pyrrolidinecarboxamide**

Compound CID: 1951  
MF: C<sub>28</sub>H<sub>29</sub>F<sub>5</sub>N<sub>4</sub>O<sub>3</sub> MW: 564.5g/mol  
IUPAC Name: 1-[2-(methylamino)-3-phenylpropanoyl]-N-[4,4,5,5-pentafluoro-1-(1H-indol-3-yl)-3-oxopentan-2-yl]pyrrolidine-2-carboxamide

ACTIONS ON RESULTS WITH ID TYPE:  
Compounds

- Push to Entrez**
- Save for Later
- Linked Data Sets



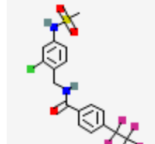
NIH National Library of Medicine  
National Center for Biotechnology Information


PubChem Compound #1 OR #2 OR #3 Limits Advanced

Summary 20 per page Sort by Default order

**Search results**

Items: 1 to 20 of 226435 << First < Prev Page 1 of 11322

1.  [CHEMBL5086882](#)  
MW: 456.800 g/mol MF: C<sub>17</sub>H<sub>14</sub>ClF<sub>5</sub>N<sub>2</sub>O<sub>3</sub>S  
IUPAC name: N-[[2-chloro-4-(methanesulfonamido)phenyl]methyl]-4-(1,1,2,2...  
Create Date: 2023-03-02  
CID: 166636311  
[Summary](#) [Same Parent, Connectivity](#)

2.  [CHEMBL5092567](#)  
MW: 663.500 g/mol MF: C<sub>23</sub>H<sub>14</sub>F<sub>9</sub>N<sub>3</sub>O<sub>6</sub>S<sub>2</sub>  
IUPAC name: methyl (2Z)-2-[(2Z)-2-[(E)-[4-(1,1,2,2,3,3,4,4,4-nonafluorob...  
Create Date: 2023-03-02  
CID: 166635140  
[Summary](#) [Same Parent, Connectivity](#)

# Advanced Search Building: Large PFAS Parts in MassBank (II)

Go to **PubChem TOC**: <https://pubchem.ncbi.nlm.nih.gov/classification/#hid=72>

## PubChem Classification Browser

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

Select classification

PubChem: PubChem Compound TOC

Search selected classification by

Keyword

Enter desired search term

### Classification description (from PubChem)

This classification was created automatically from the PubChem Compound TOC on 2023/03/14.

Note that in some cases a number of highly populated nodes - those for which all or nearly all IDs have information - have been left out of the tree.

The sections, along with their child subsections, that are not shown in this tree are: Computed Properties, Substances by Category, Computed Descriptors, Molecular Formula, Depositor-Supplied Synonyms, Removed Synonyms, Create Date, Modify Date, Record Title, Related Compounds, Related Compounds with Annotations, Related Substances, 2D Structure, 3D Conformer, and Chemical Vendors. [More...](#)

Data type counts to display

None

Compound

Yes

No

Display zero count nodes?

Filter by Entrez History

#5 Search (#4) (pccompound): 226435 results

### Browse PubChem: PubChem Compound TOC Tree (filter applied \*)

PubChem Compound TOC 226,420

Agrochemical Information 5

PubChem Compound TOC 226,420

Agrochemical Information 5

Associated Disorders and Diseases 44

Biologic Description 538

Biological Test Results 3,430

Chemical and Physical Properties 2,345

Classification 226,420

Drug and Medication Information 21

Food Additives and Ingredients 8

Identification 13

Information Sources 164,999

Interactions and Pathways 120

Literature 6,958

Names and Identifiers 30,002

Patents 131,027

Pharmacology and Biochemistry 93

Related Records 12,497

Safety and Hazards 766

Spectral Information 8,705

Structures 45,733

Toxicity 198

Use and Manufacturing 3,853

How many in MassBank?

# Advanced Search Building: Large PFAS Parts in MassBank (III)

Go to **PubChem TOC**: <https://pubchem.ncbi.nlm.nih.gov/classification/#hid=72>

Data type counts to display: **None** **Compound** Display zero count nodes? **Yes** **No** Filter by Entrez History: Choose one


### Browse PubChem: PubChem Compound TOC Tree

- PubChem Compound TOC** ? **65,945,956**
  - Agrochemical Information ? **3,090**
  - Associated Disorders and Diseases ? **29,990**
  - Biologic Description ? **2,464,499**
  - Biological Test Results ? **4,497,660**
  - Chemical and Physical Properties ? **267,837**
  - Classification ? **22,519,643**
  - Drug and Medication Information ? **19,108**
  - Food Additives and Ingredients ? **7,330**
  - Identification ? **4,679**
  - Information Sources** ? **45,543,994**
    - Athena Minerals **318**
    - Baker Lab, Chemistry Department, The University of North Carolina at Chapel Hill **1,069**

KEGG **12,382**  
KNApSACK Species-Metabolite Database **17,530**  
Krueve Lab, Ionization & Mass Spectrometry, Stockton  
Lab and Research Safety, University of Minnesota  
LIPID MAPS **38,576**  
LiverTox **1,065**  
LOTUS - the natural products occurrence database  
MarkerDB **899**  
**MassBank Europe** **15,901**  
MassBank of North America (MoNA) **609,755**  
Medical Subject Headings (MeSH) **129,557**  
Metabolomics Workbench **161,704**

SEARCH FOR: PubChem: PubChem Compound TOC: MassBank Europe  
Treating this as a previously computed list of identifiers.

Compounds  
15,901 results Filters SORT BY Relevance Download

 14992-62-2; 1-Propanaminium, 2-(acetyloxy)-3-carboxy-N,N,N-trimethyl-, Inner Salt; SCHEMBL3259109; ChEMBL1625375; DTXSID40859554; ...  
Compound CID: 2  
MF: C<sub>9</sub>H<sub>18</sub>NO<sub>4</sub><sup>+</sup> MW: 204.24g/mol  
IUPAC Name: (2-acetyloxy-3-carboxypropyl)-trimethylazanium  
Isomeric SMILES: CC(=O)OC(CC(=O)O)C[N+](C)(C)C  
InChIKey: RDHQFKQIGNGIED-UHFFFAOYSA-O

ACTIONS ON RESULTS WITH ID TYPE: Compounds  
**Push to Entrez**  
Save for Later  
Linked Data Sets

# Advanced Search Building: Large PFAS Parts in MassBank (VI)

PubChem  
Compound

PubChem Compound ▾

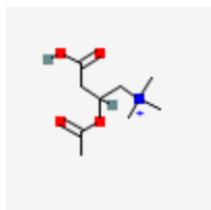
Limits **Advanced**

Summary ▾ 20 per page ▾ Sor

## Selected items

Items: 1 to 20 of 15901

1.



[14992](#)  
[SCHE](#)  
MW: 20  
IUPAC  
Create  
CID: 2

[Summary](#) [Similar Compounds](#) [Same Parent, C](#)

## History

[Download history](#) [Clear history](#)

Search	Add to builder	Query	Items found	Time
<a href="#">#7</a>	<a href="#">Add</a>	Select <b>15901</b> document(s)	<a href="#">15901</a>	07:19:35
<a href="#">#6</a>	<a href="#">Add</a>	Select <b>15901</b> document(s)	<a href="#">15901</a>	07:19:34
<a href="#">#4</a>	<a href="#">Add</a>	Search <b>#1 OR #2 OR #3</b>	<a href="#">226435</a>	07:02:25
<a href="#">#3</a>	<a href="#">Add</a>	Select <b>26435</b> doc		
<a href="#">#2</a>	<a href="#">Add</a>	Select <b>100000</b> do		
<a href="#">#1</a>	<a href="#">Add</a>	Select <b>100000</b> do		

MassBank

Larger PFAS parts

## PubChem Compound Advanced Search Builder

(#7 AND #4)

[Edit](#)

[Clear](#)

### Builder

Recent Query ▾

#7 AND #4

AND ▾

All Fields ▾

[Show index list](#)

[Search](#) or [Add to history](#)





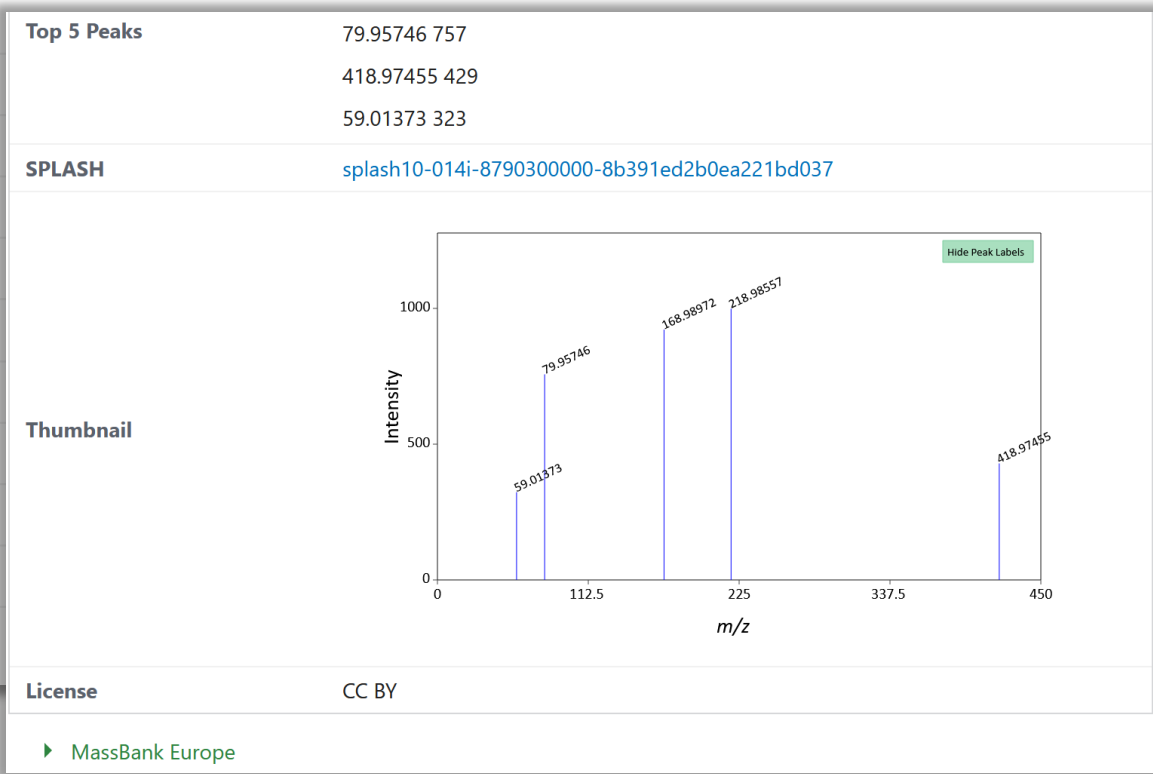
# Advanced Search Building: Large PFAS Parts in MassBank (VI)

PubChem Perfluorononanoic acid (Compound)

## 4.1.2 LC-MS

Showing 2 of 17 View More

Accession ID	MSBNK-ACES_SU-AS000012
Authors	ACESx, Martin Group
Instrument	Top 5 Peaks
Instrument Type	79.95746 757
MS Level	418.97455 429
Ionization Mode	59.01373 323
Ionization	SPLASH
Collision Energy	splash10-014i-8790300000-8b391ed2b0ea221bd037
Fragmentation Mode	Thumbnail
Column Name	
Retention Time	
Precursor m/z	



Cite Download

- CONTENTS
- Title and Summary
- 1 Structures
- 2 Names and Identifiers
- 3 Chemical and Physical Properties
- 4 Spectral Information
  - 4.1 Mass Spectrometry
    - 4.1.1 GC-MS
    - 4.1.2 LC-MS
    - 4.1.3 Other MS
  - 4.2 IR Spectra
    - 4.2.1 ATR-IR Spectra



<https://twitter.com/AcademicTox/status/1605997310726443009>

<https://pubchem.ncbi.nlm.nih.gov/compound/67821#section=LC-MS>

# Advanced Search Building: How many PFAS Agrochem? (I)

PubChem Compound TOC ? **65,945,956**

**▶ Agrochemical Information ? **3,090****

▶ Associated Disorders and Dis

SEARCH

PubChem: PubChem Compound TOC: Agrochemical Information

Treating this as a previously computed list of identifiers.

### Compounds

3,090 results Filters SORT BY Relevance Download

**1,2-dichloroethane; Ethylene Dichloride; 107-06-2; Ethylene Chloride; Ethane, 1,2-dichloro-; ...**

Compound CID: 11  
MF: C<sub>2</sub>H<sub>4</sub>Cl<sub>2</sub> MW: 98.96g/mol  
IUPAC Name: 1,2-dichloroethane  
Isomeric SMILES: C(CCl)Cl  
InChIKey: WSLDOOZREJYCGB-UHFFFAOYSA-N  
InChI: InChI=1S/C2H4Cl2/c3-1-2-4/h1-2H2  
Create Date: 2004-09-16

ACTIONS ON RESULTS WITH ID TYPE:  
Compounds

**Push to Entrez**

Save for Later

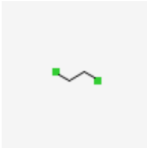
Linked Data Sets

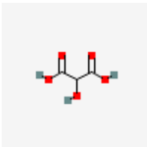
PubChem Compound PubChem Compound Limits Advanced

Summary 20 per page Sort by Default order

#### Selected items

Items: 1 to 20 of 3090

1.  [1,2-dichloroethane; Ethylene dichloride; 107-06-2 ...](#)  
MW: 98.960 g/mol MF: C<sub>2</sub>H<sub>4</sub>Cl<sub>2</sub>  
IUPAC name: 1,2-dichloroethane  
Create Date: 2004-09-16  
CID: 11  
[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [Mixture/Component Compounds](#) [PubMed \(MeSH Keyword\)](#)

2.  [Tartronic acid; 80-69-3; 2-Hydroxymalonic acid ...](#)  
MW: 120.060 g/mol MF: C<sub>3</sub>H<sub>4</sub>O<sub>5</sub>  
IUPAC name: 2-hydroxypropanedioic acid  
Create Date: 2004-09-16  
CID: 45  
[Summary](#) [Similar Compounds](#) [Same Parent, Connectivity](#) [Mixture/Component Compounds](#) [PubMed \(MeSH Keyword\)](#)

# Advanced Search Building: How many PFAS Agrochem? (I)

Data type counts to display    Display zero count nodes?

None

Compound

Yes

No

Filter by Entrez History

#12 Search (#11) (pccompound): 3090 results

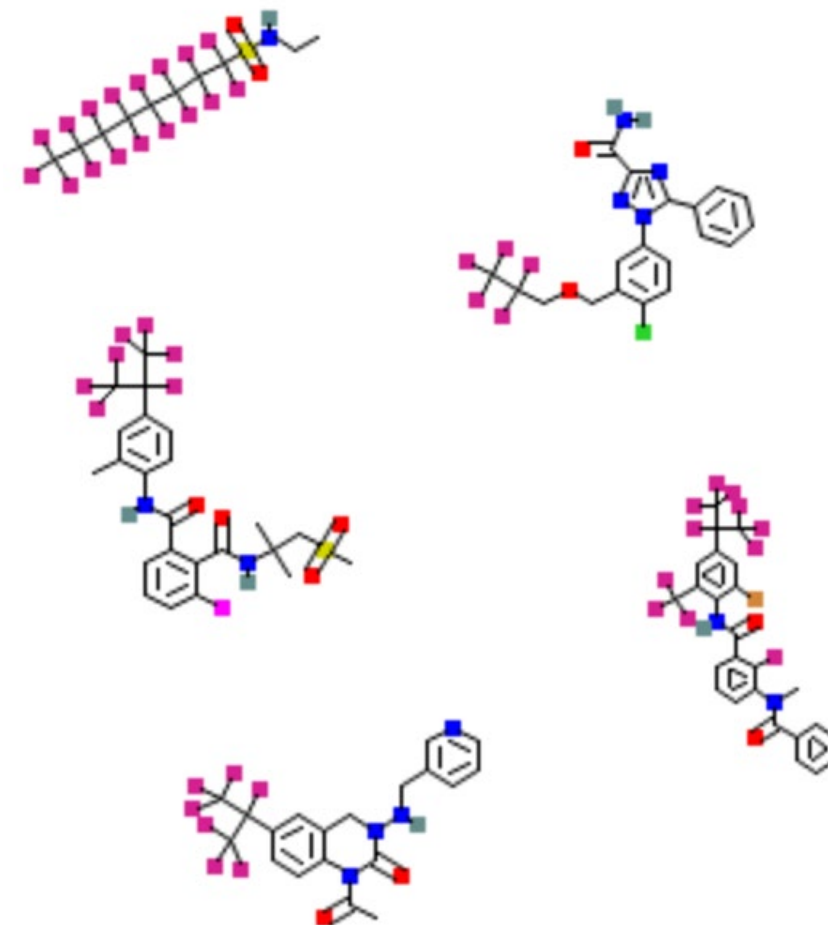
## Browse PubChem: PFAS and Fluorinated Compounds in PubChem Tree (filter applied ✖)

▼ PFAS and Fluorinated Compounds in PubChem ? ↗ 476

- ▼ OECD PFAS definition ? ↗ 293
  - ▶ Molecule contains isolated CF2 ? 13
  - ▶ Molecule contains isolated CF3 ? 283
  - ▶ Molecule contains PFAS parts larger than CF2/CF3 ? 5
- ▶ Organofluorine compounds ? ↗ 460
- ▶ Other diverse fluorinated compounds ? 2
- ▶ PFAS and fluorinated compound collections ? ↗ 326
- ▶ PFAS breakdowns by chemistry ? 304
- ▶ Regulatory PFAS collections ? 2

# Advanced Search Building: How many PFAS Agrochem? (III)

- ▼ PFAS and Fluorinated Compounds in PubChem ? ↗ 476
  - ▼ OECD PFAS definition ? ↗ 293
    - ▶ Molecule contains isolated CF2 ? 13
    - ▶ Molecule contains isolated CF3 ? 283
    - ▼ Molecule contains PFAS parts larger than CF2/CF3 ? 5
      - ▼ Breakdown by isolated PFAS part count ? 5
        - ▼ Contains 01 isolated PFAS part ? 4
          - ▼ Count of molecules 01001-10000 ? 1
            - Contains 01xC08F17-linear 1
          - ▼ Count of molecules 10001-100000 ? 3
            - Contains 01xC02F05-linear 1
            - Contains 01xC03F07-linear 2
          - ▼ Contains 02 isolated PFAS parts ? 1
            - ▼ Count of molecules 01001-10000 ? 1
              - Contains 01xCF3,01xC03F07-linear 1





# Advanced Search Building: How many PFAS Agrochem? (IV)

PFAS and Fluorinated Compounds in PubChem 476

- OECD PFAS definition 293
- Organofluorine compounds 460
- Other diverse fluorinated compounds 2
- PFAS and fluorinated compound collections 326
  - CompTox Chemicals Dashboard PFAS suspect lists 22

NORMAN-SLE PFAS suspect lists 196



- S09 | PFASTRIER | PFAS Suspect List of fluorinated substances from >
- S14 | KEMIPFAS | PFAS Highly Fluorinated Substances List from KEMI
- S25 | OECDPFAS | List of PFAS from the OECD 6
- S80 | PFASGLUEGE | Overview of PFAS Uses 3
- S89 | PRORISKPFAS | List of PFAS Compiled from NORMAN SusDat 7
- S92 | FLUOROPHARMA | List of 340 ATC classified fluoro-pharmaceuticals 4
- S94 | FLUOROPEST | List of 423 FRAC/HRAC/IRAC classified fluoro-agrochemicals 180
- S95 | PFASANEXCH | PFAS List from the NORMAN PFAS Analytical Exchange Activity 2
- S96 | ECIPFAS | Updateable List to add PFAS Structures to Public Resources from ECI (UniLu) 2
- S100 | PFASREACH | List of PFAS identified in REACH 2019 26

PFAS breakdowns by chemistry 304

Breakdown by PFAS composition 304

Neutral 291

Salt/Mixture 13

Breakdown by PFAS functional groups 13

Contains PFAS-C 9

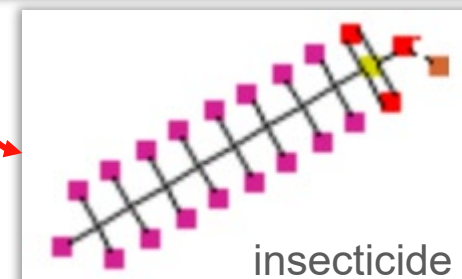
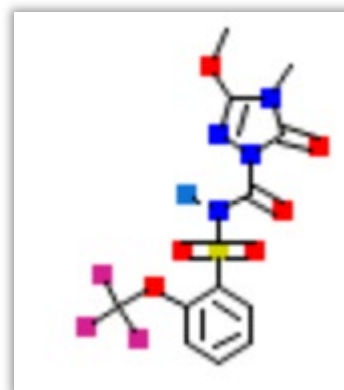
Contains PFAS-O 1

Contains PFAS-S 3

Contains PFAS-S(=O) 3

PFAS-S(=O)2-NHR 2

PFAS-S(=O)2-OH 1



# Identification with MetFrag and PubChem PFAS Tree



MetFrag

<https://msbi.ipb-halle.de/MetFrag/>

In silico fragmentation for computer assisted identification of metabolite mass spectra

Slides available at DOI:  
[10.5281/zenodo.6461325](https://doi.org/10.5281/zenodo.6461325)

**Database Settings**

Database: PubChem\_OECDPFAS\_la

Neutral Mass: 789.98232 Search ppm: 5

Formula:

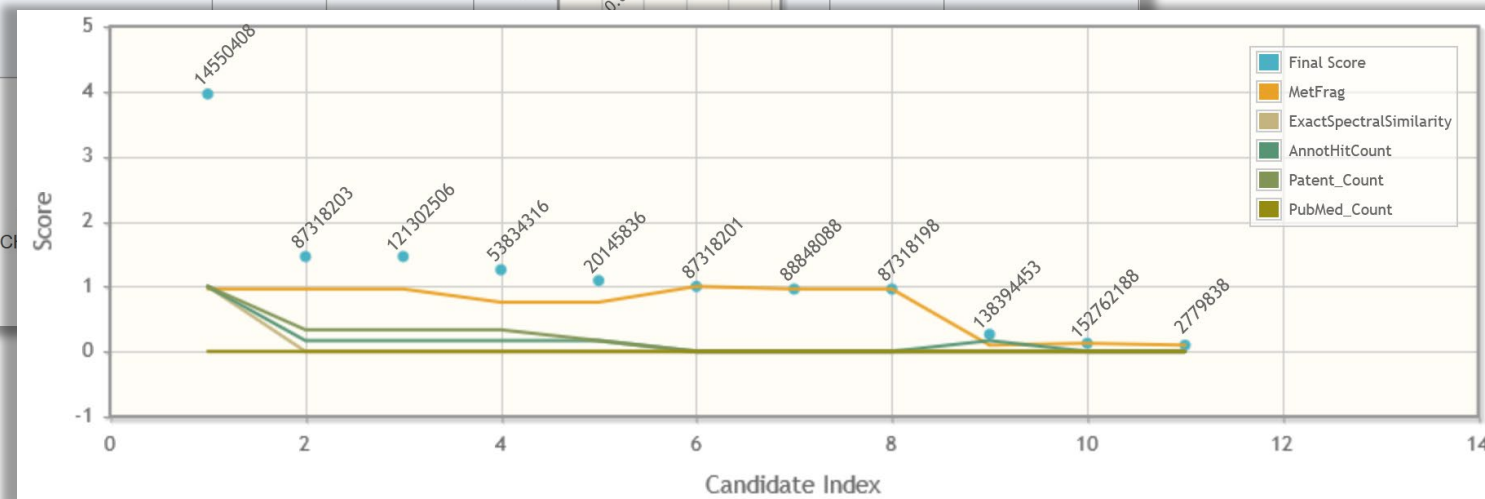
Identifiers:

Retrieve Candidates 15 Candidates

**Weights**

- MetFrag (1st)
- ExactSpectralSimilarity (2nd)
- AnnotHitCount (3rd)
- Patent\_Count (4th)
- PubMed\_Count (5th)

#	Molecule	Identifier	Mass	Formula	Normalized Scores	FinalScore	Details
1		14550408 InChIKeyBlock1 = ZDYYWMSLMLTXDM	789.98233	C <sub>16</sub> H <sub>9</sub> F <sub>26</sub> O <sub>4</sub> P		3.9607	Peaks: 2 / 2 Fragments Scores Download
2		87318203 InChIKeyBlock1 = KYZFNWUVSNMKOP	789.98233	C <sub>16</sub> H <sub>9</sub> F <sub>26</sub> O <sub>4</sub> P		1.4607	Peaks: 2 / 2 Fragments Scores
3							



SETAC EUROPE 32<sup>ND</sup> ANNUAL MEETING  
15-19 MAY 2022 | COPENHAGEN, DENMARK + ONLINE

<https://msbi.ipb-halle.de/MetFrag/> with  
<https://massbank.eu/MassBank/RecordDisplay?id=EA292203>

Ruttkies, Schymanski *et al.* (2016) DOI: [10.1186/s13321-016-0115-9](https://doi.org/10.1186/s13321-016-0115-9)

# Future topic: Expanding to Polymers/UVCBs

Functionality under development at PubChem

Data type counts to display

None Compound

Display zero count nodes?

Yes No

*PubChem PFAS Tree  
is in the compound space*

Browse PubChem: PFAS and Fluorinated Compounds in PubChem Tree

- PFAS and Fluorinated Compounds in PubChem ? ↗ 20,929,881
  - OECD PFAS definition ? ↗ 6,370,077
  - Organofluorine compounds ? ↗ 19,963,719
  - Other diverse fluorinated compounds ? 122,266
  - PFAS and fluorinated compound collections ? ↗ 1,789,330
  - PFAS breakdowns by chemistry ? 7,299,804
    - Breakdown by PFAS composition ? 7,299,804
      - Neutral ? 6,300,816
      - Salt/Mixture ? 999,000
    - Breakdown by PFAS functional groups ? 7,299,804
    - Breakdown by PFAS part connectivity degree ? 7,299,804
    - Breakdown by PFAS part formulas ? 7,299,804
  - Regulatory PFAS collections ? 26,965

UVCB = Chemical Substances of Unknown or Variable Composition, Complex Reaction Products and Biological Materials

PubChem About Docs Submit Contact Search PubChem

COMPOUND SUMMARY

Polytetrafluoroethylene

See also: Tetrafluoroethylene (has monomer).

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

Cite Download

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- Title and Summary
- 1 Synonyms
- 2 Names and Identifiers
- 3 Chemical and Physical Properties
- 4 Related Records
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<https://testpubchem.ncbi.nlm.nih.gov/rest/compounds/polytetrafluoroethylene>

# Future topic: Expanding to Polymers/UVCBs

Functionality under development at PubChem

PubChem Polytetrafluoroethylene (Compound)

## 7.1 Uses

A major use for PTFE is in tubing. PTFE is also used in applications include coatings on mechanical tapes, and is found in architectural liners, thread sealant fabric structures that have fibrillation capability.

*Gangal SV, Brothers PL, Wiley & Sons, Inc. Online*

▶ Hazardous Substances Data Bank (HSDB)

The major mechanical cylinders & nonlubricated mechanical tapes & in

*IARC. Monographs on the Organization, International Agency for Research on Cancer. <https://monographs.iarc.fr/>*

▶ Hazardous Substances Data Bank (HSDB)

PubChem Polytetrafluoroethylene (Compound)

## 5.3 Drug Warnings

Soft tissue reactions to materials in joint prostheses include discoloration, fibrosis, florid histiocytic reaction, and granulomatous inflammation with foreign body giant cell reaction. Clinical manifestations include pain and swelling. We report a case of temporomandibular joint Proplast-Teflon prosthesis, followed by the development of large cell lymphoma in the left parotid gland 10 years after joint replacement. While it is unclear whether the implant directly contributed to the development of lymphoma, this association has not been previously documented, prompting this report.

[PMID:22533111](#)

*Ong MG et al; J La State Med Soc. 164 (1): 31-2 (2012)*

▶ Hazardous Substances Data Bank (HSDB)

Expanded polytetrafluoroethylene implant is usually considered as a wonderful implant for chin cosmetic augmentation with no or less bone resorption compared with solid silicone implant. However, one severe bony erosion in expanded polytetrafluoroethylene chin augmentation was found in our clinical work. We consider that the possible reason about severe bone resorption in such situation is most relative to the mentalis muscle hyperactivity, rather than the kinds of materials. We also strongly advise that genioplasty is suitable for the cases with mentalis muscle hyperactivity caused by a dentofacial deformity.

[PMID:24036760](#)

Cite

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13:35

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COMPOUND SUMMARY

Polytetrafluoroethylene

Cite

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See also: Tetrafluoroethylene (has monomer).

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

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



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# Are there really 6 million PFAS in PubChem?



- Yes and more ... the count keeps growing
- PubChem has a lot of functionality to (help) explore this
- The annotation content is critical to understanding “PFAS Space”
  - Please reach out to us if you have structures or data to add!  
Emma: [emma.schymanski@uni.lu](mailto:emma.schymanski@uni.lu) or [@ESchymanski](https://twitter.com/ESchymanski)  
PubChem: [pubchem-help@ncbi.nlm.nih.gov](mailto:pubchem-help@ncbi.nlm.nih.gov) or [@pubchem](https://twitter.com/pubchem)

★ → *Documentation:*





# Acknowledgements!

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

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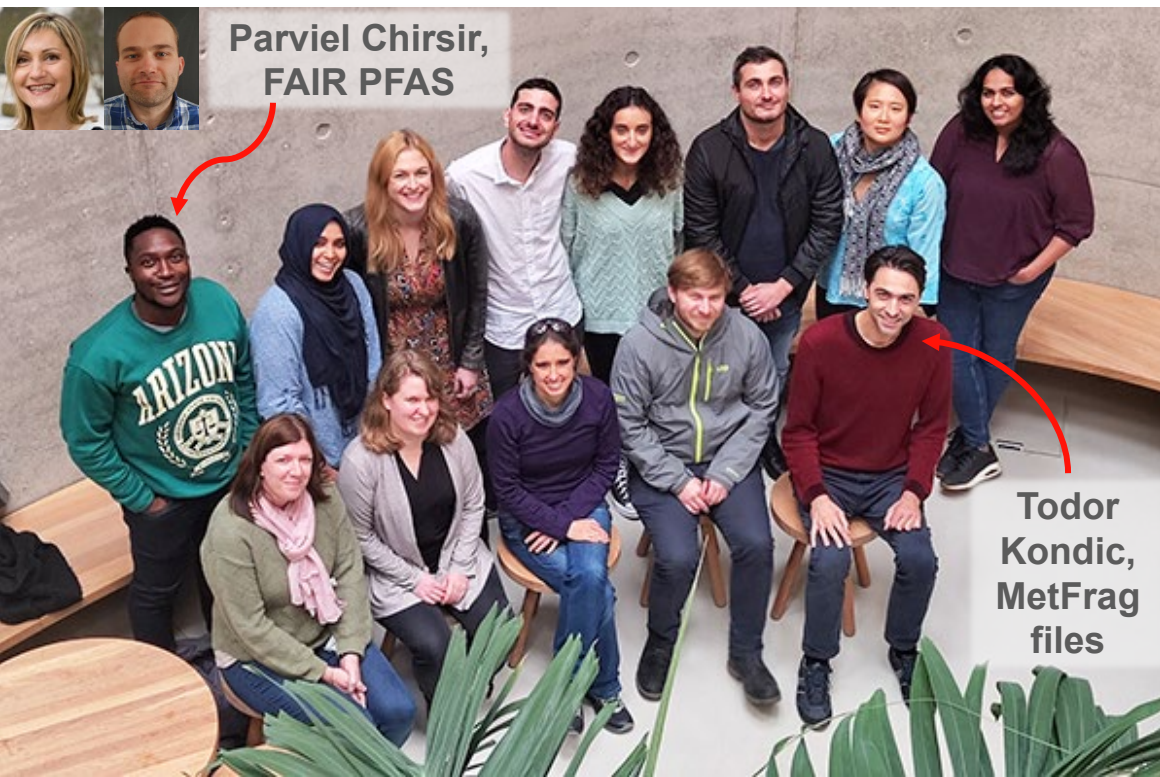
[DOI:10.5281/  
zenodo.7756622](https://doi.org/10.5281/zenodo.7756622)



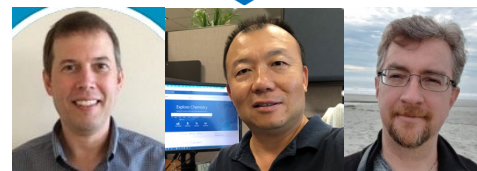
ZerO<sup>PM</sup>



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## PubChem



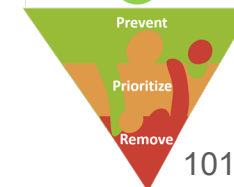
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Siqian + the whole team  
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# Outline

- Background and Motivation
- PubChem PFAS Tree
  - OECD PFAS & organofluorine compounds
  - PFAS suspect lists
  - Regulatory PFAS collections
  - PFAS breakdown by chemistry
- How many PFAS are really “out there”?
- Questions / Discussion

