

# Accessing information for Per- & Polyfluoroalkyl Substances using the US EPA CompTox Chemistry Dashboard

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*The views expressed in this presentation are those of the author and do not necessarily reflect the views or policies of the U.S. EPA*

*August 2018  
ACS Fall Meeting, Boston*

- EPA's National Center for Computational Toxicology is developing automated workflows for curating large databases within the DSSTox project, and providing accurate linkages of data to chemical structures, exposure and hazard information. The data are made available via the EPA's CompTox Chemistry Dashboard (<https://comptox.epa.gov/dashboard>), a publicly accessible website providing access to data for ~760,000 chemical substances, the majority of these represented as chemical structures. The web application delivers a wide array of computed and measured physicochemical properties, *in vitro* high-throughput screening data and *in vivo* toxicity data, as well as integrated chemical linkages to a growing list of literature, toxicology, and analytical chemistry websites. In addition, several specific search types are in development to directly support the mass spectrometry non-targeted screening community, enabling cohesive workflows to support data generation for the detection and assessment of environmental exposures to chemicals contained within DSSTox. The application provides access to segregated lists of chemicals that are of specific interest to relevant stakeholders, including, for example, scientists interested in Per- & Polyfluoroalkyl Substances (PFAS). Added lists include those sourced from the European Union as well as developed in-house and now containing thousands of chemicals. A procured testing library of hundreds of PFAS chemicals annotated into chemical categories has been integrated into the dashboard with a number of resulting benefits: a searchable database of chemical properties, with hazard and exposure predictions, and links to the open literature. This presentation will provide an overview of the dashboard, the developing library of PFAS chemicals and associated categorization, and new physicochemical property and environmental fate and transport QSAR prediction models developed for these chemicals. The application of the dashboard to support mass spectrometry non-targeted analysis studies for the identification of PFAS chemicals will also be reviewed.

# EPA activities around PFAS chemicals

<https://www.epa.gov/pfas>

## Per- and Polyfluoroalkyl Substances (PFAS)

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### What are PFAS?

PFAS is a category of man-made chemicals that are found in everyday items including food packaging, nonstick products, and stain repellent fabrics. [Learn more about PFAS](#), what they are, how people are exposed and [what EPA is doing](#).

1

2

3

"The [National Leadership Summit](#) on PFAS provided an unprecedented opportunity for stakeholders to share vital information and best practices regarding PFAS." -

*Former Administrator Pruitt*

- [Community Events](#)
- [Infographic](#)

### Basic Information

- [What are PFAS?](#)
- [Why are PFAS important?](#)
- [How people are exposed?](#)

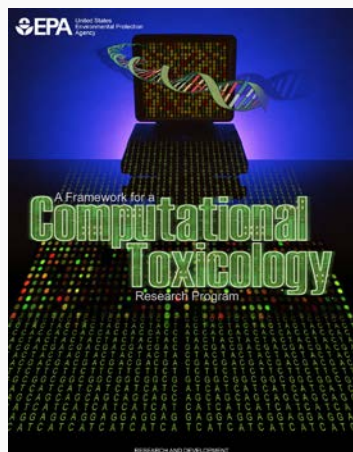
### EPA Actions to Address PFAS

- [EPA actions](#)
- [National leadership summit and engagement](#)

### Tools and Resources

- [EPA data and tools](#)
- [State information](#)
- [Site-specific resources](#)

# National Center for Computational Toxicology



- National Center for Computational Toxicology established in 2005 to integrate:
  - High-throughput and high-content technologies
  - Modern molecular biology
  - Data mining and statistical modeling
  - Computational biology and chemistry
- Researching computational approaches to quickly evaluate the safety of chemicals for potential risk.
- Outputs: a lot of data, models, algorithms and software applications
- **How can these efforts support research into PFAS chemicals?**

- A **publicly accessible website** delivering access:
  - ~762,000 chemicals with related property data
  - Experimental and predicted physicochemical property data
  - Experimental Human and Ecological hazard data
  - Integration to “biological assay data” for 1000s of chemicals
  - Information regarding consumer products containing chemicals
  - Links to other agency websites and public data resources
  - “Literature” searches for chemicals using public resources
  - “Batch searching” for thousands of chemicals
  - Real time prediction of physchem and toxicity endpoints
  - **Over 5,000 of the chemicals are classed as PFAS Chemicals**

# CompTox Dashboard

<https://comptox.epa.gov/dashboard>



United States  
Environmental Protection  
Agency

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762 Thousand Chemicals

Chemicals

Product/Use Categories

Assay/Gene

PFOS

☐ Identifier substring search

See what people are saying, read the dashboard [comments!](#)  
Cite the Dashboard Publication [click here](#)

## Latest News

[Read more news](#)

### Article "Suspect screening and non-targeted analysis of drinking water using point-of-use filters" uses the Dashboard

March 7th, 2018 at 8:59:16 AM

A recent article published by Newton et al in the National Exposure Research Laboratory focuses on [Suspect screening and non-targeted analysis of drinking water using point-of-use filters](#). The utility of the dashboard to help in the process of identifying chemicals is highlighted.



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# CompTox Dashboard

<https://comptox.epa.gov/dashboard>



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762 Thousand Chemicals

**Chemicals** [Product/Use Categories](#) [Assay/Gene](#)

Q Perfluor

Perfluorinated compounds  
DTXSID4031859



Perfluoro alkanes (linear)  
DTXSID30894934

Perfluoro compounds, C5-18  
DTXSID5029059



Perfluoro diacyl amides  
DTXSID10893889



Perfluoro dimethylethylpentane  
DTXSID50198289



Perfluoro iso n.p acrylates  
DTXSID60893637



Perfluoro tert-butylcyclohexane  
DTXSID70233868



Perfluoro-(2,5,8-trimethyl-3,6,9-trioxadodecanoic)acid  
DTXSID70276659

Perfluoro-(C6-18)-alkylphosphonic acid (Fluowet® PL 80, 80% aqueous solution)  
DTXSID20881914

## PFASEUOECD

PFAS Listed in OECD Global  
Database

## Perfluorooctanesulfonic acid

1763-23-1 | DTXSID3031864

Searched by DSSTox Substance Id.

### DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

► EXPOSURE

► BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

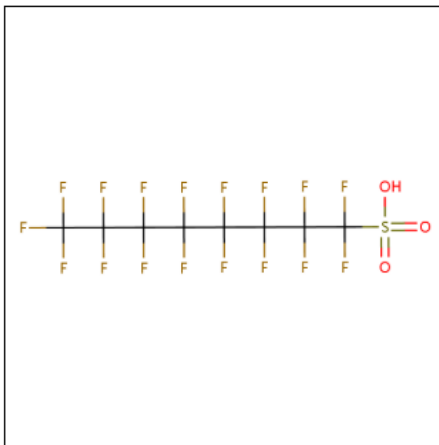
RELATED SUBSTANCES

SYNONYMS

► LITERATURE

LINKS

COMMENTS



### Wikipedia

**Perfluorooctanesulfonic acid** (conjugate base **perfluorooctanesulfonate**) (**PFOS**) is an anthropogenic fluorosurfactant and global pollutant. PFOS was the key ingredient in Scotchgard, a fabric protector made by 3M, and numerous stain repellents. It was added to Annex B of the Stockholm Convention on Persistent Organic Pollutants in May 2009. PFOS can be synthesized in industrial production or result from the degradation of precursors. PFOS levels that have been detected in wildlife

...  
[Read more](#)

### Intrinsic Properties

### Structural Identifiers

### Linked Substances

### Presence in Lists

### Record Information

### Quality Control Notes



# Executive Summary

## PFASEUOECD

PFAS Listed in OECD Global  
Database

DETAILS

**EXECUTIVE SUMMARY**

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RELATED SUBSTANCES

SYNONYMS

► LITERATURE

LINKS

COMMENTS

### Reproductive Toxicology

✓ 13 Reproductive toxicity PODs available [↗](#)

### Chronic Toxicology

✓ 15 Chronic toxicity PODs available [↗](#)

### Subchronic Toxicology

✓ 1 Subchronic toxicity PODs available [↗](#)

### Developmental Toxicology

✓ 8 Developmental toxicity PODs available [↗](#)

### Acute Toxicology

✓ 65 Acute toxicity PODs available [↗](#)

### Subacute Toxicology

✗ No subacute toxicity data available.

### Neurotoxicology

✗ No neurotoxicology data available.

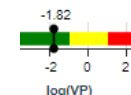
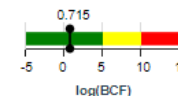
### Endocrine System

✓ Endocrine Disruption Potential. Significant Estrogen Receptor activity seen. Chemical was positive in 5 ER assays (out of 17) and was positive in 2 AR assays (tested in 10) .

Submit Comment

Search all data

HEM PARAMETERS



# Physicochemical properties

## Property



Summary



Summary

LogP: Octanol-Water

Melting Point

Boiling Point

Water Solubility

Vapor Pressure

Flash Point

Surface Tension

Index of Refraction

Molar Refractivity

Polarizability

Density

Molar Volume

Thermal Conductivity

Viscosity

Henry's Law

LogKoa: Octanol-Air

## Summary

Search query

Average	Experimental median	Predicted median	Experimental range	Predicted range	Unit
		3.43	3.32	2.40 to 3.64	
	156	138	153 to 156	125 to 157	°C
		360	200	343 to 401	°C
		1.00e-3	5.26e-4	5.44e-4 to 1.31e-3	mol/L
		3.43e-7	-	6.83e-8 to 2.59e-6	mmHg
		190	-	188 to 192	°C
			-	46.0	dyn/cm
			-	1.60	
			-	68.2	cm^3
			-	27.0	Å^3
		1.17	-	1.14 to 1.20	g/cm^3
			-	200	cm^3
			-	150	mW/(m^2K)

## An automated curation procedure for addressing chemical errors and inconsistencies in public datasets used in QSAR modelling

K. Mansouri, C. M. Grulke, A. M. Richard, R. S. Judson & A. J. Williams

To cite this article: K. Mansouri, C. M. Grulke, A. M. Richard, R. S. Judson & A. J. Williams (2016)

An automate  
datasets use  
DOI: [10.1081](https://doi.org/10.1081)

Mansouri et al. *J Cheminform* (2018) 10:10  
<https://doi.org/10.1186/s13321-018-0263-1>

 Journal of Cheminformatics

To link to th

RESEARCH ARTICLE

Open Access



## OPERA models for predicting physicochemical properties and environmental fate endpoints

Kamel Mansouri<sup>1,2,3\*</sup> , Chris M. Grulke<sup>1</sup>, Richard S. Judson<sup>1</sup> and Antony J. Williams<sup>1</sup>

# Detailed OPERA Prediction Reports

Source

Result

Calculation Details

Experimental Values

PhysPropNCCT

Predicted Values

EPISUITE

NICEATM

ACD/Labs Conse

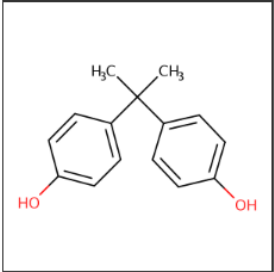
ACD/Labs

OPERA

OPERA Models: LogP: Octanol-Water

Bisphenol A

80-05-7 | DTXSID7020182



Model Results

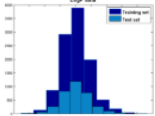
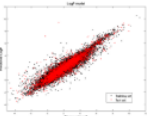
Predicted value: 3.35

Global applicability domain: Inside

Local applicability domain index: 0.88

Confidence level: 0.75

Model Performance

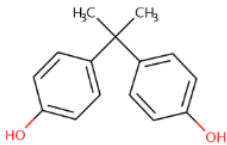


Weighted KNN model

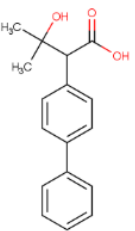
5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.89	0.85	0.87	0.88	0.78

QMRF

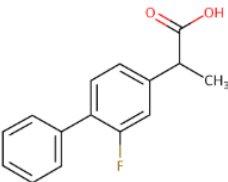
Nearest Neighbors from the Training Set



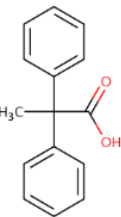
Bisphenol A  
Measured: 3.32  
Predicted: 3.35



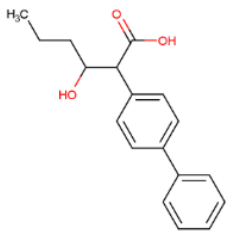
BUTANOIC ACID, 2-(4-BIPHENYL)-3-HYDROXY-  
Measured: 3.25  
Predicted: 3.45



Flurbiprofen  
Measured: 4.18  
Predicted: 3.83



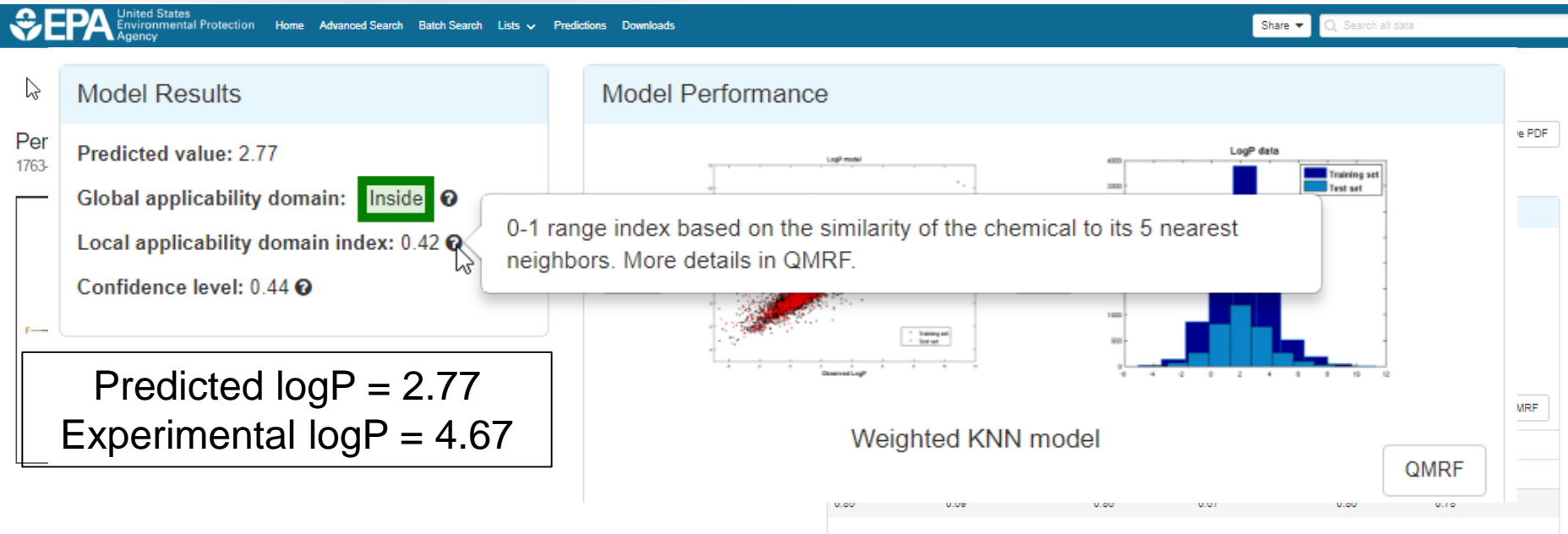
2,2-Diphenylpropionic acid  
Measured: 2.89  
Predicted: 2.93



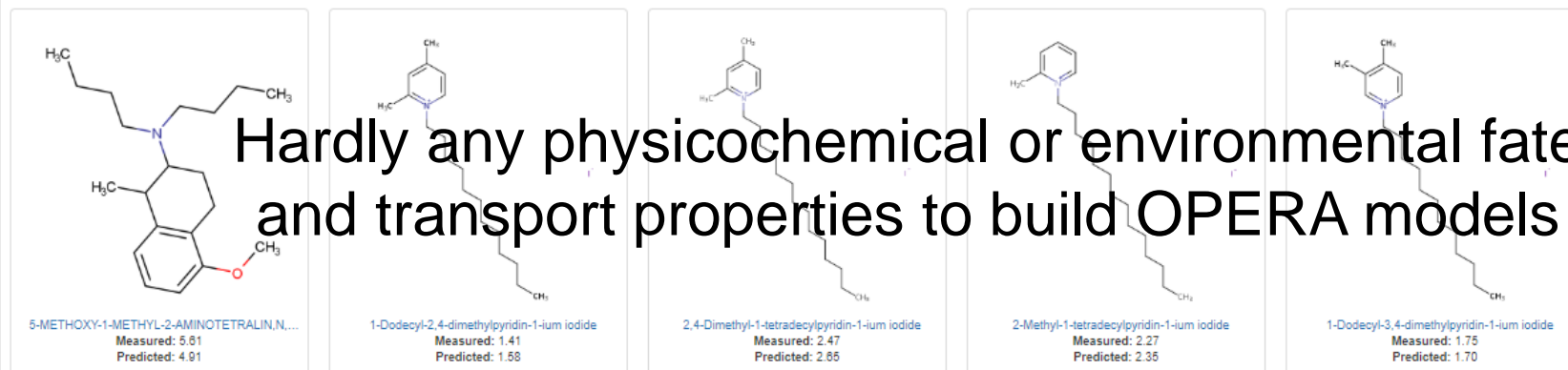
3-OH-2-(4-BIPHENYL)HEXANOIC ACID  
Measured: 3.75  
Predicted: 3.88

11

# Not much data for PFAS - yet



## Nearest Neighbors from the Training Set



- Physicochemical property and environmental fate and transport data has been extracted from the literature
- OPERA models will be rebuilt with these data for new predictions
- Data and predictions available Spring 2019



# Hazard Data – Human and Eco



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Environmental Protection  
Agency

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DETAILS

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**HAZARD**

ADME

► EXPOSURE

► BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES


SYNONYMS

► LITERATURE

LINKS

COMMENTS

DataType









 Ecotox Effect Level

 Download

 Human

 Eco


Columns

More	Priority	Toxval type	Subtype	Risk assessment class	Value	Units	Study type	Exposure route	Species	Subsource	Source
	6	EC10	-	growth:acute	2.6	mg/L	growth	static	sea urchin, echinoderm	J. Environ. Monit.14(5): 1375-1382	ECOTOX
	6	EC10	-	mortality:acute	3.2	mg/L	mortality	static	mysid	J. Environ. Monit.14(5): 1375-1382	ECOTOX
	6	EC50	-	mortality:acute	141.7	mg/L	mortality	renewal	black sandshell	Environ. Toxicol. Chem.31(7): 1611-1620	ECOTOX
	6	EC50	-	mortality:acute	158.1	mg/L	mortality	renewal	lamp-mussel	Environ. Toxicol. Chem.31(7): 1611-1620	ECOTOX
	6	EC50	-	mortality:acute	6.9	mg/L	mortality	static	mysid	J. Environ. Monit.14(5): 1375-1382	ECOTOX
	6	EC50	-	mortality:acute	158.1	mg/L	mortality	renewal	lamp-mussel	Environ. Toxicol. Chem.31(7): 1611-1620	ECOTOX
	6	EC50	-	growth:acute	20	mg/L	growth	static	sea urchin, echinoderm	J. Environ. Monit.14(5): 1375-1382	ECOTOX
	6	EC50	-	mortality:acute	158.1	mg/L	mortality	renewal	black sandshell	Environ. Toxicol. Chem.31(7): 1611-1620	ECOTOX

- ToxVal Database contains following data:
  - 30,050 chemicals
  - 772,721 toxicity values
  - 29 sources of data
  - 21,507 sub-sources
  - 4585 journals cited
  - 69,833 literature citations

### RELATED SUBSTANCES

## Download

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Environmental Protection  
Agency

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PFASEUOECD  
PFAS Listed in OECD Global  
Database

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EXPOSURE

BIOACTIVITY

TOXCAST: SUMMARY

PUBCHEM

TOXCAST: DATA

TOXCAST: MODELS

TOXCAST: MODELS

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

Perfluorooctanesulfonic acid  
1763-23-1 | DTXSID3031864  
Searched by DSSTox Substance Id.

QC Data ID	Grade	Description
Tox21_400083	Not determined	Analysis in progress

Assay Selection 1 Selected

A Single Assay Can Have Multiple Charts

Number of Charts: 4

☒ Active☐ Inactive☐ All

Filter

Filter assays

Assay Set: ER (0 of 18 Selected)

Assay Set: AR (1 of 11 Selected)

☐ ATG\_AR\_TRANS\_up

☐ NVS\_NR\_cAR

☒ NVS\_NR\_hAR

☐ NVS\_NR\_rAR

☐ OT\_AR\_ARELUC\_AG\_1440

☐ OT\_AR\_ARSRC1\_0480

☐ OT\_AR\_ARSRC1\_0960

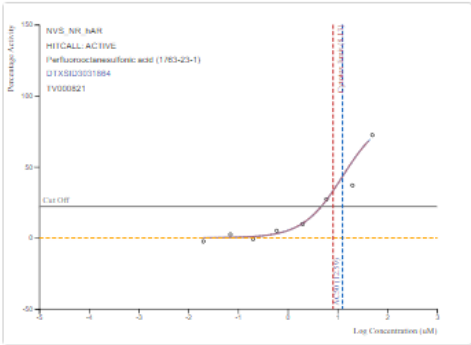
☐ Tox21\_AR\_BLA\_Agonist\_ratio

☐ Tox21\_AR\_BLA\_Antagonist\_ratio

☐ Tox21 AR LUC MDAKB2 Aagonist

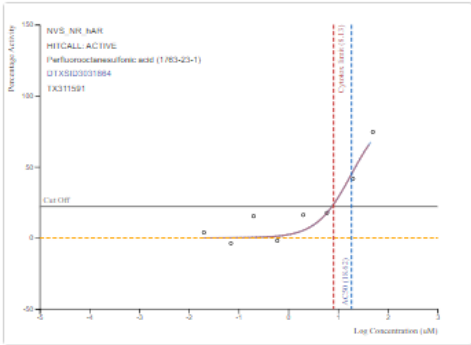
Percentage Activity

NVS\_NR\_hAR  
MITCALL: ACTIVE  
Perfluorooctanesulfonic acid (1763-23-1)  
DTXSID3031864  
TV000821




Percentage Activity

NVS\_NR\_hAR  
MITCALL: ACTIVE  
Perfluorooctanesulfonic acid (1763-23-1)  
DTXSID3031864  
TXK11591




Percentage Activity

NVS\_NR\_hAR  
MITCALL: ACTIVE  
Perfluorooctanesulfonic acid (1763-23-1)  
DTXSID3031864  
TXK11591



Percentage Activity

NVS\_NR\_hAR  
MITCALL: ACTIVE  
Perfluorooctanesulfonic acid (1763-23-1)  
DTXSID3031864  
TXK11591



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# What is PFOS Called?

## DETAILS

## EXECUTIVE SUMMARY

## PROPERTIES

## ENV. FATE/TRANSPORT

## HAZARD

## ADME

## ► EXPOSURE

## ► BIOACTIVITY

## SIMILAR COMPOUNDS

## GENRA (BETA)

## RELATED SUBSTANCES

## SYNONYMS

## ► LITERATURE

## LINKS

## COMMENTS

Per	Perfluorooctanesulfonic acid
17	Heptadecafluorooctane-1-sulfonic acid
Seal	1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-
	1763-23-1 <b>Active CAS-RN</b>
Syn	Heptadecafluorooctanesulfonic acid
Per	1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-
Hept	1-Octanesulfonic acid, heptadecafluoro-
1-O	EF 101
176	heptadecafluorooctane-1-sulfonic acid
Hept	heptadecafluorooctane-1-sulphonic acid
1-O	PFOS
1-O	EINECS 217-179-8
EF	1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-Heptadecafluoro-1-octanesulfonic acid
hep	
hep	
PFOS	
EIN	
1,1,	
1-P	
Eto	
UNI	
Per	
hep	

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Search all data

Search query

Quality

Valid

Valid

Valid

Valid

Valid

Valid

Valid

Valid

Valid

Valid

Good

Other

Other

Other

Other

Other

Other


Other

# Literature Searching - PubMed

## Perfluorooctanesulfonic acid

1763-23-1 | DTXSID3031864

Searched by Synonym from Valid Source.

1) Select PubMed starting point query then 2) click on Retrieve. 

Hazard ▼

Select a Query Term

Hazard

Fate and Transport

Metabolism/PK/PD

Chemical Properties

Exposure

Mixtures

Male Reproduction

Androgen Disruption

Female Reproduction

GeneTox

Cancer

Clinical Trials

Embryo and embryonic development

Child (infant through adolescent)

Dust and Exposure

Food and Exposure

Water and Exposure

Algae

Disaster / Emergency

Retrieve Articles 

Optionally, edit the query before retrieving.

("1763-23-1" OR "Perfluorooctanesulfonic acid" OR "perfluorooctane sulfonic acid")  
AND (NOAEL or NOEL OR LOEL or Rfd OR "reference dose" OR "reference  
concentration" OR "adverse effect level"[tiab] OR "cancer slope factor"[tiab])



# Literature Searching - PubMed

## Perfluorooctanesulfonic acid

1763-23-1 | DTXSID3031864

Searched by Synonym from Valid Source.

1) Select PubMed starting point query then 2) click on Retrieve.

Hazard

Retrieve Articles

23 of 23 articles loaded...

Optionally, edit the query before retrieving.

("1763-23-1" OR "Perfluorooctanesulfonic acid" OR "perfluorooctane sulfonic acid")  
AND (NOAEL or NOEL OR LOEL or Rfd OR "reference dose" OR "reference  
concentration" OR "adverse effect level"[tiab] OR "cancer slope factor"[tiab])

To find articles quickly, enter terms to sift abstracts.

Download / Send to...

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<input type="checkbox"/>	PMID	Year	Title	Authors	Journal	Rev
<input type="checkbox"/>	<a href="#">29525662</a>	2018	Modeling avian exposures to perfluoroalkyl substances in aquatic habitats...	Larson; Conder; Arblaster	Chemosphere	
<input type="checkbox"/>	<a href="#">28521193</a>	2017	Issues raised by the reference doses for perfluorooctane sulfonate and pe...	Dong; Bahar; Jit; Kennedy; Priestly; Ng; Lamb; Liu; ...	Environment international	
<input type="checkbox"/>	<a href="#">24046276</a>	2013	Dosimetric anchoring of in vivo and in vitro studies for perfluorooctanoate ...	Wambaugh; Setzer; Pitruzzello; Liu; Reif; Kleinstreu...	Toxicological sciences : an official journal of the Soc...	
<input type="checkbox"/>	<a href="#">22441698</a>	2012	Perfluorooctane sulfonate increases $\beta$ -oxidation of palmitic acid in chicke...	Nordén; Westman; Venizelos; Engwall	Environmental science and pollution research intern...	
<input type="checkbox"/>	<a href="#">21467747</a>	2011	Induction of apoptosis and CYP4A1 expression in Sprague-Dawley rats e...	Kim; Jun Kwack; Sik Han; Seok Kang; Hee Kim; Yo...	The Journal of toxicological sciences	
<input type="checkbox"/>	<a href="#">21207445</a>	2011	Aquatic predicted no-effect-concentration derivation for perfluorooctane s...	Qi; Wang; Mu; Wang	Environmental toxicology and chemistry	
<input type="checkbox"/>	<a href="#">20879709</a>	2010	Distribution of perfluorooctane sulfonate and other perfluorochemicals in t...	Wang; Fu; Wang; Liang; Pan; Cai; Jiang	Environmental science & technology	
<input type="checkbox"/>	<a href="#">20709355</a>	2010	Brominated flame retardants and perfluorinated compounds in indoor dust...	D'Hollander; Roossens; Covaci; Cornelis; Reynders; ...	Chemosphere	
<input type="checkbox"/>	<a href="#">19569327</a>	2009	Perfluoroalkyl contaminants in an Arctic marine food web: trophic magnific...	Kelly; Ikonoum; Blair; Surridge; Hoover; Grace; Go...	Environmental science & technology	
<input type="checkbox"/>	<a href="#">19343326</a>	2009	Chronic effects of perfluorooctanesulfonate exposure on immunotoxicity i...	Dong; Zhang; Zheng; Liu; Jin; He	Archives of toxicology	
<input type="checkbox"/>	<a href="#">19162172</a>	2009	Gestational and lactational exposure to potassium perfluorooctanesulfona...	Butenhoff; Ehresman; Chang; Parker; Stump	Reproductive toxicology (Elmsford, N.Y.)	
<input type="checkbox"/>	<a href="#">19110351</a>	2008	Behaviour of damselfly larvae (Enallagma cyathigerum) (Insecta, Odonata...	Van Gossuin; Bots; Snijders; Meyer; Van Wassenbe...	Environmental pollution (Barking, Essex : 1987)	

# Literature Searching - PubMed

## Perfluorooctanesulfonic acid

1763-23-1 | DTXSID3031864

Searched by Synonym from Valid Source.

1) Select PubMed starting point query then 2) click on Retrieve.

Hazard [Retrieve Articles](#)

23 of 23 articles loaded...

Optionally, edit the query before retrieving.

("1763-23-1" OR "Perfluorooctanesulfonic acid" OR "perfluorooctane sulfonic acid") AND (NOAEL or NOEL OR LOEL or Rfd OR "reference dose" OR "reference concentration" OR "adverse effect level"[tiab] OR "cancer slope factor"[tiab])

To find articles quickly, enter terms to sift abstracts.

exposure RfD immunotox [Clear Terms](#)

[Download / Send to...](#) [Download Sifter for Excel](#)

<input type="checkbox"/>	exposure	RfD	immunotox	Total	PMID	Year	Title	Authors	Journal	Rev
<input type="checkbox"/>	8	0	0	8	2952662	2018	Modeling avian exposures to perfluoroalkyl substan...	Larson; Conder; Arblaster	Chemosphere	
<input type="checkbox"/>	2	5	1	8	28521193	2017	Issues raised by the reference doses for perfluoroo...	Dong; Bahar; Jit; Kennedy; Priestly; Ng; Lamb; Liu; ...	Environment international	
<input type="checkbox"/>	0	0	0	0	24046276	2013	Dosimetric anchoring of in vivo and in vitro studies f...	Wambaugh; Setzer; Pitruzzello; Liu; Reif; Kleinstreu...	Toxicological sciences : an official journal of the Soc...	
<input type="checkbox"/>	0	0	0	0	22441698	2012	Perfluorooctane sulfonate increases $\beta$ -oxidation of ...	Nordén; Westman; Venizelos; Engwall	Environmental science and pollution research intern...	
<input type="checkbox"/>	0	0	0	0	21467747	2011	Induction of apoptosis and CYP4A1 expression in S...	Kim; Jun Kwack; Sik Han; Seok Kang; Hee Kim; Yo...	The Journal of toxicological sciences	
<input type="checkbox"/>	0	0	0	0	21207445	2011	Aquatic predicted no-effect-concentration derivation...	Qi; Wang; Mu; Wang	Environmental toxicology and chemistry	
<input type="checkbox"/>	0	0	0	0	20879709	2010	Distribution of perfluorooctane sulfonate and other p...	Wang; Fu; Wang; Liang; Pan; Cai; Jiang	Environmental science & technology	
<input type="checkbox"/>	1	0	0	1	20709355	2010	Brominated flame retardants and perfluorinated co...	D'Hollander; Roosens; Covaci; Cornelis; Reynders; ...	Chemosphere	
<input type="checkbox"/>	2	0	0	2	19569327	2009	Perfluoroalkyl contaminants in an Arctic marine food...	Kelly; Ikonou; Blair; Surridge; Hoover; Grace; Go...	Environmental science & technology	
<input type="checkbox"/>	3	0	1	4	19343326	2009	Chronic effects of perfluorooctanesulfonate exposur...	Dong; Zhang; Zheng; Liu; Jin; He	Archives of toxicology	
<input type="checkbox"/>	3	0	0	3	19162172	2009	Gestational and lactational exposure to potassium p...	Butenhoff; Ehresman; Chang; Parker; Stump	Reproductive toxicology (Elmsford, N.Y.)	
<input type="checkbox"/>	2	0	0	2	19110351	2008	Behaviour of damselfly larvae (Enallagma cyathiger...	Van Gossum; Bots; Snijders; Meyer; Van Wassenbe...	Environmental pollution (Barking, Essex : 1987)	

### Issues raised by the reference doses for perfluorooctane sulfonate and perfluorooctanoic acid.

On 25th May 2016, the U.S. EPA released reference doses (RfDs) for Perfluorooctane Sulfonate (PFOS) and Perfluorooctanoic Acid (PFOA) of 20ng/kg/day, which were much more conservative than previous values. These RfDs rely on the choices of animal point of departure (PoD) and the toxicokinetics (TK) model. At this stage, considering that the human evidence is not strong enough for RfD determination, using animal data may be appropriate but with more uncertainties. In this article, the uncertainties concerning RfDs from the choices of PoD and TK models are addressed. Firstly, the candidate PoDs should include more critical endpoints (such as immunotoxicity), which may lead to lower RfDs. Secondly, the reliability of the adopted three-compartment TK model is compromised: the parameters are not non-biologically plausible; and this TK model was applied to simulate gestation and lactation exposures, while the two exposure scenarios were not actually included in the model structure.

# Generalized Read-Across (GenRA)

**EPA** United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Copy Share Submit Comment Search all data

PFAS EUCED  
PFAS Listed in OECD Global Database

**Perfluorooctanesulfonic acid**  
1763-23-1 | DTXSID3031864  
Searched by DSSTox Substance Id.

DETAILS  
EXECUTIVE SUMMARY  
PROPERTIES  
ENV. FATE/TRANSPORT  
HAZARD  
ADME  
EXPOSURE  
BIOACTIVITY  
SIMILAR COMPOUNDS  
**GENRA (BETA)**  
RELATED SUBSTANCES  
SYNONYMS  
LITERATURE  
LINKS  
COMMENTS

**Step One: Analog Identification and Evaluation**

Neighbors by: Chem: Morgan Fgrpts Filter by: invivo data

**PFOS**

PFOS-K Sulfonamid PFBS-K PFOA, ammon... PFHxA Sulfury fluoride Sodium perfluor...

# of Analogs 10

Next

Summary Data Step Analogs

Substance	Invivo	Invivo	Invivo	Invivo
PFOS	1	1	1	1
PFOS-K	1	1	1	1
Sulfonamid	1	1	1	1
PFBS-K	1	1	1	1
PFOA, ammon...	1	1	1	1
PFHxA	1	1	1	1
Sulfury fluoride	1	1	1	1
Sodium perfluor...	1	1	1	1
PFOS-K	1	1	1	1
PFBS-K	1	1	1	1

Select and Review Analogs

# Generalized Read-Across (GenRA)

PFAS EUCED  
PFAS Listed in OECD Global  
Database

## Perfluorooctanesulfonic acid

1763-23-1 | DTXSID3031864

Searched by DSSTox Substance Id.

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

EXPOSURE

BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

LITERATURE

LINKS

COMMENTS

### Step Two: Data Gap Analysis & Generate Data Matrix

Neighbors by: Chem: Morgan Fgprts Filter by: invivo data Summary Data Gap Analysis Group: ToxRef By: Tox Fingerprint Generate Data Matrix

**Summary Data Gap Analysis**

	bio_b21	bio_tox	chem_ct	tox_bnf
PFOS	31	821	21	95
PFOS-K	38	714	21	307
Sulfuramid	29	714	21	282
PFBS-K	2	714	19	187
PFOA, ammonium salt	19	714	20	345
PFHxA	24	714	17	85
Sodium perfluorohexano...	0	0	18	282
Sulfuryl fluoride	0	0	8	345
Bis(trichloromethyl)sulfone	0	0	8	158
Tetrakis(hydroxymethyl)...	25	0	8	408
Aldoxycarb	9	228	6	83

**Generate Data Matrix**

	PFOS	PFOS-K	Sulfuramid	PFBS-K	PFOA, ammonium	PFHxA	Sodium perfluorohexano...	Sulfuryl fluoride	Bis(trichloromethyl)sulfone	Tetrakis(hydroxymethyl)sulfone	Aldoxycarb
CHR:Abdominal Cavity											
CHR:Adrenal Gland											
CHR:Artery (General)											
CHR:Auditory Stairle Re...											
CHR:Bile duct											
CHR:Blood											
CHR:Blood vessel											
CHR:Body Weight											
CHR:Bone											
CHR:Bone Marrow											
CHR:Brain											
CHR:Bronchus											

Select and Review Analogs

Review Available Data

Fingerprint indicating available data

# Generalized Read-Across (GenRA)



Red : Toxicity effects.  
Blue: No Toxicity effects  
Grey : Absence of data

# Are there Similar Compounds?

**EPA** United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Copy Share Submit Comment Search all data

## Perfluorooctanesulfonic acid

1763-23-1 | DTXSID3031864

Searched by Synonym from Valid Source.

Searched with a similarity threshold of 0.8

83 chemicals

Download / Send

Sort by: TOXCAST 8

Show info: DTXSID CASRN TOXCAST Select all

Filter by: Name or CASRN Hide

<p>Potassium perfluorooctanesulfonate DTXSID: DTXSID08037706 CASRN: 2766-39-3 TOXCAST: 84/576</p>	<p>Lithium perfluorooctanesulfonate DTXSID: DTXSID2032421 CASRN: 29457-72-5 TOXCAST: 8/116</p>	<p>Potassium perfluorohexanesulfonate DTXSID: DTXSID2037709 CASRN: 3871-99-6 TOXCAST: 29/611</p>	<p>Potassium perfluorobutanesulfonate DTXSID: DTXSID3037707 CASRN: 29420-49-3 TOXCAST: 2/534</p>	<p>Sodium 1,1,2,2,3,3,4,4,4-nonafluoro-1-b... DTXSID: DTXSID10893309 CASRN: 102061-62-5 TOXCAST: 0</p>	<p>Sodium Perfluorononanesulfonate DTXSID: DTXSID50893308 CASRN: 98789-57-2 TOXCAST: 0</p>
<p>Perfluoro(7-methyloctanesulfonate) pot... DTXSID: DTXSID90893281 CASRN: 40365-28-4 TOXCAST: 0</p>	<p>Perfluoropropane sulfonate DTXSID: DTXSID00892967 CASRN: 110676-15-6 TOXCAST: 0</p>	<p>Heptadecafluorooctane-1-(2H)sulfonic a... DTXSID: DTXSID00892720 CASRN: NOCAS_892720 TOXCAST: 0</p>	<p>Perfluoroheptanesulfonate DTXSID: DTXSID20892505 CASRN: 146689-46-5 TOXCAST: 0</p>	<p>Perfluoropentanesulfonate DTXSID: DTXSID70892479 CASRN: 175905-36-9 TOXCAST: 0</p>	<p>Sodium perfluorohexanesulfonate DTXSID: DTXSID60892476 CASRN: 82382-12-5 TOXCAST: 0</p>



# Relationships in the data

## Perfluorooctanesulfonic acid

1763-23-1 | DTXSID3031864

Searched by Synonym from Valid Source.

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

EXPOSURE

BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

LITERATURE

LINKS

COMMENTS

12 chemicals

Download / Send

Sort by: Relationship

Show info: DTXSID CASRN

Select all

Filter by: Name or CASRN

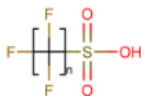
Hide

Searched Chemical



Perfluorooctanesulfonic acid  
DTXSID: DTXSID3031864  
CASRN: 1763-23-1

Markush Parent



Perfluoroalkyl sulfonates  
DTXSID: DTXSID70892979  
CASRN: NOCAS\_892979

Predecessor: Component

3 related chemical  
structures with this  
substance

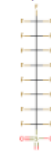
Mixture of PFOS and PFOA  
DTXSID: DTXSID20872983  
CASRN: NOCAS\_872983

Predecessor: Component

3 related chemical  
structures with this  
substance

1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5...  
DTXSID: DTXSID40880545  
CASRN: 84202-77-3

Component



Perfluorooctanesulfonate  
DTXSID: DTXSID80108992  
CASRN: 45298-90-6

Salt Form



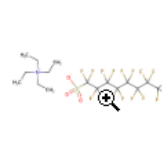
Potassium perfluorooctanesulfonate  
DTXSID: DTXSID8037706  
CASRN: 2795-39-3

Salt Form



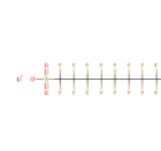
Ammonium perfluorooctanesulfonate  
DTXSID: DTXSID9097435  
CASRN: 29081-56-9

Salt Form



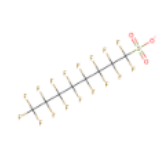
Tetraethylammonium perfluorooctanes...  
DTXSID: DTXSID5089128  
CASRN: 56773-42-3

Salt Form



Lithium perfluorooctanesulfonate  
DTXSID: DTXSID2032421  
CASRN: 29457-72-5

Salt Form



Sodium perfluorooctanesulfonate  
DTXSID: DTXSID50635462  
CASRN: 4021-47-0

# 7 salt forms of PFOS (and the ion)

Component



Perfluorooctanesulfonate

DTXSID: DTXSID80108992  
CASRN: 45298-90-6

Salt Form



Potassium perfluorooctanesulfonate

DTXSID: DTXSID8037708  
CASRN: 2795-39-3

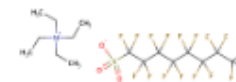
Salt Form



Ammonium perfluorooctanesulfonate

DTXSID: DTXSID9087435  
CASRN: 29081-56-9

Salt Form



Tetraethylammonium perfluorooctanesu...

DTXSID: DTXSID5069128  
CASRN: 56773-42-3

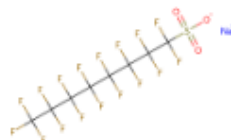
Salt Form



Lithium perfluorooctanesulfonate

DTXSID: DTXSID2032421  
CASRN: 29457-72-5

Salt Form



Sodium perfluorooctanesulfonate

DTXSID: DTXSID50635462  
CASRN: 4021-47-0

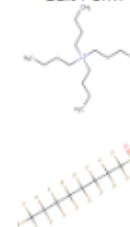
Salt Form



Magnesium bis(perfluorooctane...

DTXSID: DTXSID80881314  
CASRN: 91036-71-4

Salt Form



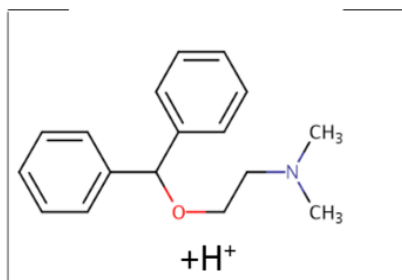
Tetrabutylammonium perfluorooctanesu...

DTXSID: DTXSID40584995  
CASRN: 111873-33-7

# Using data relationships

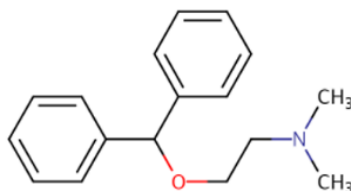
- We have purposely built relationships in the data. Specifically, “MS-Ready mappings”

A) Molecular Ion



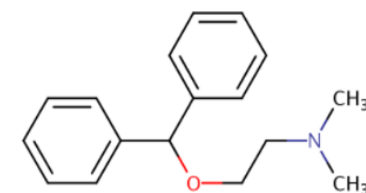
$m/z \approx 256.1702$

B) MS-Ready Form

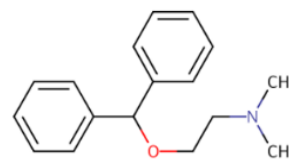


monoisotopic mass= 255.1623  
 $C_{17}H_{21}NO$   
DTXCID802949

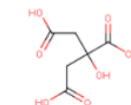
C) Mappings from MS-Ready



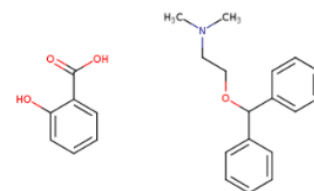
Diphenhydramine  
 $C_{17}H_{21}NO$  | 255.1623  
DTXSID4022949



Diphenhydramine  
hydrochloride  
 $C_{17}H_{22}ClNO$  | 291.1390  
DTXSID4020537



Diphenhydramine citrate  
 $C_{23}H_{29}NO_8$  | 447.1893  
DTXSID80237211



Diphenhydramine salicylate  
 $C_{24}H_{27}NO_4$  | 393.1940  
DTXSID10225883

# Advanced Search


## Supporting Target/Non-Target MS

### Advanced Search


#### Mass Search


**Select Adduct:**  ▼

Mass  Da  Error Da

Search 

#### Molecular Formula Search


☐ MS Ready Formula 

☒ Exact Formula 

Search 

#### Generate Molecular Formula(e)

Mass  Da  Error

Search 

# 2 Chemicals match the formula

## Search Results

Searched by Exact Molecular Formula: C<sub>8</sub>HF<sub>17</sub>O<sub>3</sub>S.

2 of 2 chemicals visible

Download / Send ▾

Show info: Data Picker ▾

Select all



Sort by: DTXSID ▾

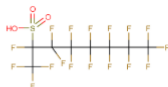


Filter by: Name or CASRN

Multicomponent Chemicals ✕ ▾



Perfluorooctanesulfonic acid



Heptaecafluorooctane-2-sulfonic acid

# Advanced Search


## Supporting Target/Non-Target MS

### Advanced Search ?



#### Mass Search


**Select Adduct:**  ▼

Da ±




#### Molecular Formula Search

☒ **MS Ready Formula **  
☐ **Exact Formula **



#### Generate Molecular Formula(e)

Da ±





# 22 Chemicals match the formula

## Search Results

Searched by MS Ready Formula: C8HF17O3S.

22 chemicals

Download / Send

Show info:

DTXSID

CASRN

TOXCAST

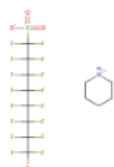
Select all

Sort by: DTXSID

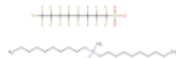


Filter by: Name or CASRN

Hide



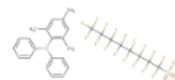
Piperidinium perfluorooctanesulfonate  
DTXSID: DTXSID0072352  
CASRN: 71483-74-8  
TOXCAST: 0



N-Decyl-N,N-dimethyl-1-decanaminium...  
DTXSID: DTXSID00882964  
CASRN: 261099-16-8  
TOXCAST: 0



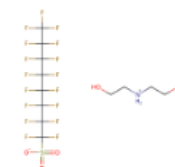
Heptadecafluorooctane-1-(2H)sulfonic a...  
DTXSID: DTXSID00892720  
CASRN: NOCAS\_892720  
TOXCAST: 0



Diphenyl(2,4,8-trimethylphenyl)sulfoni...  
DTXSID: DTXSID00893373  
CASRN: 268341-99-0  
TOXCAST: 0



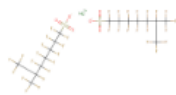
Lithium perfluorooctanesulfonate  
DTXSID: DTXSID2032421  
CASRN: 29457-72-8  
TOXCAST: 8/116



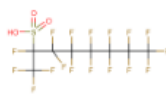
Bis(2-hydroxyethyl)ammonium perfluor...  
DTXSID: DTXSID2072049  
CASRN: 70225-14-8  
TOXCAST: 0



Perfluorooctanesulfonic acid  
DTXSID: DTXSID3031864  
CASRN: 1763-23-1  
TOXCAST: 175/889



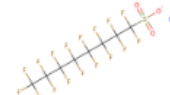
Magnesium heptadecafluoroisooctanes...  
DTXSID: DTXSID30881127  
CASRN: 93894-73-6  
TOXCAST: 0



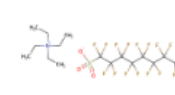
Heptadecafluorooctane-2-sulfonic acid  
DTXSID: DTXSID30885921  
CASRN: 927870-12-0  
TOXCAST: 0



Tetrabutylammonium perfluorooctanesu...  
DTXSID: DTXSID40584995  
CASRN: 111873-33-7  
TOXCAST: 0



Sodium perfluorooctanesulfonate  
DTXSID: DTXSID50835482  
CASRN: 4021-47-0  
TOXCAST: 0



Tetraethylammonium perfluorooctanesu...  
DTXSID: DTXSID5089128  
CASRN: 66773-42-3  
TOXCAST: 0

# 22 Chemicals match the formula



## Search Results

Searched by MS Ready Formula: C<sub>8</sub>HF<sub>17</sub>O<sub>3</sub>S.

22 chemicals

Download / Send

Select all



Sort by: Sources



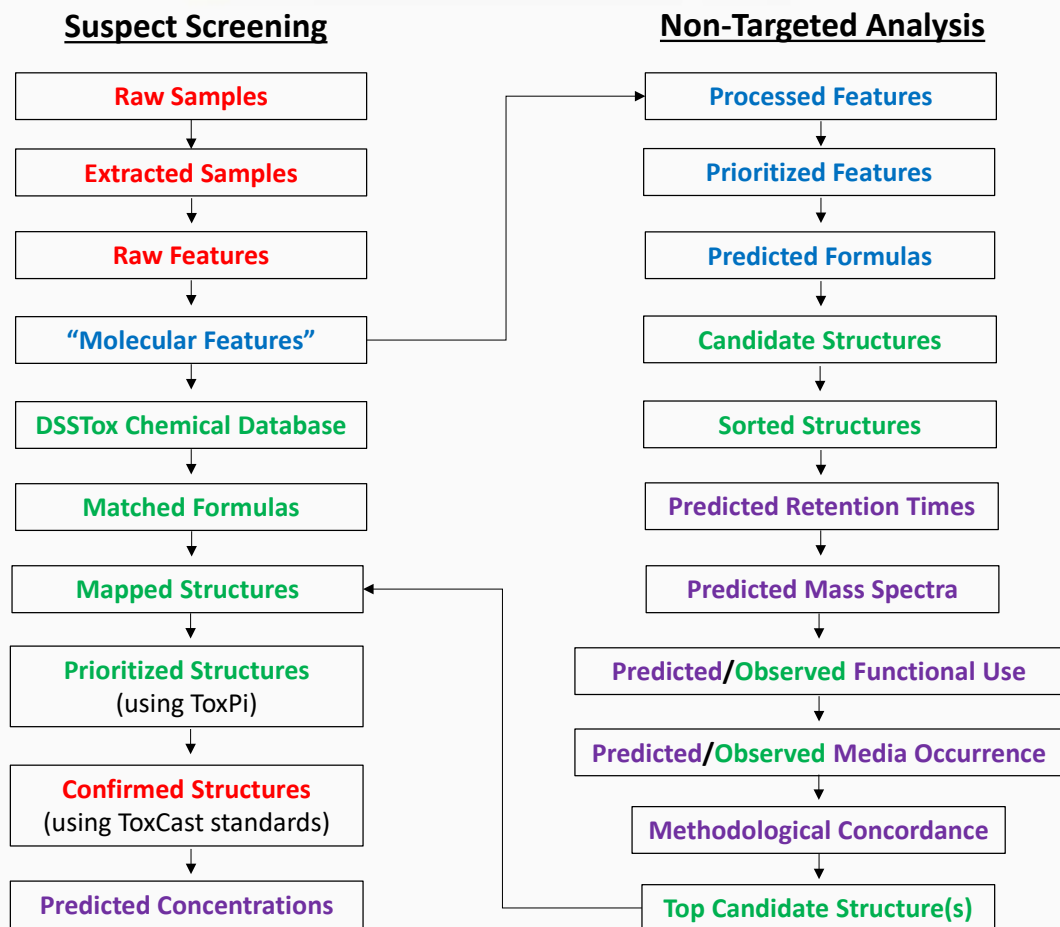
Filter by: Name or CASRN

Hide

Structure	DTXSID	Preferred Name	CASRN	QC Level	CPDat Count	Number of Sources	PubChem Data Sources	PubMed Ref. Counts	Monoisotopic Mass
	<a href="#">DTXSID3031864</a> ToxCast™	Perfluorooctanesulfonic acid	1763-23-1	Level 1	10	88	68	1124	499.937494
	<a href="#">DTXSID8037706</a> ToxCast™	Potassium perfluorooctanesulfonate	2795-39-3	Level 1	18	51	59	0	537.893375
	<a href="#">DTXSID2032421</a> ToxCast™	Lithium perfluorooctanesulfonate	29457-72-5	Level 1	14	36	32	0	505.945672
	<a href="#">DTXSID5069128</a>	Tetraethylammonium perfluorooctanesulfonate	56773-42-3	Level 2	13	27	42	0	629.089243

<https://epa.gov>

# Suspect Screening and Non-Targeted Analysis Workflow



## Color Key

**Red** = Analytical Chemistry  
**Blue** = Data Processing & Analysis  
**Purple** = Mathematical & QSPR Modeling  
**Green** = Informatics & Web Services



# How to search 1000s of formulae?

# Batch Searches








## Batch Search?



### Step Three: Select Download Data or Display Chemicals

Please enter one identifier per line

#### Select Input Type(s)

- ☒ Identifiers
  - ☐ Chemical Name 
  - ☒ CASRN 
  - ☐ InChIKey 
  - ☐ DSSTox Substance ID 
- ☐ InChIKey Skeleton 
- ☐ MS-Ready Formula(e) 
- ☐ Exact Formula(e) 
- ☐ Monoisotopic Mass

 Display All Chemicals

... Download Chemical Data

#### Enter Identifiers to Search (searches should be limited to <5000 identifiers)

2795-39-3  
29457-72-5  
56773-42-3  
45298-90-6  
29081-56-9  
70225-14-8  
251099-16-8  
71463-74-6  
4021-47-0






# Batch Searches

## Select Output Format.






Download as...

TSV  
CSV  
Excel  
SDF






### Chemical Identifiers

- ☒ DTXSID 
- ☒ Chemical Name 
- ☐ CAS-RN 
- ☐ InChIKey 
- ☐ IUPAC Name 

### Structures

- ☐ Mol File 
- ☐ SMILES 
- ☐ InChI String 
- ☒ MS-Ready SMILES 
- ☐ QSAR-Ready SMILES 

### Intrinsic And Predicted Properties

- ☒ Molecular Formula 
- ☐ Average Mass 
- ☐ Monoisotopic Mass 
- ☒ TEST Model Predictions 
- ☒ OPERA Model Predictions 

### Metadata

 Download

### Presence in Lists:

- ☐ ICCVAM test method evaluation report: in vitro ocular toxicity test methods
- ☐ 40CFR355
- ☐ A list of all PBDEs (Polybrominated diphenyl ethers)
- ☐ A list of all PCBs (Polychlorinated biphenyls)
- ☐ A list of polycyclic aromatic hydrocarbons
- ☒ Acute exposure guideline levels
- ☐ Algal Toxins
- ☐ Androgen Receptor Chemicals
- ☐ APCRA Chemicals for Prospective Analysis
- ☐ APCRA Chemicals for Retrospective Analysis
- ☐ APCRA Chemicals for Retrospective Analysis\_App\_List\_448\_Chemicals
- ☒ ATSDR Minimal Risk Levels (MRLs) for Hazardous Substances
- ☐ ATSDR Toxic Substances Portal Chemical List
- ☐ Bisphenol Compounds
- ☒ California Office of Environmental Health Hazard Assessment
- ☐ Chemicals with interesting names
- ☐ CMAP
- ☐ DNT Screening Library
- ☒ Drinking Water Suspects, KWR Water, Netherlands
- ☐ EDSP Universe
- ☐ EPA Chemicals associated with hydraulic fracturing
- ☐ EPA Consumer Products Suspect Screening Results

- Specific subsets of chemicals, “lists”, can be displayed on the dashboard
- If there are chemicals that map together then these link to existing:
  - Property data
  - Hazard data
  - Exposure data
  - *In vitro* bioassay data
  - Documents and Literature



# Batch Searches to Support MS-Analysis

## MS-Ready Structures Underpin Analysis

**Mass Search** ⓘ

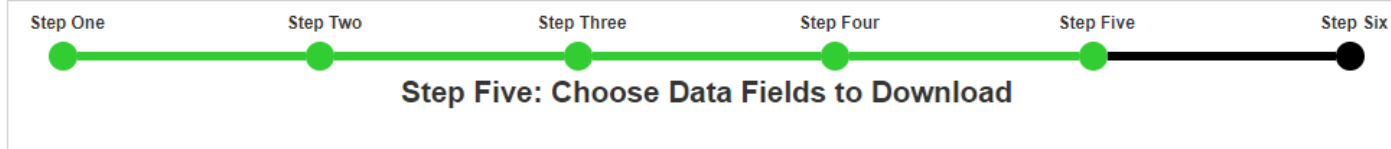
Da

**Molecular Formula Search** ⓘ

☒ MS Ready Formula ⓘ  
☐ Exact Formula ⓘ

**Generate Molecular Formula(e)** ⓘ

Da



Please enter one identifier per line

Select Input Type(s)

- ☐ Chemical Name ⓘ
- ☐ CASRN ⓘ
- ☐ InChIKey ⓘ ☐ Skeleton ⓘ
- ☐ DSSTox Substance ID ⓘ
- ☒ MS-Ready Formula(e) ⓘ
- ☐ Exact Formula(e) ⓘ
- ☐ Monoisotopic Mass

Enter Identifiers to Search (searches should be limited to <1000 identifiers)

C14H22N2O3  
C10H12N2O  
C14H18N4O3  
C12H11N7  
C8H9NO2

# A List of Lists of Chemicals

[https://comptox.epa.gov/dashboard/chemical\\_lists](https://comptox.epa.gov/dashboard/chemical_lists)



## Chemistry Dashboard

Aa ▼

Aa

Aa ▲

### Select List



List Name	Number of Chemicals	List Description
40CFR355	354	Extremely Hazardous Substance List and Threshold Planning Quantities; Emergency Planning and Release Notification Requirements; Final Rule. (52 FR 13378)
Algal Toxins	54	A set of algal toxins of interest
Androgen Receptor Chemicals	110	The list of chemicals used to identify references with in vitro AR binding . From Kleinstrauer et al <a href="http://pubs.acs.org/doi/abs/10.1021/acs.chemrestox.6b00347">http://pubs.acs.org/doi/abs/10.1021/acs.chemrestox.6b00347</a>
ATSDR Toxic Substances Portal Chemical List	200	The Agency for Toxic Substances and Disease Registry (ATSDR) is a federal public health agency of the U.S. Department of Health and Human Services.
Bisphenol Compounds	52	This list represents a collection of Bisphenol Compounds
California Office of Environmental Health Hazard Assessment	972	The OEHHA Chemical Database is a compilation of health hazard information including reference exposure levels, California public health goals, child-specific reference doses, Propos. 65 safe harbor numbers, soil-screening levels, and fish advisories
Chemicals with interesting names	17	This is a list of chemicals with interesting and fun names
EPA Integrated Risk Information System (IRIS)	510	EPA's IRIS Program identifies and characterizes the health hazards of chemicals found in the environment. Each IRIS assessment can cover a chemical, a group of related chemicals, or a complex mixture.
EPAHFR - EPA Chemicals associated with hydraulic fracturing	1640	EPAHFR lists chemicals associated with hydraulic fracturing from 2005-20013, as reported in EPA's Hydraulic Fracturing Drinking Water Assessment Final Report (Dec 2016)
EU Cosmetic Ingredients Inventory (Combined 2000/2006)	2878	EUCOSMETICS contains the Combined Inventory of Ingredients Employed in Cosmetic Products (2000, SCCNFP/0389/00 Final) and Revised Inventory (2006, Decision 2006/257/EC), prepared for NORMAN by P. von der Ohe (UBA) and R. Aalizadeh (Uni. Athens).
EU ToxRisk Dataset	230	Compounds of interest to the EU-ToxRisk Case Studies.
French Monitoring List	1171	FRENCHLIST contains substances for prospective monitoring activities in France, developed in cooperation with the NORMAN Network Working Group 1 on Prioritization. Provided by Valeria Dulio, INERIS, France. Further details on the website.

# 11 PFAS Lists

[http://comptox-prod.epa.gov/dashboard/chemical\\_lists](http://comptox-prod.epa.gov/dashboard/chemical_lists)

## Select List

Show 10 entries

Search: pfas

Download

List Acronym	List Name	Last Updated	Number of Chemicals	List Description
EPAPFAS75S1	<a href="#">EPA PFAS List of 75 Test Samples (Set 1)</a>	2018-06-29	74	PFAS list corresponds to 75 samples (Set 1) submitted for initial testing screens conducted by EPA researchers in collaboration with researchers at the National Toxicology Program.
EPAPFASCAT	<a href="#">Registered DSSTox "category substances" representing Per- and Polyfluoroalkyl Substances (PFAS) categories</a>	2018-06-29	64	List of registered DSSTox "category substances" representing PFAS categories created using ChemAxon's Markush structure-based query representations.
EPAPFASINSOL	<a href="#">PFAS in EPA's Chemical Inventory Insoluble in DMSO</a>	2018-06-29	43	PFAS chemicals included in EPA's expanded ToxCast chemical inventory found to be insoluble in DMSO above 5mM.
EPAPFASINV	<a href="#">PFAS in EPA's ToxCast Chemical Inventory</a>	2018-06-29	430	PFAS chemicals included in EPA's expanded ToxCast chemical inventory and available for testing.
EPAPFASRL	<a href="#">EPA PFAS Cross-Agency Research List</a>	2018-07-27	194	EPAPFASRL is a manually curated listing of mainly straight-chain and branched PFAS (Per- & Poly-fluorinated alkyl substances) compiled from various internal, literature and public sources by EPA researchers and program office representatives.
PFASEPA	<a href="#">PFAS_EPA List of Perfluorinated alkyl substances</a>	2017-11-03	190	PFAS_EPA (Perfluorinated alkyl substances) is a manually curated listing of mainly straight-chain and branched PFAS substances
PFASEUOECD	<a href="#">PFAS Listed in OECD Global Database</a>	2018-07-26	4725	OECD released a New Comprehensive Global Database of Per- and Polyfluoroalkyl Substances, (PFASs) listing approximately 4700 new PFAS
PFASGRACE	<a href="#">PFASforGrace</a>	2017-02-16	35	A list of polyfluorinated chemicals of interest to Grace Patlewicz
PFASKEMI	<a href="#">PFAS List from the Swedish Chemicals Agency (KEMI) Report</a>	2017-02-09	2397	Perfluorinated substances from a Swedish Chemicals Agency (KEMI) Report on the occurrence and use of highly fluorinated substances.
PFASMASTER	<a href="#">PFAS Master List of PFAS Substances</a>	2018-07-26	5061	PFASMASTER is a consolidated list of PFAS substances spanning and bounded by the below lists of current interest to researchers and regulators worldwide.

Showing 1 to 10 of 11 entries (filtered from 96 total entries)



Port

HOME



## The OECD releases a new list of PFASs

The OECD releases a new list of Per- and Polyfluoroalkyl Substances (PFASs) based on a comprehensive analysis of information available in the public domain. In total, 4730 PFAS-related CAS numbers have been identified and categorised in this study, including several new groups of PFASs that fulfil the common definition of PFASs (i.e. they contain at least one perfluoroalkyl moiety) but have not yet been commonly regarded as PFASs.

This work has been conducted under the OECD/UN Environment Global PFC Group in support of the Strategic Approach to International Chemicals Management (SAICM) and shifting to safer alternatives for PFASs.

The [New Comprehensive Global Database of Per- and Polyfluoroalkyl Substances \(PFASs\)](#) comes with a [methodology report](#) also detailing the major findings with respect to the total numbers and types of PFASs identified, the limitations, gaps and challenges identified in the development of the new list, and opportunities for improving the future understanding of PFASs production, use on the global market, and presence in the environment, biota, and other matrices.



INARS



# The OECD List of PFAS

<http://www.oecd.org/chemicalsafety/portal-perfluorinated-chemicals/>



## PFAS Listed in OECD Global Database

Search PFASEUOECD Chemicals



☐ Substring search

### List Details

**Description:** OECD released a New Comprehensive Global Database of Per- and Polyfluoroalkyl Substances (PFASs) listing approximately 4700 new PFAS, including several new groups of PFASs that fulfill the common definition of PFASs (i.e. they contain at least one perfluoroalkyl moiety) but have not yet been commonly regarded as PFASs. The list can be used in conjunction with the methodology report summarising the major findings with respect to the total numbers and types of PFASs identified, the limitations, gaps and challenges identified, and opportunities for improving the future understanding of PFASs production, use on the global market, and presence in the environment, biota, and other matrices.

Source website: <http://www.oecd.org/chemicalsafety/portal-perfluorinated-chemicals>

A major effort was undertaken to register this list within DSSTox, adding chemical structures for as many PFAS entries as possible using both manual and auto-mapping (structures using CAS-matching) curation methods. The result is that approximately 1/3 of the list is curated at the highest two curation levels (DSSTox\_High or DSSTox\_Low) currently, whereas more than half of this list is registered at the Public\_Low curation level (based on PubChem content). The PFASOECD list is undergoing continuous registration and curation.

Number of Chemicals: 4725

4725 chemicals

Download / Send ▾

Show info:

DTXSID ×

CASRN ×

TOXCAST × ▾

Select all



Sort by: DTXSID ▾



Filter by: Name or CASRN

Hide ▾

## **Chemical Substances of Unknown or Variable Composition, Complex Reaction Products and Biological Materials (UVCB Substance) on the TSCA Inventory**

This paper is a compendium of information related to the broad class of chemical substances referred to as UVCBs for the Toxic Substances Control Act (TSCA) Chemical Substance Inventory. These chemical substances cannot be represented by unique structures and molecular formulas.



# Example PFAS-UVCBs

0 related chemical  
structures with this  
substance

Ethene, tetrafluoro-, oxidized, polymd., ...  
DTXSID: DTXSID00108075  
CASRN: 274917-96-3

0 related chemical  
structures with this  
substance

Sulfonamides, C4-8-alkane, perfluoro, ...  
DTXSID: DTXSID00108095  
CASRN: 160901-25-7

0 related chemical  
structures with this  
substance

1-Propene, 1,1,2,3,3,3-hexafluoro-, pol...  
DTXSID: DTXSID00108732  
CASRN: 149935-01-3

↳ Ethene, tetrafluoro-, oxidized, polymd., reduced, decarboxylated, C6 fraction  
274917-96-3 | DTXSID00108075

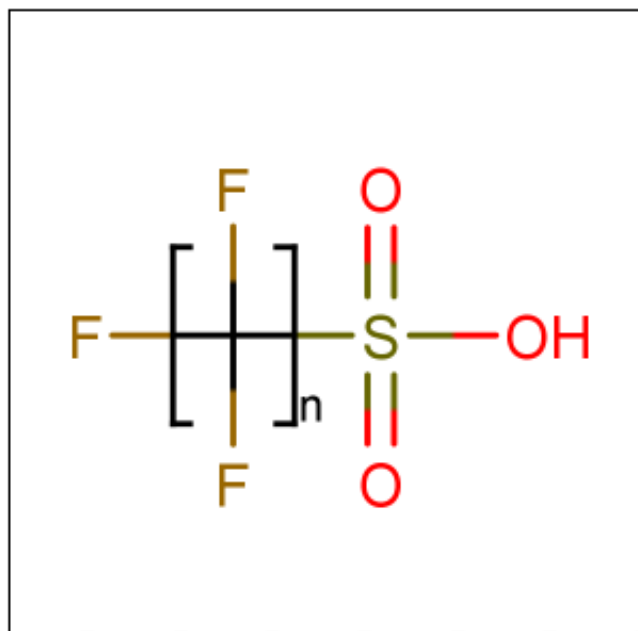
↳ 1-Propene, 1,1,2,3,3,3-hexafluoro-, polymer with 1,1-difluoroethene, ethene, 1,1,2,2-tetrafluoroethene and 1,1,2-trifluoro-2-(trifluoromethoxy)ethene  
149935-01-3 | DTXSID00108732

- PFOS is a member of linear perfluoroalkyl sulfonates

## Perfluoroalkyl sulfonates

NOCAS\_892979 | DTXSID70892979

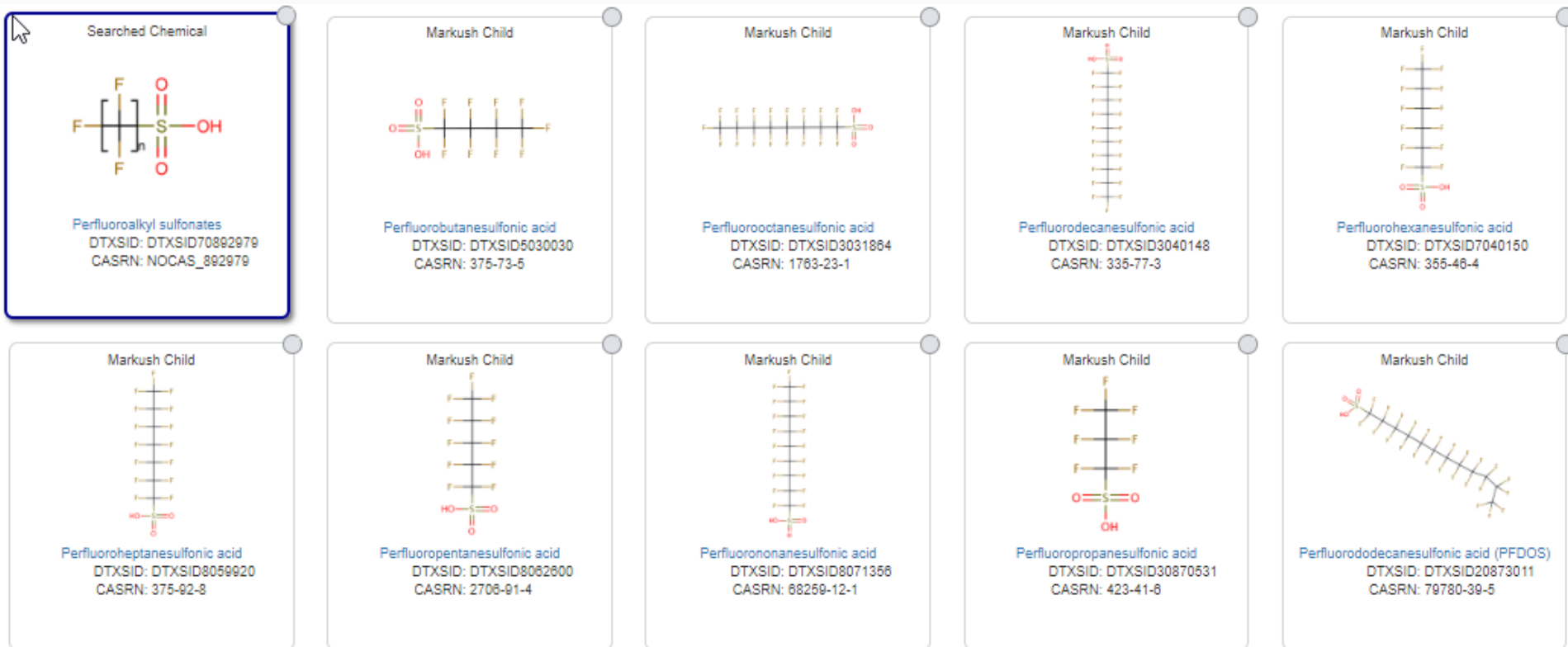
Searched by DSSTox Substance Id.





# ...and their Markush Children...

- Linear perfluoroalkyl sulfonates has children...



# PFAS Categories in Development

## Registered DSSTox “category substances” representing Per- and Polyfluoroalkyl Substances (PFAS) categories

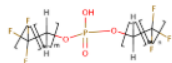
☐ Substring search

### List Details

**Description:** List of registered DSSTox “category substances” representing Per- and Polyfluoroalkyl Substances (PFAS) categories created using ChemAxon’s Markush structure-based query representations. Markush categories can be broad and inclusive of more specific categories, or can represent a unique category not overlapping with other registered categories. Each PFAS category registered with a unique DTXSID is considered a generalized substance or “parent ID” that can be associated with one or many “child IDs” (i.e. many parent-child mappings) within the full DSSTox database. These category DTXSIDs can be used to search and retrieve all currently registered DSSTox substances within the category group, and offer an objective, transparent and reproducible structure-based means of defining a category of chemicals. This list and the corresponding category mappings is undergoing continuous curation and expansion.

**Number of Chemicals:** 64

# PFAS Categories in Development



Fluorotelomer (linear) phosphate esters...



Fluorotelomer (linear) n:2 amines (prim...



Fluorotelomer (linear) amines (tertiary) (...)



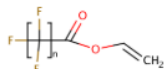
Perfluoroalkyl (linear) carboxylic acids



Fluorotelomer (linear) alcohols



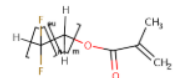
Fluorotelomer (linear) carboxylic acids



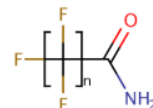
Perfluoroalkyl esters (vinyl)



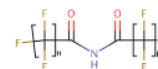
Perfluoroalkyl acyl fluorides



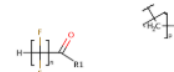
Fluorotelomer (linear) methacrylates (-...



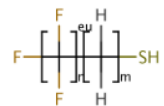
Perfluoroalkyl (linear) amides (primary)



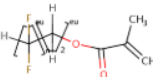
Perfluoro diacyl amides



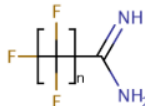
Polyfluoroalkyl (linear) (-CF2H) alkyl (lin...



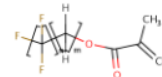
Fluorotelomer (linear) thiols



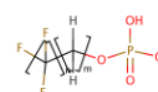
Fluorotelomer (linear) n:2 methacrylate...



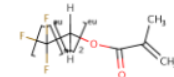
Perfluoroalkyl amidines



Fluorotelomer (linear) n:2 methacrylates

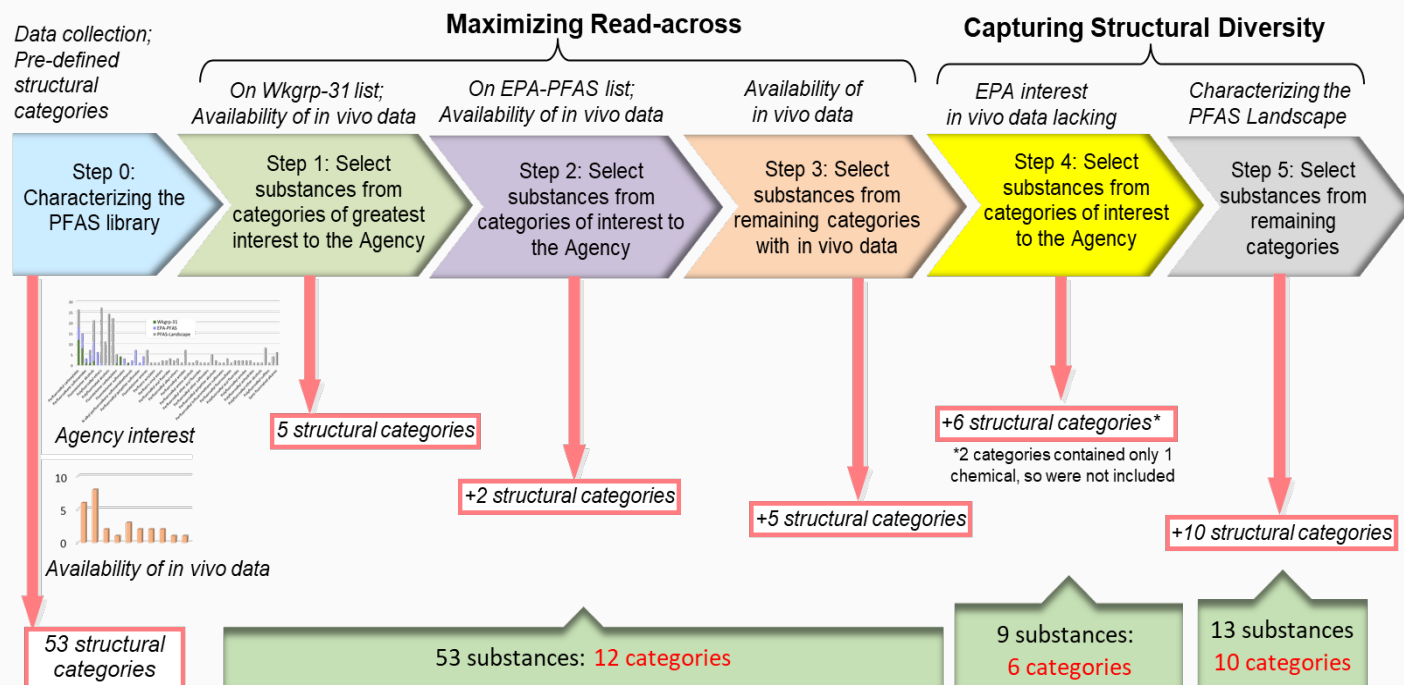


Fluorotelomer (linear) phosphate esters...



Fluorotelomer (linear) methacrylates

- Development of a high-throughput screening library and collection of physical samples (~400)
- 75 PFAS chemicals for screening based on categories, diversity, exposure considerations, procurability and testability, availability of existing toxicity data



## Four Chemical Trends Will Shape the Next Decade's Directions in Perfluoroalkyl and Polyfluoroalkyl Substances Research

*Matthias Kotthoff\* and Mark Bücking*

*Department Environmental and Food Analysis, Fraunhofer Institute for Molecular Biology and Applied Ecology, Schmallenberg, Germany*

- 1. Mobility: A wide and dynamic distribution of short chain PFAS due to their high polarity, persistency and volatility. (**OPERA Predictions**)
- 2. Substitution of regulated substances: The ban or restrictions of individual molecules will lead to a replacement with substitutes of similar concern. (**Database content and Markush Enumeration**)
- 3. Increase in structural diversity of existing PFAS molecules: Introduction of e.g., hydrogens and chlorine atoms instead of fluorine, as well as branching and cross-linking lead to a high versatility of unknown target molecules. (**Database content**)
- 4. Unknown “Dark Matter”: The amount, identity, formation pathways, and transformation dynamics of polymers and PFAS precursors are largely unknown. (**Working with agency analytical scientists and collaborators to link and host data**)

- The CompTox Dashboard supports PFAS research at EPA in numerous ways
  - Delivery of curated lists of PFAS chemicals (growing)
  - Flexible search capabilities – support for Mass Spec
  - Relationships in the data enrich navigation between chemicals
- Ongoing research efforts for PFAS chemicals
  - Physical library of ~400 chemicals has been acquired
  - High-throughput screening of ~75 chemicals
  - Classification approaches and Markush representations

- The CompTox Dashboard development team
- The DSSTox database curation team
- NERL colleagues:
  - Jon Sobus, Elin Ulrich, Mark Strynar, Seth Newton (NTA Analysis)
- Emma Schymanski – Luxembourg Center for Systems Biomedicine (MS-ready/NTA)

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**ORCID:** <https://orcid.org/0000-0002-2668-4821>