

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

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2) *ORAU*

3) *NERL*

4) *ILS*

5) *University of Luxembourg*

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.

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?](#)

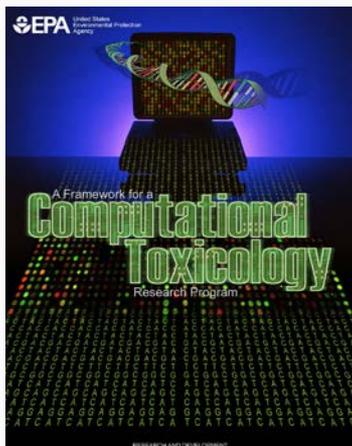
EPA Actions to Address PFAS

- [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**



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>



762 Thousand Chemicals

Chemicals Product/Use Categories Assay/Gene

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)

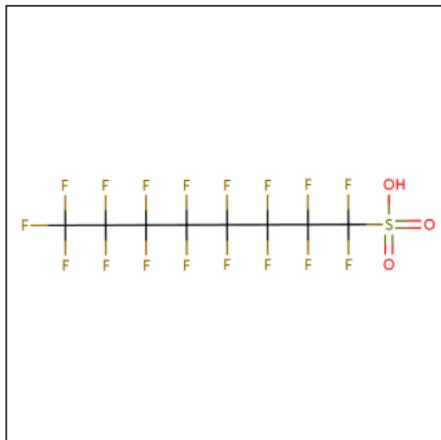
RELATED SUBSTANCES

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

PFASEUOEC
PFAS Listed in OECD Global
Database

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▶ BIOACTIVITY

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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.

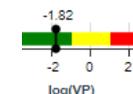
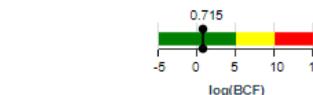
Endocrine System

✓ 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



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

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 ² K)

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^{1,2,3*} , Chris M. Grulke¹, Richard S. Judson¹ and Antony J. Williams¹

Detailed OPERA Prediction Reports

[Source](#)
[Result](#)
[Calculation Details](#)

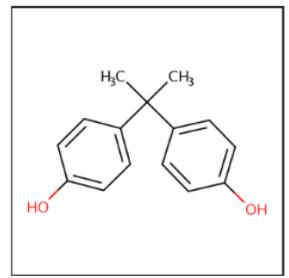
Experimental Values

- PhysPropNCCT
- Predicted Values
- EPISUITE
- NICEATM
- ACD/Labs Conse
- ACD/Labs
- OPERA

OPERA Models: LogP: Octanol-Water

Bisphenol A
80-05-7 | DTXSID7020182

[Save PDF](#)



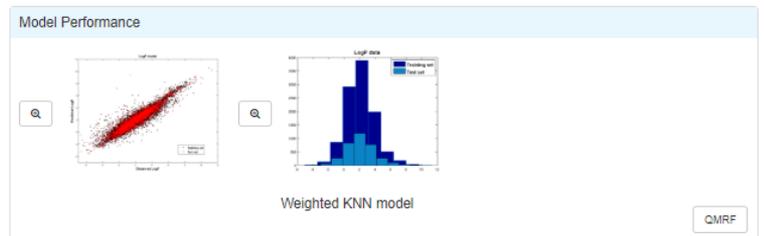
Model Results

Predicted value: 3.35

Global applicability domain: inside

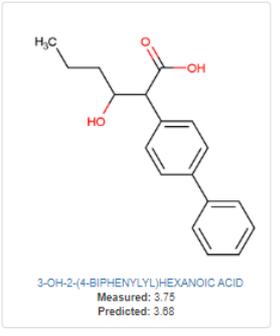
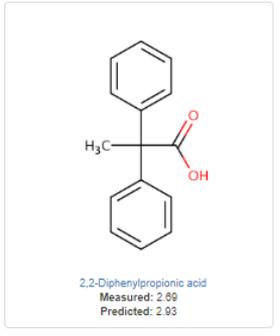
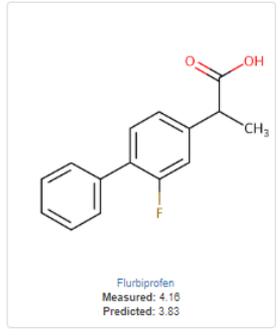
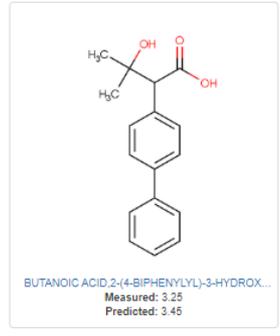
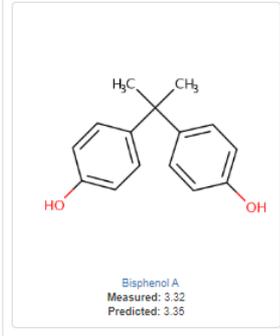
Local applicability domain index: 0.88

Confidence level: 0.75



5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.89	0.86	0.87	0.88	0.78

Nearest Neighbors from the Training Set



Not much data for PFAS - yet

Model Results

Per 1763-

Predicted value: 2.77

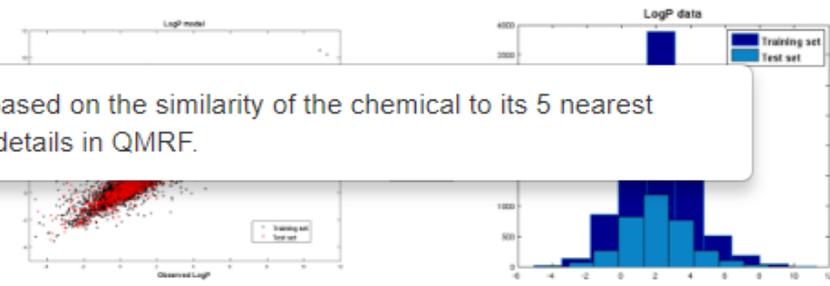
Global applicability domain: Inside ⓘ

Local applicability domain index: 0.42 ⓘ

Confidence level: 0.44 ⓘ

Predicted logP = 2.77
Experimental logP = 4.67

Model Performance

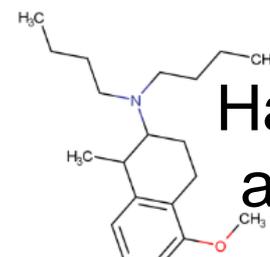
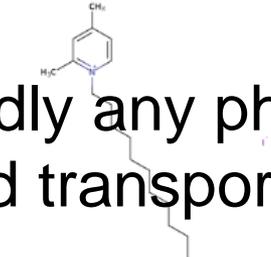
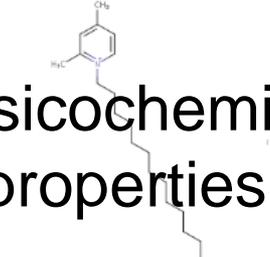
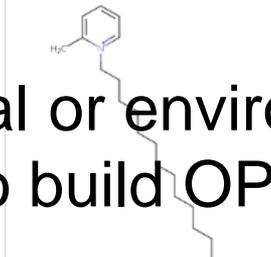
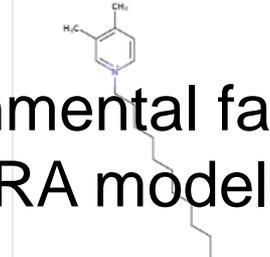


0-1 range index based on the similarity of the chemical to its 5 nearest neighbors. More details in QMRF.

Weighted KNN model

QMRf

Nearest Neighbors from the Training Set

 <p>5-METHOXY-1-METHYL-2-AMINOTETRALIN, N...</p> <p>Measured: 5.81 Predicted: 4.91</p>	 <p>1-Dodecyl-2,4-dimethylpyridin-1-ium iodide</p> <p>Measured: 1.41 Predicted: 1.58</p>	 <p>2,4-Dimethyl-1-tetradecylpyridin-1-ium iodide</p> <p>Measured: 2.47 Predicted: 2.85</p>	 <p>2-Methyl-1-tetradecylpyridin-1-ium iodide</p> <p>Measured: 2.27 Predicted: 2.35</p>	 <p>1-Dodecyl-3,4-dimethylpyridin-1-ium iodide</p> <p>Measured: 1.75 Predicted: 1.70</p>
---	--	--	---	--

Hardly any physicochemical or environmental fate and transport properties to build OPERA models

- 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

EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Copy Share Submit Comment Search all data

DETAILS

EXECUTIVE SUMMARY

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HAZARD

ADME

▶ EXPOSURE

▶ BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

▶ LITERATURE

LINKS

COMMENTS

Data Type

Ecotox Effect Level

Download

Human Eco

Columns

Search query

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

PFASEUOECD
PFAS Listed in OECD Global Database

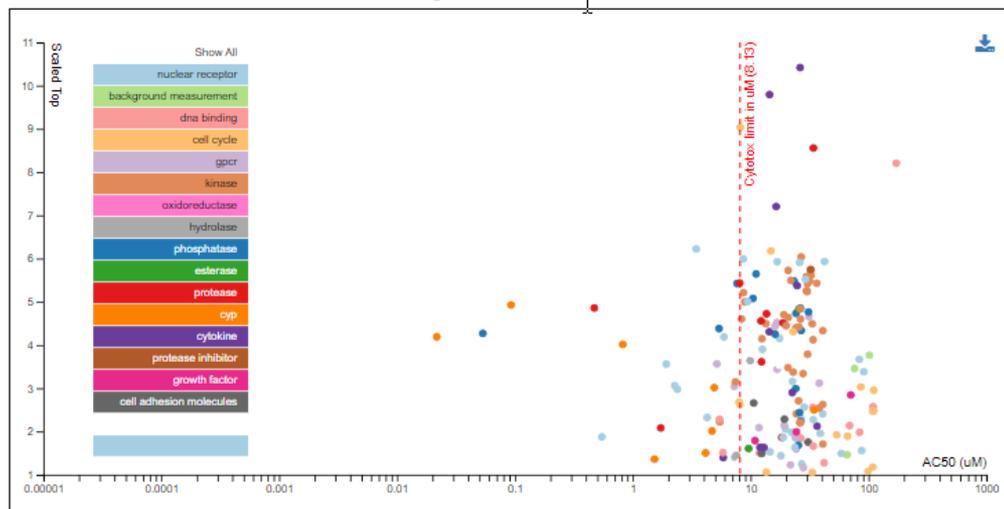
Perfluorooctanesulfonic acid

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

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- ADME
- EXPOSURE
- BIOACTIVITY
 - TOXCAST: SUMMARY**
 - PUBCHEM
 - TOXCAST: DATA
 - TOXCAST: MODELS
 - TOXCAST: MODELS
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES

Chemical Activity Summary i

TOXCAST DATA



ASSAY DETAILS

Select a data point in the plot to see associated details

Download

Boactivity Data

PFASEUOECD
PFAS Listed in OECD Global Database

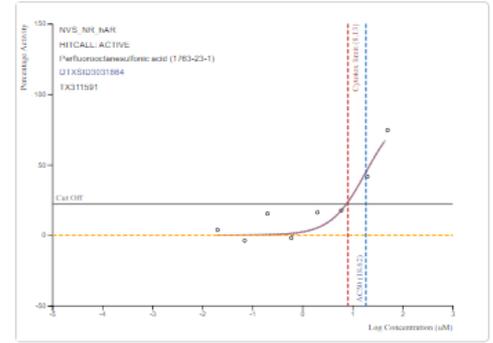
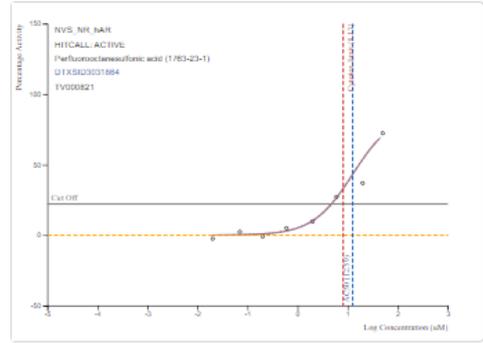
Perfluorooctanesulfonic acid
1763-23-1 | DTXSID3031864
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- DETAILS
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 - PUBCHEM
 - TOXCAST: DATA**
 - TOXCAST: MODELS
 - TOXCAST: MODELS
 - SIMILAR COMPOUNDS
 - GENRA (BETA)
 - RELATED SUBSTANCES

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 Aoonist



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
Hept	Heptadecafluorooctane-1-sulfonic acid
1-O	1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-
1763-23-1	Active CAS-RN
Hept	Heptadecafluorooctanesulfonic acid
1-O	1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-heptadecafluoro-
1-O	1-Octanesulfonic acid, heptadecafluoro-
EF	EF 101
hep	heptadecafluorooctane-1-sulfonic acid
hep	heptadecafluorooctane-1-sulphonic acid
PFOS	PFOS
EIN	EINECS 217-179-8
1,1,1	1,1,2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-Heptadecafluoro-1-octanesulfonic acid

Search query

Quality
Valid
Good
Other

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...

Download Sifter for Excel 

<input type="checkbox"/>	PMID	Year	Title	Authors	Journal	Rev
<input type="checkbox"/>	2952662	2018	Modeling avian exposures to perfluoroalkyl substances in aquatic habitats...	Larson; Conder; Arblaster	Chemosphere	
<input type="checkbox"/>	28521193	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"/>	24046276	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"/>	22441698	2012	Perfluorooctane sulfonate increases β -oxidation of palmitic acid in chicke...	Nordén; Westman; Venizelos; Engwall	Environmental science and pollution research intern...	
<input type="checkbox"/>	21467747	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"/>	21207445	2011	Aquatic predicted no-effect-concentration derivation for perfluorooctane s...	Qi; Wang; Mu; Wang	Environmental toxicology and chemistry	
<input type="checkbox"/>	20879709	2010	Distribution of perfluorooctane sulfonate and other perfluorochemicals in t...	Wang; Fu; Wang; Liang; Pan; Cai; Jiang	Environmental science & technology	
<input type="checkbox"/>	20709355	2010	Brominated flame retardants and perfluorinated compounds in indoor dust...	D'Hollander; Roosens; Covaci; Cornelis; Reynders; ...	Chemosphere	
<input type="checkbox"/>	19569327	2009	Perfluoroalkyl contaminants in an Arctic marine food web: trophic magnific...	Kelly; Ikonoum; Blair; Surridge; Hoover; Grace; Go...	Environmental science & technology	
<input type="checkbox"/>	19343326	2009	Chronic effects of perfluorooctanesulfonate exposure on immunotoxicity i...	Dong; Zhang; Zheng; Liu; Jin; He	Archives of toxicology	
<input type="checkbox"/>	19162172	2009	Gestational and lactational exposure to potassium perfluorooctanesulfona...	Butenhoff; Ehresman; Chang; Parker; Stump	Reproductive toxicology (Elmsford, N.Y.)	
<input type="checkbox"/>	19110351	2008	Behaviour of damselfly larvae (Enallagma cyathigerum) (Insecta, Odonata...	Van Gossium; Bots; Snijkers; 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 

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

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<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 β -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 Gossun; Bots; Snijkers; 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)

 United States Environmental Protection Agency

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PFASEUOECDFAS Listed in OECD Global Database

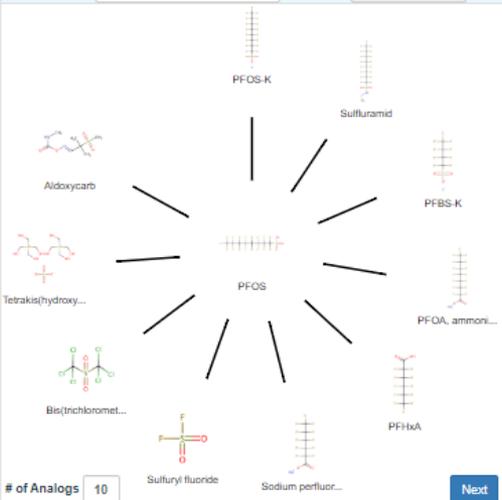
Perfluorooctanesulfonic acid

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 Fgrprts Filter by: invivo data



of Analogs 10

Next

Substance	Chemical Class	Invivo Data
PFOS	Perfluorooctanesulfonic acid	Yes
PFOS-K	Perfluorooctanesulfonate potassium salt	Yes
PFBS-K	Perfluorobutanesulfonate potassium salt	Yes
PFHxA	Perfluorohexanesulfonic acid	Yes
PFOA, ammoni...	Perfluorooctanoic acid ammonium salt	Yes
Sulfuramid	Sulfonamide	Yes
Aldoxycarb	Aldoxycarbonyl compound	Yes
Tetrakis(hydroxy...)	Tetrakis(hydroxy) compound	Yes
Bis(trichloromet...)	Bis(trichloromethyl) compound	Yes
Sulfuryl fluoride	Sulfuryl fluoride	Yes
Sodium perfluor...	Sodium perfluorooctanesulfonate	Yes

Select and Review Analogs

Generalized Read-Across (GenRA)

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PFASEUOEC
PFAS Listed in OECD Global Database

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

Perfluorooctanesulfonic acid

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

Step Two: Data Gap Analysis & Generate Data Matrix

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

of Analogs: 10

Summary Data Gap Analysis

	bio_b21	bio_tox	chem_ct	tox_b2f
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
Tetraakis(hydroxymethyl)...	25	0	8	408
Aldoxycarb	9	228	6	83

Group: ToxRef By: Tox Fingerprint

Generate Data Matrix

	PFOS	PFOS-K	Sulfuramid	PFBS-K	PFOA, ammonium	PFHxA	Sodium perfluorohexanoate	Sulfuryl fluoride	Bis(trichloromethyl)sulfone	Tetraakis(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

23

Generalized Read-Across (GenRA)



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

Are there Similar Compounds?

 United States Environmental Protection Agency

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Perfluorooctanesulfonic acid

1763-23-1 | DTXSID3031864

Searched by Synonym from Valid Source.

Searched with a similarity threshold of 0.8

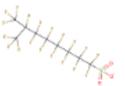
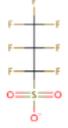
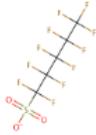
83 chemicals

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 <p>Potassium perfluorooctanesulfonate DTXSID: DTXSID6037706 CASRN: 2786-39-3 TOXCAST: 84/576</p>	 <p>Lithium perfluorooctanesulfonate DTXSID: DTXSID2032421 CASRN: 29457-72-5 TOXCAST: 8/116</p>	 <p>Potassium perfluorohexanesulfonate DTXSID: DTXSID3037709 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: 110676-15-8 TOXCAST: 0</p>	 <p>Heptadecafluorooctane-1-(¹⁹H)sulfonic a... DTXSID: DTXSID00892720 CASRN: NOCAS_892720 TOXCAST: 0</p>	 <p>Perfluoroheptanesulfonate DTXSID: DTXSID00892505 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

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Perfluorooctanesulfonic acid

1763-23-1 | DTXSID3031864

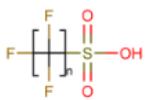
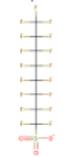
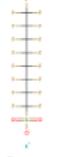
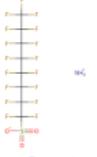
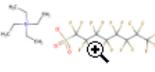
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- DETAILS
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- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- ADME
- ▶ EXPOSURE
- ▶ BIOACTIVITY
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- ▶ LITERATURE
- LINKS
- COMMENTS

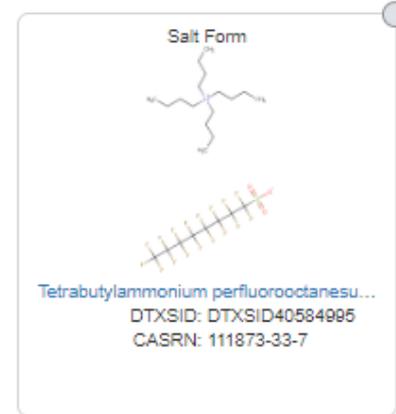
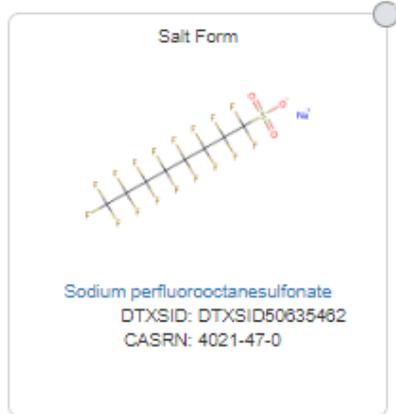
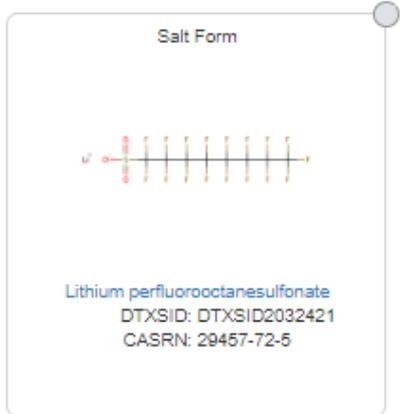
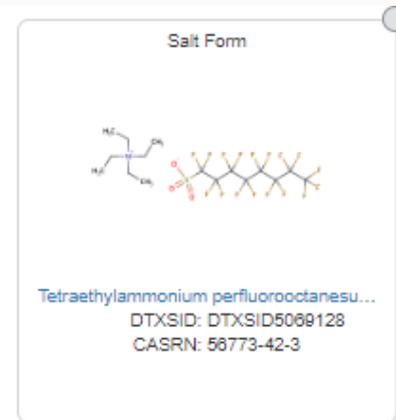
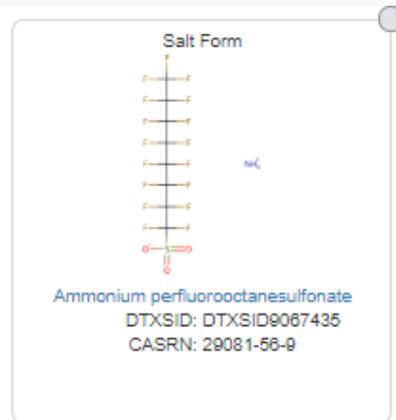
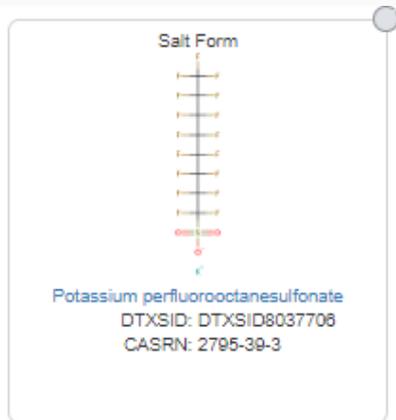
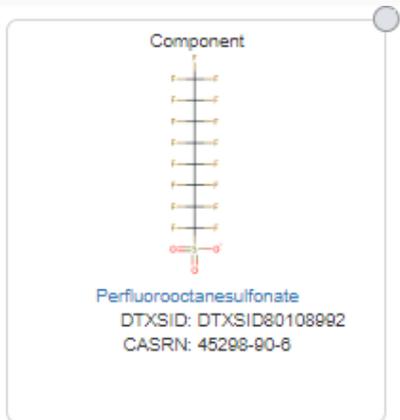
12 chemicals

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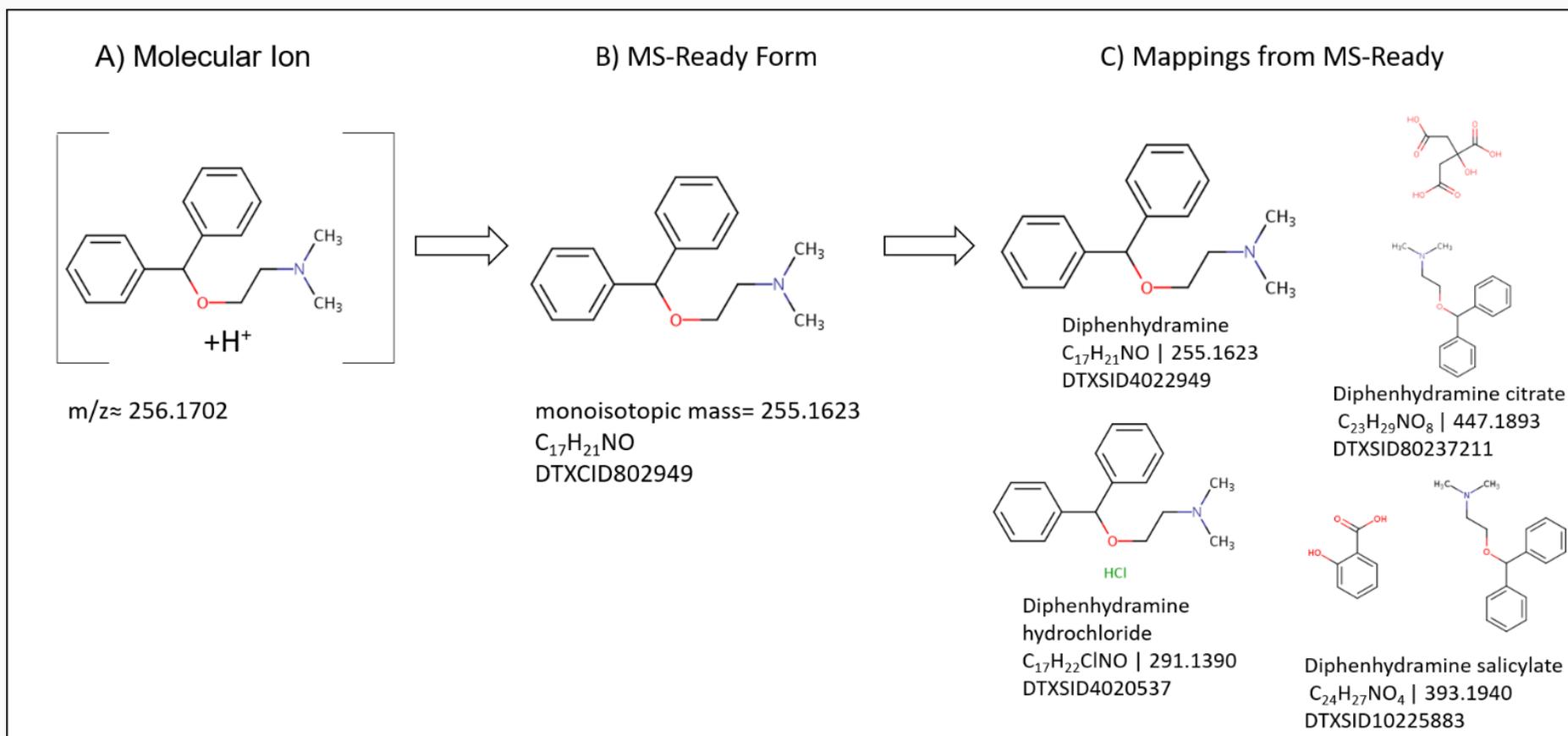
<p style="text-align: center;">Searched Chemical</p> <div style="text-align: center;">  </div> <p style="text-align: center; font-size: small;">Perfluorooctanesulfonic acid DTXSID: DTXSID3031864 CASRN: 1763-23-1</p>	<p style="text-align: center;">Markush Parent</p> <div style="text-align: center;">  </div> <p style="text-align: center; font-size: small;">Perfluoroalkyl sulfonates DTXSID: DTXSID70892979 CASRN: NOCAS_892979</p>	<p style="text-align: center;">Predecessor: Component</p> <p style="text-align: center; font-weight: bold;">3 related chemical structures with this substance</p> <p style="text-align: center; font-size: small;">Mixture of PFOS and PFOA DTXSID: DTXSID20872983 CASRN: NOCAS_872983</p>	<p style="text-align: center;">Predecessor: Component</p> <p style="text-align: center; font-weight: bold;">3 related chemical structures with this substance</p> <p style="text-align: center; font-size: small;">1-Octanesulfonic acid, 1,1,2,2,3,3,4,4,5... DTXSID: DTXSID40880545 CASRN: 64202-77-3</p>	<p style="text-align: center;">Component</p> <div style="text-align: center;">  </div> <p style="text-align: center; font-size: small;">Perfluorooctanesulfonate DTXSID: DTXSID80108992 CASRN: 45298-90-6</p>
<p style="text-align: center;">Salt Form</p> <div style="text-align: center;">  </div> <p style="text-align: center; font-size: small;">Potassium perfluorooctanesulfonate DTXSID: DTXSID8037706 CASRN: 2795-39-3</p>	<p style="text-align: center;">Salt Form</p> <div style="text-align: center;">  </div> <p style="text-align: center; font-size: small;">Ammonium perfluorooctanesulfonate DTXSID: DTXSID9087435 CASRN: 29081-58-9</p>	<p style="text-align: center;">Salt Form</p> <div style="text-align: center;">  </div> <p style="text-align: center; font-size: small;">Tetraethylammonium perfluorooctanesulfonate DTXSID: DTXSID5099128 CASRN: 56773-42-3</p>	<p style="text-align: center;">Salt Form</p> <div style="text-align: center;">  </div> <p style="text-align: center; font-size: small;">Lithium perfluorooctanesulfonate DTXSID: DTXSID2032421 CASRN: 29457-72-5</p>	<p style="text-align: center;">Salt Form</p> <div style="text-align: center;">  </div> <p style="text-align: center; font-size: small;">Sodium perfluorooctanesulfonate DTXSID: DTXSID50635462 CASRN: 4021-47-0</p>

7 salt forms of PFOS (and the ion)



Using data relationships

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



Advanced Search

Supporting Target/Non-Target MS

Advanced Search

Mass Search

Select Adduct:

Molecular Formula Search

MS Ready Formula 

Exact Formula 

Generate Molecular Formula(e)

2 Chemicals match the formula

Search Results

Searched by Exact Molecular Formula: C8HF17O3S.

2 of 2 chemicals visible

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Sort by: DTXSID

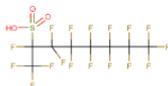


Filter by: Name or CASRN

Multicomponent Chemicals



Perfluorooctanesulfonic acid



Heptadecafluorooctane-2-sulfonic acid

Advanced Search

Supporting Target/Non-Target MS

Advanced Search

Mass Search

Min/Max

Select Adduct: Neutral 

Mass Da

±

Error Da Da ppm

Search 

Molecular Formula Search

MS Ready Formula 

Exact Formula 

Search 

Generate Molecular Formula(e)

Min/Max

Mass Da

±

Error Da ppm

Search 

22 Chemicals match the formula

Search Results

Searched by MS Ready Formula: C8HF17O3S.

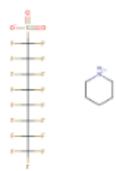
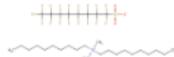
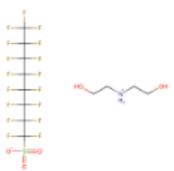
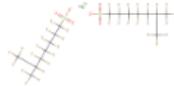
22 chemicals

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Show info: **DTXSID** **CASRN** **TOXCAST** Select all

Sort by: **DTXSID**

Filter by: Name or CASRN Hide

 <p>Piperidinium perfluorooctanesulfonate DTXSID: DTXSID0072352 CASRN: 71483-74-6 TOXCAST: 0</p>	 <p>N-Decyl-N,N-dimethyl-1-decanaminium... DTXSID: DTXSID00882964 CASRN: 261099-16-8 TOXCAST: 0</p>	 <p>Heptadecafluorooctane-1-(2H)sulfonic a... DTXSID: DTXSID00892720 CASRN: NOCAS_892720 TOXCAST: 0</p>	 <p>Diphenyl(2,4,6-trimethylphenyl)sulfoni... DTXSID: DTXSID00893373 CASRN: 268341-99-0 TOXCAST: 0</p>	 <p>Lithium perfluorooctanesulfonate DTXSID: DTXSID2032421 CASRN: 29457-72-6 TOXCAST: 8/116</p>	 <p>Bis(2-hydroxyethyl)ammonium perfluor... DTXSID: DTXSID2072049 CASRN: 70226-14-8 TOXCAST: 0</p>
 <p>Perfluorooctanesulfonic acid DTXSID: DTXSID3031864 CASRN: 1783-23-1 TOXCAST: 175/889</p>	 <p>Magnesium heptadecafluoroisooctanes... DTXSID: DTXSID30881127 CASRN: 93894-73-6 TOXCAST: 0</p>	 <p>Heptadecafluorooctane-2-sulfonic acid DTXSID: DTXSID30896921 CASRN: 927870-12-0 TOXCAST: 0</p>	 <p>Tetrabutylammonium perfluorooctanesu... DTXSID: DTXSID40584995 CASRN: 111873-33-7 TOXCAST: 0</p>	 <p>Sodium perfluorooctanesulfonate DTXSID: DTXSID50835482 CASRN: 4021-47-0 TOXCAST: 0</p>	 <p>Tetraethylammonium perfluorooctanesu... DTXSID: DTXSID5089128 CASRN: 66773-42-3 TOXCAST: 0</p>
					

22 Chemicals match the formula

Search Results

Searched by MS Ready Formula: C₈HF₁₇O₃S.

22 chemicals

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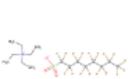


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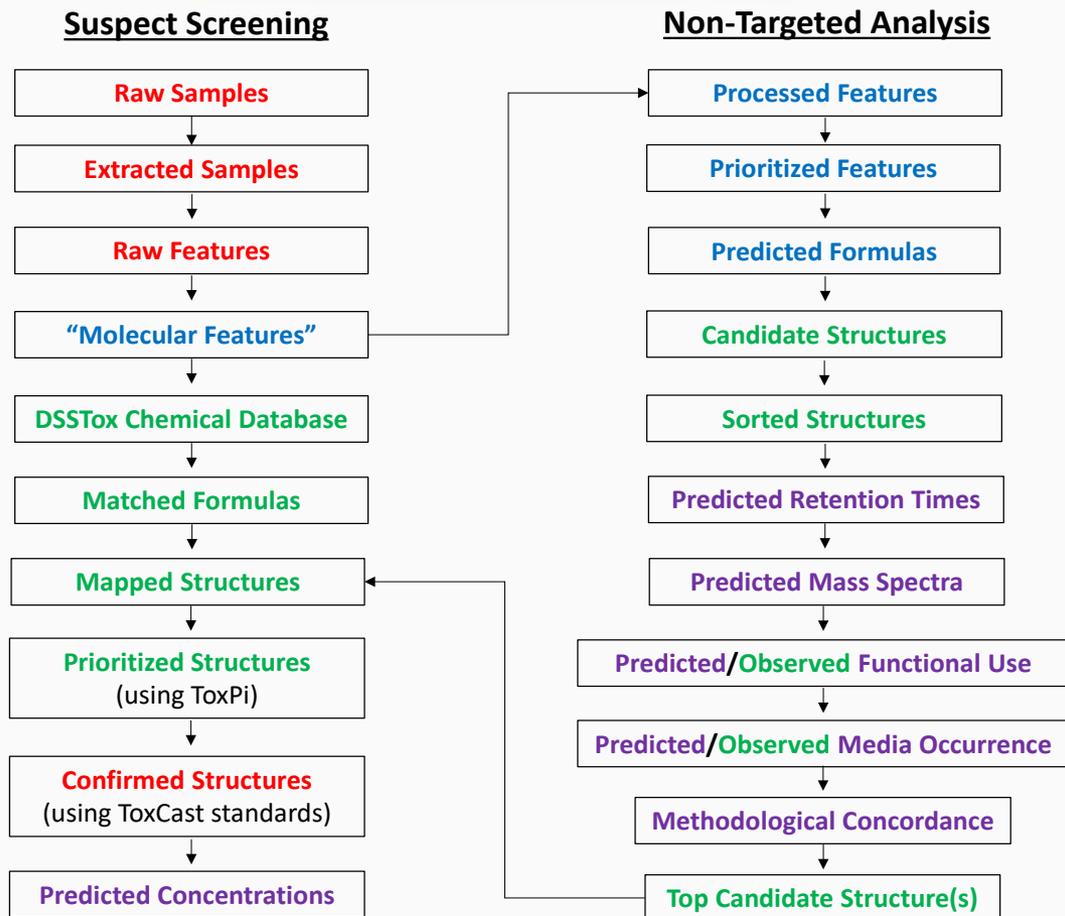


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Structure	DTXSID	Preferred Name	CASRN	QC Level	CPDat Count	Number of Sources	PubChem Data Sources	PubMed Ref. Counts	Monoisotopic Mass
	DTXSID3031864 ToxCast™	Perfluorooctanesulfonic acid	1763-23-1	Level 1	10	88	68	1124	499.937494
	DTXSID8037706 ToxCast™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

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 ⓘ

± Min/Max M

Mass Da ± Error Da ppm

Molecular Formula Search ⓘ

Molecular Formula MS Ready Formula ⓘ Exact Formula ⓘ

Generate Molecular Formula(e) ⓘ

± Min/Max

Mass Da

Default Options: C[1-50] H[0-100] O[0-20] N[0-20]
Include Halogens: F[0-20] Cl[0-20] Br[0-20]

Options ▾

Select Input Type(s)

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

Step One Step Two Step Three Step Four Step Five Step Six

Step Five: Choose Data Fields to Download

Please enter one identifier per line

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

C14H22N2O3
C10H12N2O
C14H18N4O3
C12H11N7
C8H9NO2

Display All Chemicals Download Chemical Data

A List of Lists of Chemicals

https://comptox.epa.gov/dashboard/chemical_lists



Home

Advanced Search

Batch Search

Lists

Predictions

Downloads

Search All Data



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 http://pubs.acs.org/doi/abs/10.1021/acs.chemrestox.6b00347
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

Select List

Show 10 entries

Search: pfas|

Download

List Acronym	List Name	Last Updated	Number of Chemicals	List Description
EPAPFAS75S1	EPA PFAS List of 75 Test Samples (Set 1)	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	Registered DSSTox "category substances" representing Per- and Polyfluoroalkyl Substances (PFAS) categories	2018-06-29	64	List of registered DSSTox "category substances" representing PFAS categories created using ChemAxon's Markush structure-based query representations.
EPAPFASINSOL	PFAS in EPA's Chemical Inventory Insoluble in DMSO	2018-06-29	43	PFAS chemicals included in EPA's expanded ToxCast chemical inventory found to be insoluble in DMSO above 5mM.
EPAPFASINV	PFAS in EPA's ToxCast Chemical Inventory	2018-06-29	430	PFAS chemicals included in EPA's expanded ToxCast chemical inventory and available for testing.
EPAPFASRL	EPA PFAS Cross-Agency Research List	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	PFAS_EPA List of Perfluorinated alkyl substances	2017-11-03	190	PFAS_EPA (Perfluorinated alkyl substances) is a manually curated listing of mainly straight-chain and branched PFAS substances
PFASEOECED	PFAS Listed in OECD Global Database	2018-07-26	4725	OECD released a New Comprehensive Global Database of Per- and Polyfluoroalkyl Substances, (PFASs) listing approximately 4700 new PFAS
PFASGRACE	PFASforGrace	2017-02-16	35	A list of polyfluorinated chemicals of interest to Grace Patlewicz
PFASKEMI	PFAS List from the Swedish Chemicals Agency (KEMI) Report	2017-02-09	2397	Perfluorinated substances from a Swedish Chemicals Agency (KEMI) Report on the occurrence and use of highly fluorinated substances.
PFASMASTER	PFAS Master List of PFAS Substances	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

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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

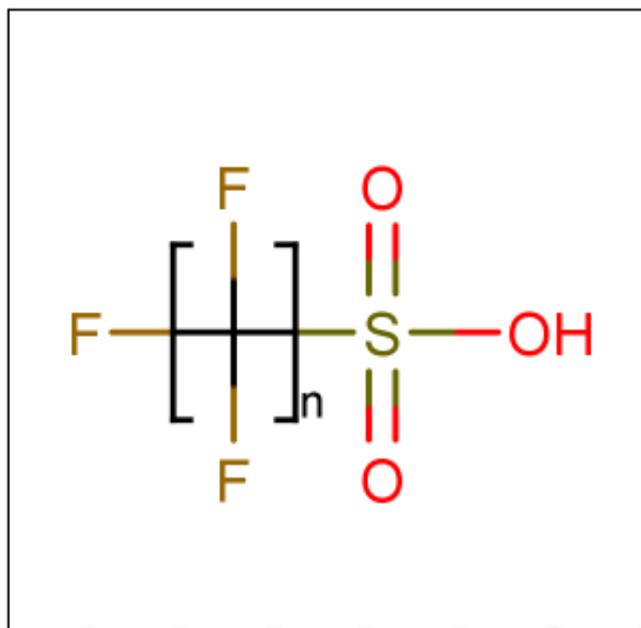
↑ 1-Propene, 1,1,2,3,3,3-hexafluoro-, polymer with 1,1-difluoroethene, ethene, 1,1,2,2-tetrafluoroethene and 1,1,2-trifluoro-2-(trifluoromethoxy)ethene
149935-01-3 | DTXSID00108732

- PFOS is a member of linear perfluoroalkyl sulfonates

Perfluoroalkyl sulfonates

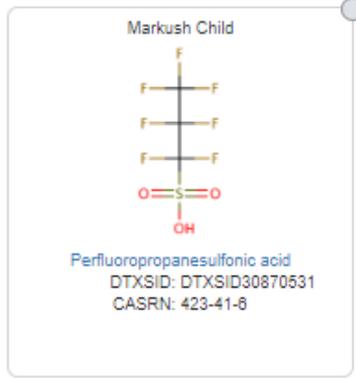
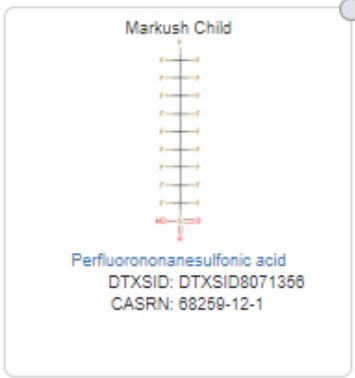
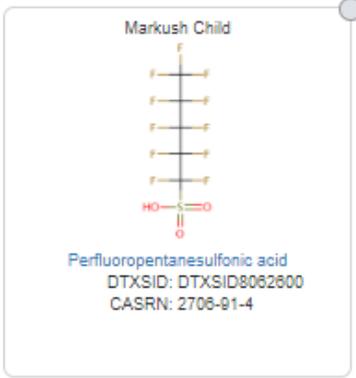
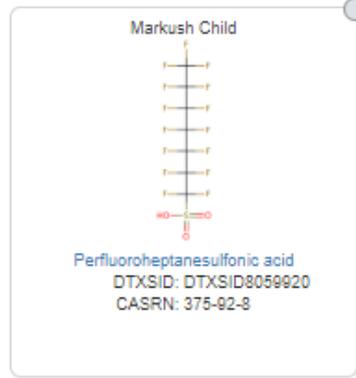
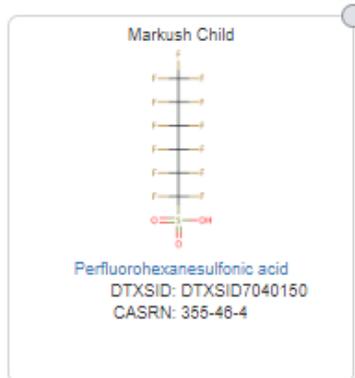
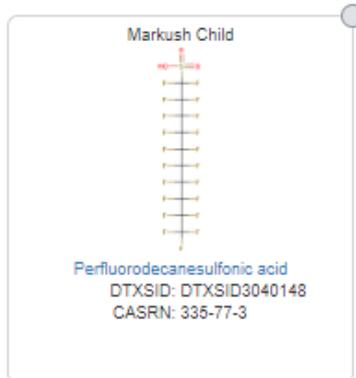
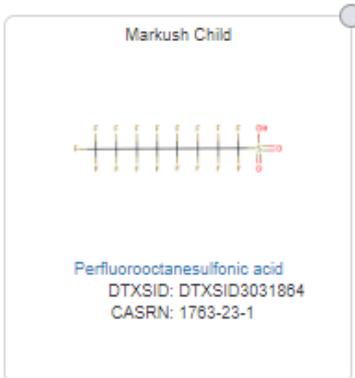
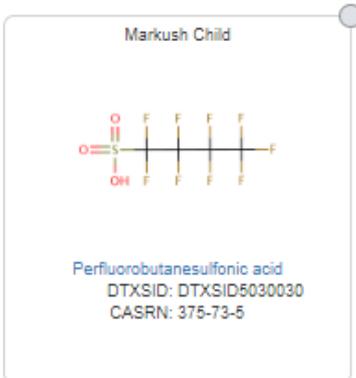
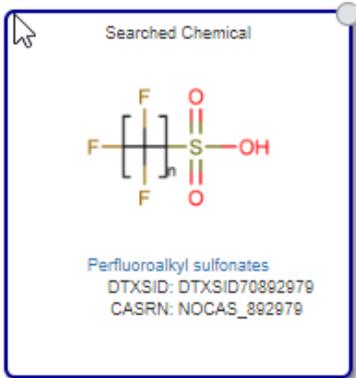
NOCAS_892979 | DTXSID70892979

Searched by DSSTox Substance Id.



...and their Markush Children...

- Linear perfluoroalkyl sulfonates has children...



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

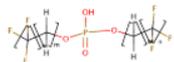
 Substring search

List Details

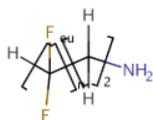
Description: List of registered DSSTox “category substances” representing Per- and Polyfluoroalkyl Substances (PFAS) categories created using ChemAxon’s Markush structure-based query representations. Markush categories can be broad and inclusive of more specific categories, or can represent a unique 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...



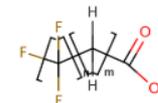
Fluorotelomer (linear) amines (tertiary) (...)



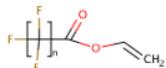
Perfluoroalkyl (linear) carboxylic acids



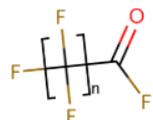
Fluorotelomer (linear) alcohols



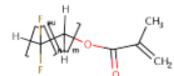
Fluorotelomer (linear) carboxylic acids



Perfluoroalkyl esters (vinyl)



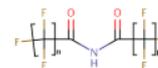
Perfluoroalkyl acyl fluorides



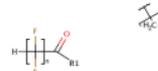
Fluorotelomer (linear) methacrylates (-...)



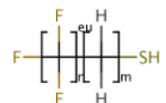
Perfluoroalkyl (linear) amides (primary)



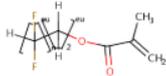
Perfluoro diacyl amides



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



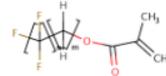
Fluorotelomer (linear) thiols



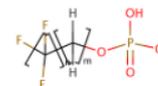
Fluorotelomer (linear) n:2 methacrylate...



Perfluoroalkyl amidines



Fluorotelomer (linear) n:2 methacrylates

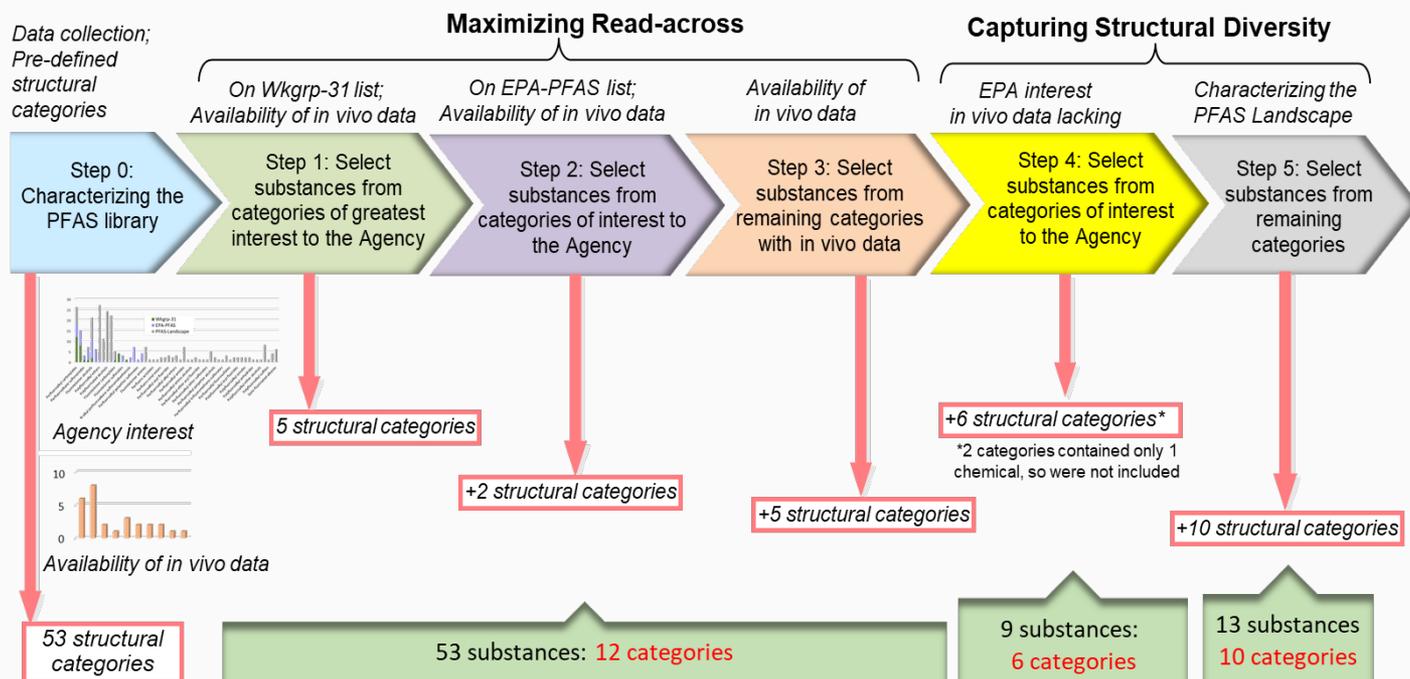


Fluorotelomer (linear) phosphate esters...



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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National Center for Computational Toxicology (NCCT)

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