

# EPA's CompTox Chemicals Dashboard, a tool with information on ~900,000 chemicals

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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*


*CREEC  
April 2020*



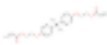
# BASIC Search

**Chemicals** **Product/Use Categories** **Assay/Gene**

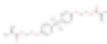
 Bisphenol



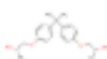
Bisphenol A  
DTXSID7020182



Bisphenol A bis(2-hydroxyethyl ether) diacrylate  
DTXSID6066991

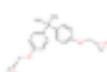


Bisphenol A bis(2-hydroxyethyl ether) dimethacrylate  
DTXSID1066992

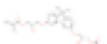


Bisphenol A bis(2-hydroxypropyl) ether  
DTXSID8051592

Bisphenol A carbonate polymer  
DTXSID6027840



Bisphenol A diglycidyl ether  
DTXSID6024624



Bisphenol A glycidyl methacrylate  
DTXSID7044841

# Detailed Chemical Pages

## DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

▶ ADME

▶ EXPOSURE

▶ BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

▶ LITERATURE

LINKS

COMMENTS

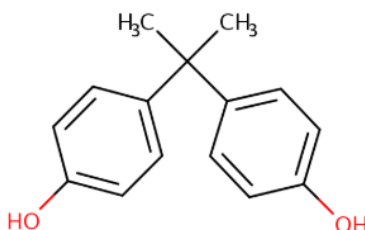
Home Advanced Search Batch Search Lists Predictions Downloads

Copy Share Submit Comment Search all data

### Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.








**Wikipedia**


**Bisphenol A (BPA)** is an organic synthetic compound with the chemical formula  $(\text{CH}_3)_2\text{C}(\text{C}_6\text{H}_4\text{OH})_2$  belonging to the group of diphenylmethane derivatives and bisphenols, with two hydroxyphenyl groups. It is a colorless solid that is soluble in organic solvents, but poorly soluble in water (0.344 wt % at 83 °C). BPA is a starting material for the synthesis of plastics, primarily certain polycarbonates

[Read more](#)

**Intrinsic Properties**

 **Molecular Formula:**  $\text{C}_{15}\text{H}_{16}\text{O}_2$   Mol File  Find All Chemicals

 **Average Mass:** 228.291 g/mol  Isotope Mass Distribution

 **Monoisotopic Mass:** 228.11503 g/mol

**Structural Identifiers**

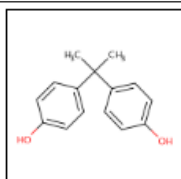
**Linked Substances**

**Presence in Lists**

**Record Information**

**Quality Control Notes**

# Properties, Fate and Transport



## Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

Property

Summary

## Summary

Download

Columns

Property	Experimental average	Predicted average	Experimental median	Predicted median
LogKow: Octanol-Water	3.32 (1)	3.30		3.39
Melting Point	155 (7)	140	156	144
Boiling Point	200 (1)	360		355
Water Solubility	8.55e-4 (3)	8.78e-4	5.26e-4	7.56e-4
Vapor Pressure	-	6.83e-7		1.51e-7
Flash Point	-	190		190
Surface Tension	-	46.0		
Index of Refraction	-	1.60		
Molar Refractivity	-	68.2		

# Properties, Fate and Transport

## e.g. Solubility

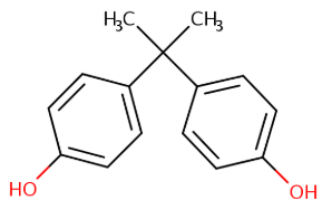
 Download Experimental Data ▼

Source	Result	
<a href="#">PhysPropNCCT</a>	5.26e-4	
<a href="#">Tetko et al. J. Chem. Inf. and Comp. Sci. 41.6 (2001): 1488-1493</a>	1.51e-3	
<a href="#">Kovdienko, et. al. Molecular informatics 29.5 (2010): 394-406.</a>	5.25e-4	

Source	Result	Calculation Details
<a href="#">EPISUITE</a>	7.56e-4	Not Available
<a href="#">NICEATM</a>	1.31e-3	Not Available
<a href="#">TEST</a>	1.24e-3	<a href="#">TEST Report</a>
<a href="#">OPERA</a>	5.44e-4	<a href="#">OPERA Model Report [Inside AD]</a>
<a href="#">OPERA2</a>	5.35e-4	Not Available

# Properties, Fate and Transport

## e.g. logP



### Model Results

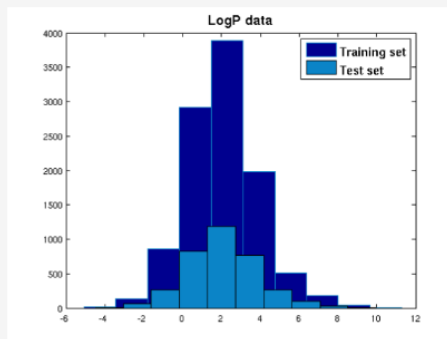
**Predicted value:** 3.35

**Global applicability domain:** Inside

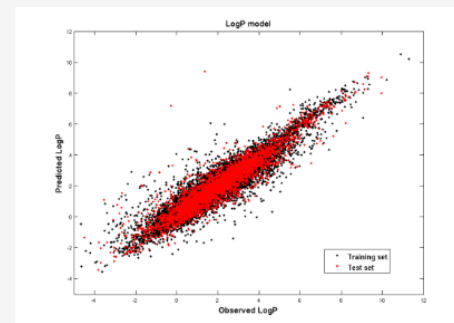
**Local applicability domain index:** 0.877

**Confidence level:** 0.748

### Model Performance



QMRP




Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.850	0.690	0.860	0.670	0.860	0.780

[od.epa.gov/dashboard/advanced\\_search/index](https://od.epa.gov/dashboard/advanced_search/index)

# Sources of Exposure to Chemicals

United States  
Environmental Protection  
Agency

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## Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

DETAILS

EXECUTIVE SUMMARY

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ENV. FATE/TRANSPORT

HAZARD

▶ ADME

Download ▼

Columns ▼10 ▼

### Product and Use Categories (PUCs) i

Product or Use Categorization	Categorization type	Number of Unique Products
manufacturing, metals	CPCat Cassette	17
adhesive	CPCat Cassette	17
	CPCat Cassette	16
	CPCat Cassette	12
	CPCat Cassette	11
	CPCat Cassette	8
	CPCat Cassette	8
	CPCat Cassette	8
	CPCat Cassette	7
	CPCat Cassette	6

First<<<12345678910>>>Last

EXPOSURE

PRODUCT & USE CATEGORIES

CHEMICAL WEIGHT FRACTION

CHEMICAL FUNCTIONAL USE

TOXICS RELEASE INVENTORY

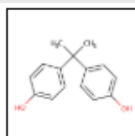
MONITORING DATA

EXPOSURE PREDICTIONS

PRODUCTION VOLUME



# Identifiers to Support Searches



## Bisphenol A

80-05-7 | DTXSID7020182

Searched by Approved Name.

### Synonyms

Download

25

Search query

Synonym	Quality
Bisphenol A	Valid
4,4'-(Propane-2,2-diyl)diphenol	Valid
Phenol, 4,4'-(1-methylethylidene)bis-	Valid
80-05-7 <span>Active CAS RN</span>	Valid
BPA	Valid
4,4'-Propane-2,2-diylidiphenol	Valid
Phenol, 4,4'-(1-methylethylidene)bis-	Valid
4-06-00-06717 <span>Beilstein Registry Number</span>	Beilstein
(4,4'-Dihydroxydiphenyl)dimethylmethane	Good
2,2-Bis(4'-hydroxyphenyl) propane	Good
2,2'-Bis(4-hydroxyphenyl)propane	Good
2,2-BIS-(4-HYDROXY-PHENYL)-PROPANE	Good
2,2-Bis(4'-hydroxyphenyl)propane	Good
2,2-Bis(p-hydroxyphenyl)propane	Good
2,2-Di(4-Hydroxyphenyl) Propane	Good

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▶ EXPOSURE

▶ BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

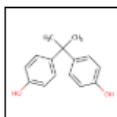
RELATED SUBSTANCES

SYNONYMS

▶ LITERATURE

LINKS

COMMENTS



## Bisphenol A

80-05-7 | DTXSID7020182

Searched by Approved Name.

### DETAILS

#### EXECUTIVE SUMMARY

#### PROPERTIES

#### ENV. FATE/TRANSPORT

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#### ▶ ADME

#### ▶ EXPOSURE

#### ▶ BIOACTIVITY

#### SIMILAR COMPOUNDS

#### GENRA (BETA)

#### RELATED SUBSTANCES


#### SYNONYMS

#### ▶ LITERATURE


#### LINKS

#### COMMENTS

### General

 EPA Substance Registry Service

 Household Products Database

 Chemical Entities of Biological Interest (ChEBI)

 PubChem

 ChempSpider

 CPCat

 DrugBank


 HMDB

 Wikipedia

 MSDS Lookup


 ChEMBL

 Chemical Vendors

 CalEPA Office of Environmental Health Hazard Assessment

 NIOSH Chemical Safety Cards

 ToxPlanet


 ACS Reagent Chemicals

 Wikidata

 ChemHat: Hazards and Alternatives Toolbox

 Wolfram Alpha

 ScrubChem

 ECHA Brief Profile

### Toxicology

 ACToR

 DrugPortal

 CCRIS

 ChemView

 CTD

 eChemPortal


 Gene-Tox


 HSDB


 ToxCast Dashboard 2

 LactMed

 International Toxicity Estimates for Risk

 ATSDR Toxic Substances Portal

 Superfund Chemical Data matrix

 NIOSH IDLH Values

 ACToR PDF Report

 Toxics Release Inventory

 CREST

 National Air Toxics Assessment

### Publications

 Toxline

 Environmental Health Perspectives


 NIEHS

 National Toxicology Program

 Google Books


 Google Scholar

 Google Patents


 PPRTVWEB

 PubMed

 IRIS Assessments

 EPA HERO


 NIOSH Skin Notation Profiles

 NIOSH Pocket Guide


 RSC Publications

 BioCaddie DataMed

 Springer Materials


 Federal Register


 Regulations.gov

 Bielefeld Academic Search Engine

 CORE Literature Search


### Analytical

 FOR-IDENT

 NEMI: National Environmental Methods Index

 RSC Analytical Abstracts

 Tox21 Analytical Data

 MONA: MassBank North America

 mzCloud

 NIST NIST IR Spectrum

 NIST NIST MS Spectrum

### Prediction

 2D NMR HSQC/HMBC Prediction

 Carbon-13 NMR Prediction

 Proton NMR Prediction

 ChemRTP Predictor

 LSERD

## Analytical



[RSC Analytical Abstracts](#)



[Tox21 Analytical Data](#)



[MONA: MassBank North America](#)



[mzCloud](#)



[NIST IR Spectrum](#)



[NIST MS Spectrum](#)



[MassBank](#)



[NEMI: National Environmental Methods Index](#)



[NIST Antoine Constants](#)



[IR Spectra on PubChem](#)





[NIST Kovats Index values](#)


# NIST WebBook

<https://webbook.nist.gov/chemistry/>


## Analytical

 FOR-IDENT

 NEMI: National Environmental  
Methods Index

 RSC Analytical Abstracts

 Tox21 Analytical Data

 MONA: MassBank North  
America

 mzCloud

 NIST IR Spectrum

 NIST MS Spectrum

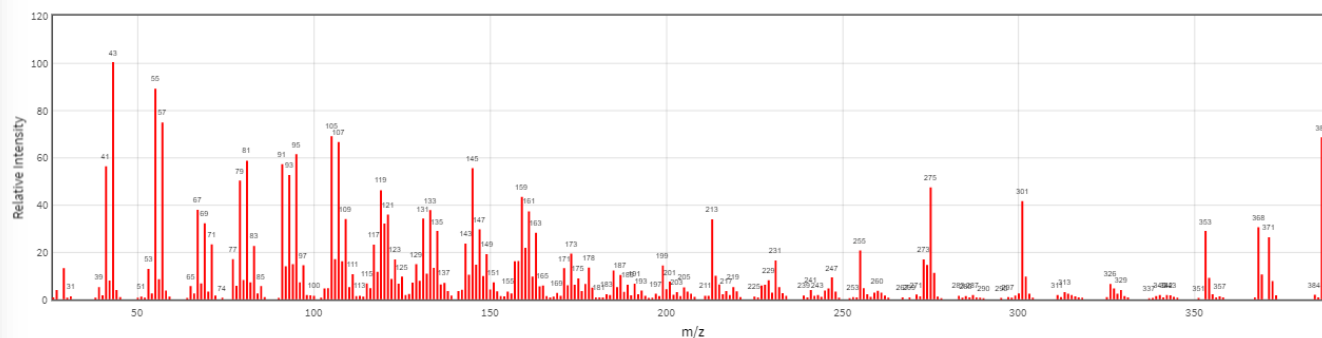
## Spectrum

Plot

Help / Software credits

Cholesterol


Mass Spectrum





# MassBank of North America

<https://mona.fiehnlab.ucdavis.edu>


## Analytical


 FOR-IDENT

 NEMI: National Environmental  
Methods Index


 RSC Analytical Abstracts





 Tox21 Analytical Data



 MONA: MassBank North  
America

 mzCloud





 NIST NIST IR Spectrum

 NIST NIST MS Spectrum

MoNA - MassBank of North America  Spectra  Downloads  Upload  Help

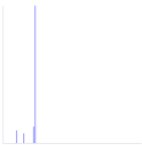
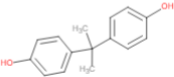
Search...  

Display Generated Query

    9




10 records/page ▾

Bisphenol A Score: ★★★★★

Q instrument	LTQ Orbitrap XL Thermo Sc...
Q instrument type	LC-ESI-ITFT
Q ms level	MS2
Q ionization	ESI
Q collision energy	30 % (nominal)
Q retention time	14.0 min
Q precursor m/z	229.1223
Q precursor type	[M+H] <sup>+</sup>
Q ionization mode	positive
Q accession	EA016309

Originally submitted to the MassBank High Quality Mass Spectral Database

# ***Batch Searching***



## Trends in Environmental Analytical Chemistry

Volume 20, October 2018, e00059



### Opioid occurrence in environmental water samples—A review

Marina Celia Campos-Mañas <sup>a</sup>, Imma Ferrer <sup>b</sup>  , E.Michael Thurman <sup>b</sup>, Ana Agüera <sup>a</sup>

 [Show more](#)

<https://doi.org/10.1016/j.teac.2018.e00059>

[Get rights and content](#)

# Batch Search Names

Buprenorphine  
 Codeine  
 Dextromethorphan  
 Dihydrocodeine  
 Dihydromorphine  
 Ethylmorphine  
 Fentanyl  
 Heroin  
 Hydrocodone  
 Hydromorphone  
 Ketamine  
 Meperidine  
 Methadone  
 Morphine  
 Morphinone  
 Naloxone  
 Naltriben  
 Oxycodone  
 Oxymorphone  
 Propoxyphene  
 Sufentanil  
 Tramadol

Step 1 Step 2 Step 3 Step 4 Step 5 Step 6

Step Five: Choose Data Fields to Download

Please enter one identifier per line

Select Input Type(s)

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

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

Buprenorphine  
 Codeine  
 Dextromethorphan  
 Dihydrocodeine  
 Dihydromorphine  
 Ethylmorphine  
 Fentanyl  
 Heroin  
 Hydrocodone  
 Hydromorphone







Excel  
Download

INPUT	FOUND_BY	DTXSID
Buprenorphine	Approved Name	DTXSID2022705
Codeine	Approved Name	DTXSID2020341
Dextromethorphan	Approved Name	DTXSID3022908
Dihydrocodeine	Approved Name	DTXSID5022936
Dihydromorphine	Approved Name	DTXSID7048908
Ethylmorphine	Approved Name	DTXSID1046760
Fentanyl	Approved Name	DTXSID9023049
Heroin	Synonym	DTXSID6046761
Hydrocodone	Approved Name	DTXSID8023131
Hydromorphone	Approved Name	DTXSID8023133
Ketamine	Approved Name	DTXSID8023187
Meperidine	Approved Name	DTXSID9023253
Methadone	Approved Name	DTXSID7023273
Morphine	Approved Name	DTXSID9023336








# Add Other Data of Interest






## Chemical Identifiers

- ☒ DTXSID 
- ☒ Chemical Name 
- ☐ DTXCID 
- ☒ 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 

INPUT	DTXSID	CASRN	MOLECULAR_FORMULA	MONOISOTOPIC	MS_READY_SMILES
Buprenorphine	<a href="#">DTXSID202</a>	52485-79-7	C29H41NO4	467.3035588	[H]C12CC3=C4C
Codeine	<a href="#">DTXSID202</a>	76-57-3	C18H21NO3	299.1521435	[H]C12CC3=C4C
Dextromethamphetamine	<a href="#">DTXSID302</a>	125-71-3	C18H25NO	271.1936144	[H]C12CC3=C(C=
Dihydrocodone	<a href="#">DTXSID502</a>	125-28-0	C18H23NO3	301.1677936	[H]C12CC3=C4C
Dihydromorphine	<a href="#">DTXSID704</a>	509-60-4	C17H21NO3	287.1521435	[H]C12CC3=C4C
Ethylmorphine	<a href="#">DTXSID104</a>	76-58-4	C19H23NO3	313.1677936	[H]C12CC3=C4C
Fentanyl	<a href="#">DTXSID902</a>	437-38-7	C22H28N2O	336.2201635	CCC(=O)N(C1CC
Heroin	<a href="#">DTXSID604</a>	561-27-3	C21H23NO5	369.1576228	[H]C12CC3=C4C
Hydrocodone	<a href="#">DTXSID802</a>	125-29-1	C18H21NO3	299.1521435	[H]C12CC3=C4C
Hydromorphone	<a href="#">DTXSID802</a>	466-99-9	C17H19NO3	285.1364935	[H]C12CC3=C4C
Ketamine	<a href="#">DTXSID802</a>	6740-88-1	C13H16ClNO	237.0920418	CNC1(CCCCC1=
Meperidine	<a href="#">DTXSID902</a>	57-42-1	C15H21NO2	247.1572289	CCOC(=O)C1(CC
Methadone	<a href="#">DTXSID702</a>	76-99-3	C21H27NO	309.2092645	CCC(=O)C(CC(C)
Morphine	<a href="#">DTXSID902</a>	57-27-2	C17H19NO3	285.1364935	[H]C12CC3=C4C
Morphinone	<a href="#">DTXSID501</a>	467-02-7	C17H17NO3	283.1208434	[H]C12CC3=C4C
Naloxone	<a href="#">DTXSID802</a>	465-65-6	C19H21NO4	327.1470582	[H]C12CC3=C4C
Naltrexone	-	-	-	-	-
Oxycodone	<a href="#">DTXSID502</a>	76-42-6	C18H21NO4	315.1470582	[H]C12CC3=C4C
Oxymorphone	<a href="#">DTXSID502</a>	76-41-5	C17H19NO4	301.1314081	[H]C12CC3=C4C
Propoxyphene	<a href="#">DTXSID102</a>	469-62-5	C22H29NO2	339.2198292	CCC(=O)OC(CC1
Sufentanil	<a href="#">DTXSID602</a>	56030-54-7	C22H30N2O2S	386.2027994	CCC(=O)N(C1=C
Tramadol	<a href="#">DTXSID908</a>	27203-92-5	C16H25NO2	263.188529	COC1=CC=CC(=

# ***Chemical Lists of Interest...***

# 225 Chemical Lists (and growing)

[Home](#)[Advanced Search](#)[Batch Search](#)[Lists ▾](#)[Predictions](#)[Downloads](#)[Lists of Chemicals](#)[List of Assays](#) Download ▾

Columns ▾

 Copy Filtered Lists URL

List Acronym ▾	List Name ▾	Last Updated ▾	Number of Chemicals ▾	List Description ▾
<a href="#">HDXEXCH</a>	<a href="#">MASSPECDB: Hydrogen Deuterium Exchange Standard Set - Under HDX Conditions</a>	2018-11-07	592	Observed species (deuterated and undeuterated) from the HDXNOEX list under hydrogen deuterium exchange conditions (Ruttkies, Schymanski et al. in prep.)
<a href="#">HDXNOEX</a>	<a href="#">MASSPECDB: Hydrogen Deuterium Exchange Standard Set - No Exchange</a>	2018-11-07	765	Environmental standard set used to investigate hydrogen deuterium exchange in small molecule high resolution mass spectrometry (Ruttkies, Schymanski et al. in prep.)
<a href="#">MASSBANKEUSP</a>	<a href="#">MASSPECDB: MassBank.EU Collection: Special Cases</a>	2017-07-16	263	The MassBank.EU list contains curated chemicals (Schymanski/Williams) associated with the literature/tentative/unknown/SI spectra available on MassBank.EU that are not available as part of the full MassBank collection of reference standard spectra.
<a href="#">MASSBANKREF</a>	<a href="#">MASSPECDB: MassBank Reference Spectra Collection</a>	2017-07-13	1267	This MassBank list contains chemicals associated with the full MassBank collection of reference standard spectra available on MassBank.EU, MassBank.JP and MassBank of North America as well as the Open Data collection, curated by Williams/Schymanski.
<a href="#">MYCOTOXINS</a>	<a href="#">MASSPECDB: Mycotoxins from MassBank.EU</a>	2017-08-02	88	This is a set of mycotoxins, initiated by the contribution of spectra of 90 mycotoxins to MassBank.EU by Justin Renaud and colleagues from Agriculture and Agri-Food Canada, Government of Canada

# "Volatilome" Human Breath

## LIST: VOLATILOME: Human Breath

Search VOLATILOME Chemicals

☐ Identifier substring search

### List Details

**Description:** This list is a subset of compounds detected in human breath and reported in the peer-reviewed literature and identified in experimental work at US-EPA. The bulk of the collection is extracted from the article "The human volatilome: volatile organic compounds (VOCs) in exhaled breath, skin emanations, urine, feces and saliva" by de Lacy Costello et al in J. Breath Res. 8 (2014) 034001 ([DOI:10.1088/1752-7155/8/3/034001](https://doi.org/10.1088/1752-7155/8/3/034001)), from the article "On-line analysis of exhaled breath", by Bruderer et al in Chemical Reviews ([DOI:10.1021/acs.chemrev.9b00005](https://doi.org/10.1021/acs.chemrev.9b00005)) as well as an increasing number of chemicals identified in our own laboratory studies.

**Number of Chemicals:** 1075

1075 chemicals

Select all

Download

Send to Batch Search

Default



CASRN



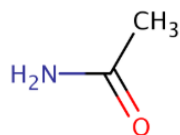
DTXSID



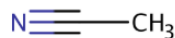
DTXSID

Hide chemicals that are:

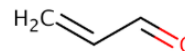
Filter by Name or CASRN



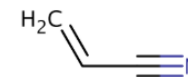
Acetamide  
CASRN:60-35-5  
DTXSID:DTXSID7020005



Acetonitrile  
CASRN:75-05-8  
DTXSID:DTXSID7020009



Acrolein  
CASRN:107-02-8  
DTXSID:DTXSID5020023



Acrylonitrile  
CASRN:107-13-1  
DTXSID:DTXSID5020029

# “Volatilome” Saliva

## LIST: VOLATILOME: Saliva

☐ Identifier substring search

### List Details

**Description:** This list is a subset of compounds detected in saliva and reported in the peer-reviewed literature and identified in experimental work at US-EPA. The collection is extracted from the article "The human volatilome: volatile organic compounds (VOCs) in exhaled breath, skin emanations, urine, feces and saliva" by de Lacy Costello et al in J. Breath Res. 8 (2014) 034001 ([DOI:10.1088/1752-7155/8/3/034001](https://doi.org/10.1088/1752-7155/8/3/034001)).

**Number of Chemicals:** 307

307 chemicals

Select all

Download

Send to Batch Search

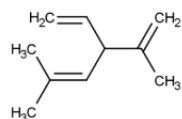
Name

CASRN

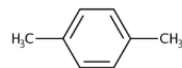
DTXSID

Hide chemicals that are:

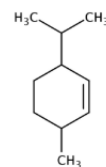
Filter by Name or CASRN



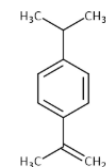
santolina triene  
CASRN:2153-66-4  
DTXSID:DTXSID90880656



p-Xylene  
CASRN:106-42-3  
DTXSID:DTXSID2021868



p-Menth-2-ene  
CASRN:5256-65-5  
DTXSID:DTXSID30333757



p-Isopropyl-alpha-methylstyrene  
CASRN:2388-14-9  
DTXSID:DTXSID90178580

# PFAS lists of Chemicals

## Select List

Download

Columns

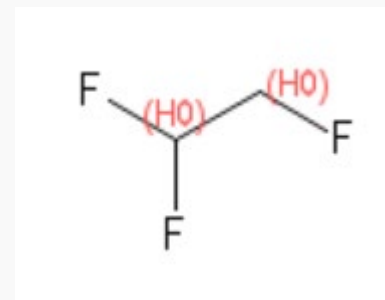
PFAS

Copy Filtered Lists URL

List Acronym	List Name	Last Updated	Number of Chemicals	List Description
EPAPFAS75S1	PFAS[EPA: 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.
EPAPFAS75S2	PFAS[EPA: List of 75 Test Samples (Set 2)]	2019-02-21	75	PFAS list corresponds to a second set of 75 samples (Set 2) submitted for testing screens conducted by EPA researchers in collaboration with researchers at the National Toxicology Program.
EPAPFASCAT	PFAS[EPA Structure-based 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[EPA: 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[EPA: ToxCast Chemical Inventory]	2018-06-29	430	PFAS chemicals included in EPA's expanded ToxCast chemical inventory and available for testing.
EPAPFASRL	PFAS[EPA: Cross-Agency Research List]	2017-11-16	199	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.
PFASKEMI	PFAS: List from the Swedish Chemicals Agency (KEMI) Report	2017-02-09	2416	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.
PFASOECD	PFAS: Listed in OECD Global Database	2018-05-16	4729	OECD released a New Comprehensive Global Database of Per- and Polyfluoroalkyl Substances, (PFASs) listing more than 4700 new PFAS
PFASTRIER	PFAS Community-Compiled List (Trier et al, 2015)	2017-07-16	597	PFASTRIER community-compiled public listing of PFAS (Trier et al, 2015)

# Building a “reference” PFAS list

- PFAS structure list (PFASSTRUCT) is expanded from public databases, agency lists and literature
- Approaching ~7000 structures – 98.8% have associated CAS Numbers
- Compare with PubChem 220,720 structures



[DATA SOURCES](#) > [CONTRIBUTOR INFORMATION](#)

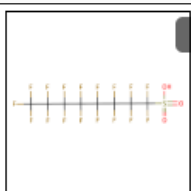
## SureChEMBL

 Share  Tweet  Email

SureChEMBL automatically extracts chemistry from the full text patent documents provided by the three major patent authorities (WIPO, USPTO, EPO). Compounds are derived from the chemical names found in text, images and attached MOL files, where available.



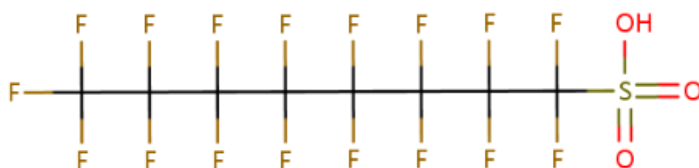
# Formula Search can find isomers



## Perfluorooctanesulfonic acid

1763-23-1 | DTXSID3031864

Searched by Synonym from Valid Source.



### Wikipedia

**Perfluorooctanesulfonic acid** (conjugate base **perfluorooctanesulfonate**) (**PFOS**) is an anion was the key ingredient in Scotchgard, a fabric protector made by 3M, and numerous stain removers. It was listed under the Convention on Persistent Organic Pollutants in May 2009. PFOS can be synthesized in industrial processes from precursors. PFOS levels that have been detected in wildlife

...

[Read more](#)

### Quality Control Notes

### Intrinsic Properties



**Molecular Formula:** C<sub>8</sub>HF<sub>17</sub>O<sub>3</sub>S



**Mol File**



**Find All Chemicals**



**Average Mass:** 500.13 g/mol



**Isotope Mass Distribution**



**Monoisotopic Mass:** 499.937494 g/mol




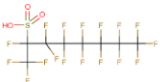

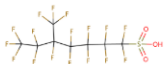

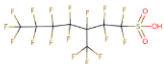
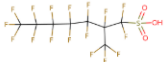
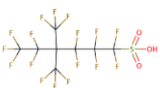
# Active expansion of the PFAS list

## From 2 to 8 variants of PFOS

Searched by Exact Molecular Formula: C8HF17O3S.

8 chemicals

Select all Download Send to Batch Search Default  DTXSID X CASRN X TOXCAST X Hide chemicals that are: Filter by Name or CASRN

 <p>Perfluorooctanesulfonic acid DTXSID:DTXSID3031864 CASRN:1763-23-1 TOXCAST:207/979</p>	 <p>Heptadecafluorooctane-2-sulfonic acid DTXSID:DTXSID30895921 CASRN:927670-12-0 TOXCAST:-</p>	 <p>IsoPFOS DTXSID:DTXSID701019144 CASRN:NOCAS_1019144 TOXCAST:-</p>	 <p>1,1,2,2,3,3,4,4,5,5,6,6,7,7,7-tetradecafluoro... DTXSID:DTXSID401019145 CASRN:NOCAS_1019145 TOXCAST:-</p>	 <p>1,1,2,2,3,3,4,5,5,6,6,7,7,7-tetradecafluoro... DTXSID:DTXSID101019146 CASRN:NOCAS_1019146 TOXCAST:-</p>	 <p>1,1,2,2,3,4,4,5,5,6,6,7,7,7-tetradecafluoro... DTXSID:DTXSID801019147 CASRN:NOCAS_1019147 TOXCAST:-</p>
 <p>1,1,2,3,3,4,4,5,5,6,6,7,7,7-tetradecafluoro... DTXSID:DTXSID501019148 CASRN:NOCAS_1019148 TOXCAST:-</p>	 <p>1,1,2,2,3,3,5,5,6,6,6-undecafluoro-4,4-bis... DTXSID:DTXSID201019149 CASRN:NOCAS_1019149 TOXCAST:-</p>				

# Disinfection By-Products

## LIST: Disinfection By-Products

Search DBPRODUCTS Chemicals

☐ Identifier substring search

### List Details

**Description:** Disinfection by-products (DBPs) result from chemical reactions between organic and inorganic matter in water with chemical treatment agents during the water disinfection process. DBPs are present in most drinking water supplies that have been subject to chlorination, chloramination, ozonation, or treatment with chlorine dioxide.

**Number of Chemicals:** 87

87 chemicals

Select all

Download

Send to Batch Search

Default

↑

CASRN

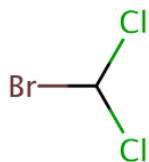
DTXSID

▼

Hide chemicals that are: ▼

Filter by Name or CASRN

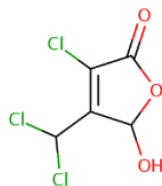
☰



Bromodichloromethane

CASRN:75-27-4

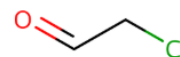
DTXSID:DTXSID1020198



3-Chloro-4-(dichloromethyl)-5-hydroxy-...

CASRN:77439-76-0

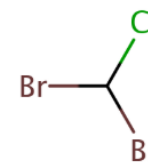
DTXSID:DTXSID6020276



Chloroacetaldehyde

CASRN:107-20-0

DTXSID:DTXSID4020292



Chlorodibromomethane

CASRN:124-48-1

DTXSID:DTXSID1020300

## MASSPECDB: Mycotoxins from MassBank.EU

☐ Identifier substring search

### List Details

**Description:** This is a set of mycotoxins, initiated by the contribution of spectra of 90 mycotoxins to [MassBank.EU](#) by Justin Renaud and colleagues from Agriculture and Agri-Food Canada, Government of Canada. This list is also a part of the [MASSBANKREE](#) list and the [NORMAN Suspect Exchange](#) and will be expanded as new contributions arrive.

**Number of Chemicals:** 88

88 chemicals

Select all

Download

Send to Batch Search

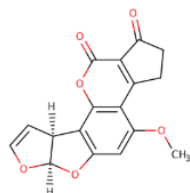
Default

CASRN

DTXSID

Hide chemicals that are:

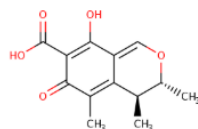
Filter by Name or CASRN



Aflatoxin B1

CASRN:1162-65-8

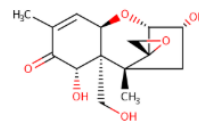
DTXSID:DTXSID9020035



Citrinin

CASRN:518-75-2

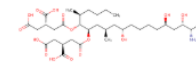
DTXSID:DTXSID8020333



Vomitoxin

CASRN:51481-10-8

DTXSID:DTXSID3020382



Fumonisin B1

CASRN:116355-83-0

DTXSID:DTXSID6020644

# Tire Crumb Rubber (298)

Related Topics: [Safer Chemicals Research](#)

[CONTACT US](#)

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## July 2019 Report: Tire Crumb Rubber Characterization

### Key Takeaways:

- EPA is releasing a new report that addresses exposure (that is, chemicals and how people come in contact with these) to tire crumb rubber on synthetic turf fields. **This report is not a risk assessment**, nor can the information be used to identify a level above which health effects could occur.
- In general, the findings for human exposure appear to be limited.
- Only Part 1 is being released for public comment and risk assessment.
- Part 1 of this report presents the findings of the literature search.
- The scope of this study was to identify potential chemical constituents in tire crumb rubber.

### Tire Crumb Rubber

 Search TIRECRUMB Chemicals

☐ Identifier substring search

#### List Details

**Description:** This chemical list is based on data contained within the [Federal Research Action Plan \(FRAP\) on Recycled Tire Crumb Used on Playing Fields and Playgrounds](#). The chemical list is obtained from the [Toxicity reference information spreadsheet](#) compiled for the potential tire crumb rubber chemical constituents identified in the State-of-Science Literature Review/Gaps Analysis, White Paper Summary of Results. Eleven sources of publicly available toxicity reference information were searched. It is important to recognize that not all potential chemical constituents identified through the literature search were confirmed through measurements made under the Federal Research Action Plan.

**Number of Chemicals:** 298

Select all

 Download

Send to Batch Search

Default



CASRN

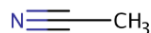
DTXSID



298 chemicals

Hide chemicals that are:

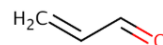
Filter by Name or CASRN



Acetonitrile

CASRN:75-05-8

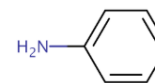
DTXSID:DTXSID7020009



Acrolein

CASRN:107-02-8

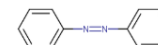
DTXSID:DTXSID5020023



Aniline

CASRN:62-53-3

DTXSID:DTXSID8020090



Azobenzene

CASRN:103-33-3

DTXSID:DTXSID8020123

# Terpenes in Vape (37)

## LIST: Terpenes in vape

☐ Identifier substring search

### List Details

**Description:** Terpenes are organic compounds found in the marijuana plant that give strains their distinct aromatic and flavor profiles. They are now being isolated and concentrated into oils for individual vaping.

**Number of Chemicals:** 37

37 chemicals

Select all

Download

Send to Batch Search

Default



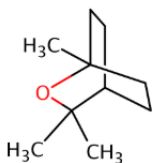
CASRN

DTXSID



Hide chemicals that are:

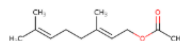
Filter by Name or CASRN



1,8-Cineol

CASRN:470-82-6

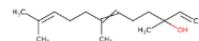
DTXSID:DTXSID4020616



Geranyl acetate

CASRN:105-87-3

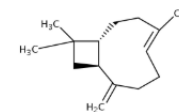
DTXSID:DTXSID0020654



Nerolidol

CASRN:7212-44-4

DTXSID:DTXSID3022247



beta-Caryophyllene

CASRN:87-44-5

DTXSID:DTXSID8024739

# Hydraulic Fracturing (1640)

## EPA's Study of Hydraulic Fracturing and Its Potential Impact on Drinking Water Resources

[Contact Us](#)

Hydraulic Fracturing Study  
Home

**Final Assessment**

EPA Published Research

Fact Sheets

Questions & Answers about  
the final assessment

Multi-agency collaboration  
on unconventional oil and  
gas research

EPA Hydraulic Fracturing -  
Agency Main Page

## Hydraulic Fracturing For Oil And Gas: Impacts From The Hydraulic

WATER|EPA; Chemicals associated with hydraulic fracturing

☐ Identifier substring search

### List Details

**Description:** Chemicals used in hydraulic fracturing fluids and/or identified in produced water from 2005-2013, corresponding to chemicals listed in Appendix H of EPA's Hydraulic Fracking Drinking Water Assessment Final Report (Dec 2016). Citation: U.S. EPA, Hydraulic Fracturing for Oil and Gas: Impacts from the Hydraulic Fracturing Water Cycle on Drinking Water Resources in the United States (Final Report). U.S. Environmental Protection Agency, Washington, D.C. EPA/600/R-16/236F, 2016. <https://www.epa.gov/hfstudy>

\*Note that Appendix H chemical listings in Tables H-2 and H-4 were mapped to current DSSTox content, which has undergone additional curation since the publication of the original EPA HF Report (Dec 2016). In the few cases where a Chemical Name and CASRN from the original report map to distinct substances (as of Jan 2018), both were included in the current EPAHFR chemical listing for completeness; additionally, 34 previously unmapped chemicals in Table H-5 are now registered in DSSTox (all but 2 assigned CASRN) and, thus, have been added to the current EPAHFR listing.

**Number of Chemicals:** 1640

Select all

Download

Send to Batch Search

Default

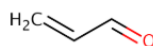
CASRN x

DTXSID x

1640 chemicals

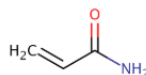
Hide chemicals that are:

Filter by Name or CASRN



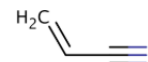
Acrolein

CASRN:107-02-8  
DTXSID:DTXSID5020023



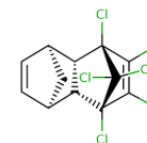
Acrylamide

CASRN:79-06-1  
DTXSID:DTXSID5020027



Acrylonitrile

CASRN:107-13-1  
DTXSID:DTXSID5020029



Aldrin

CASRN:309-00-2  
DTXSID:DTXSID8020040

# Opioids and Metabolites (160)

## DRUGS: Opioids and related metabolites

☐ Identifier substring search

### List Details

**Description:** This list of opioids and related metabolites is assembled primarily from public resources (e.g. Wikipedia, databases and literature articles) and is under ongoing curation and expansion.  
**Number of Chemicals:** 180

Select all

Download

Send to Batch Search

Default

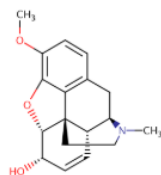
CASRN

DTXSID

180 chemicals

Hide chemicals that are:

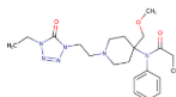
Filter by Name or CASRN



Codeine

CASRN:76-57-3

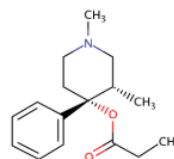
DTXSID:DTXSID2020341



Alfentanil

CASRN:71195-58-9

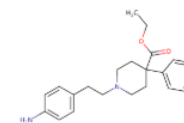
DTXSID:DTXSID9022570



Alphaprodine

CASRN:77-20-3

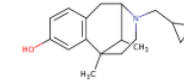
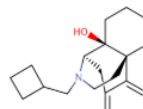
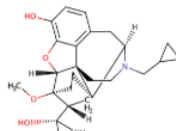
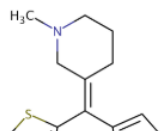
DTXSID:DTXSID4022575



Anileridine

CASRN:144-14-9

DTXSID:DTXSID8022610



# ***“MS-ready” structures***

McEachran et al. *J Cheminform* (2018) 10:45  
<https://doi.org/10.1186/s13321-018-0299-2>

Journal of Cheminformatics

METHODOLOGY

Open Access

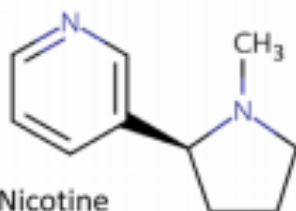
**“MS-Ready” structures for non-targeted  
high-resolution mass spectrometry screening  
studies**



Andrew D. McEachran<sup>1,2\*</sup>, Kamel Mansouri<sup>1,2,3</sup>, Chris Grulke<sup>2</sup>, Emma L. Schymanski<sup>4</sup>, Christoph Ruttkies<sup>5</sup>  
and Antony J. Williams<sup>2\*</sup>

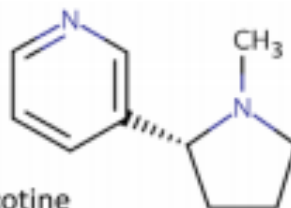


- All structure-based chemical substances are algorithmically processed to
  - Split multicomponent chemicals into individual structures
  - Desalt and neutralize individual structures
  - Remove stereochemical bonds from all chemicals
- MS-Ready structures are then mapped to original substances to provide a path between chemicals detected by mass spectrometry to original substances



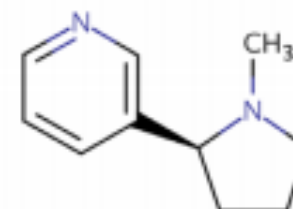
## Nicotine

CN1CCC[C@H]1C1=CN=CC=C1  
 DTXSID1020930 | SNICXCGAKADSCV  
 54-11-5 | **162.1157** | 0.929 | **72**  
 Tox: **yes** | Expo: **yes** | Bioassay: **yes**



D-Nicotine

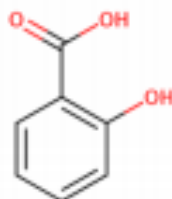
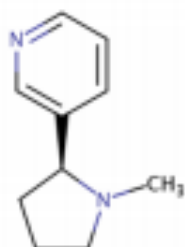
CN1CCC[C@@H]1C1=CN=CC=C1  
 DTXSID004635 | SNICXCGAKADSCV  
 25162-00-9 | **162.1157** | 0.929 | **20**  
 Tox: **no** | Expo: **yes** | Bioassay: **yes**



HCl

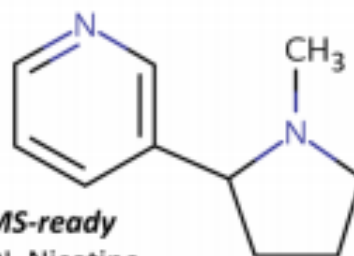
Nicotine hydrochloride

Cl.CN1CCC[C@H]1C1=CN=CC=C1  
DTXSID602093 | HDJBTAJIMNXEW  
2820-51-1 | **198.0924** | 0.929 | **9**  
Tox: **no** | Expo: **yes** | Bioassay: **yes**



Benzoic acid, 2-hydroxy-, compd. with  
3-[(2S)-1-methyl-2-pyrrolidinyl]pyridine (1:1)

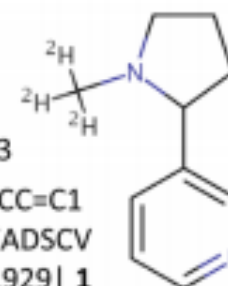
OC(=O)C1=C(O)C=CC=C1.CN1CCC[C@H]1C1=CN=CC=C1  
DTXSID5075319| AIBWPBUAKCMKNS  
29790-52-1| **300.1474**| 0.929| **6**  
Tox: **no**| Expo: **yes**| Bioassay: **no**



**MS-ready**

DL-Nicotine

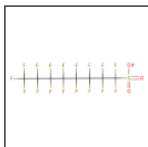
CN1CCCC1C1=CN=CC=C1  
 DTXSID3048154 | SNICXCGAKADSCV  
 22083-74-5 | **162.1157** | 0.953 | 9  
 Tox: **yes** | Expo: **no** | Bioassay: **yes**



DL-Nicotine-d3

[2H]C([2H])([2H])N1CCCC1C1=CN=CC=C1  
DTXSID80442666 | SNICXCGAKADSCV  
69980-24-1 | **165.1345** | 0.929 | **1**  
Tox: **no** | Expo: **no** | Bioassay: **no**

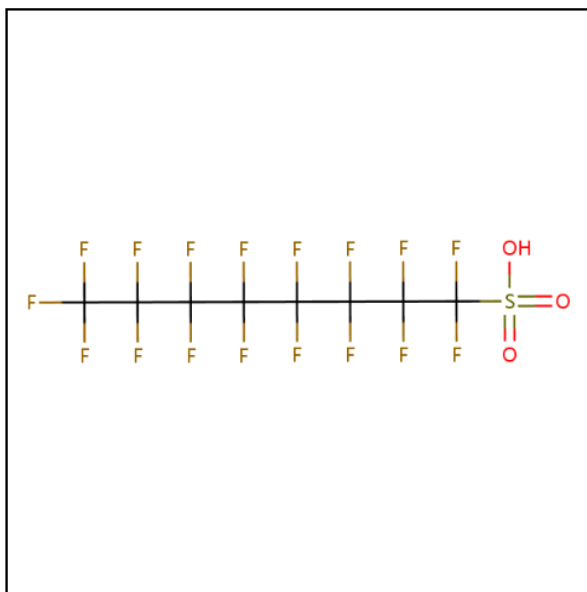
# MS-Ready Mappings from Details Page



## Perfluorooctanesulfonic acid

1763-23-1 | DTXSID3031864

Searched by Synonym from Valid Source.



### 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](#)

### Quality Control Notes

### Intrinsic Properties

### Structural Identifiers

### Linked Substances

**Same Connectivity:** [4 records](#) (based on first layer of InChI)

**Mixtures, Components and Neutralized Forms:** [9 records](#) (based on QSAR ready mappings and with the compound as a component of a mixture)

**MS-Ready Mappings:** [DTXCID1011864: 18 records;](#)

**Similar Compounds:** [83 records](#) (based on Tanimoto coefficient >0.8)

[ed search/index](#)

# MS-Ready Mappings Set of 20 substances for "PFOS"

**EPA** United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads




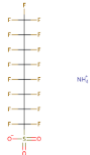
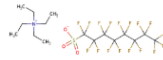

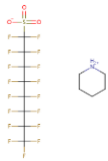

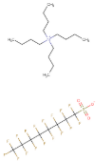
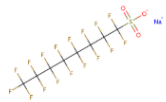

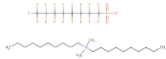
Share Search all data

## MS-Ready Mappings of Perfluorooctanesulfonic acid (Isotopes pre-filtered)

18 of 20 chemicals visible

Select all Download Send to Batch Search Default CASRN DTXSID

Isotopes Filter by Name or CASRN

 <p>Perfluorooctanesulfonic acid CASRN:1763-23-1 DTXSID:DTXSID3031864</p>	 <p>Lithium perfluorooctanesulfonate CASRN:29457-72-5 DTXSID:DTXSID2032421</p>	 <p>Potassium perfluorooctanesulfonate CASRN:2795-39-3 DTXSID:DTXSID8037706</p>	 <p>Ammonium perfluorooctanesulfonate CASRN:29081-56-9 DTXSID:DTXSID9067435</p>	 <p>Tetraethylammonium perfluorooctanesulfonate CASRN:56773-42-3 DTXSID:DTXSID5069128</p>	 <p>Bis(2-hydroxyethyl)ammonium perfluorooctanesulfonate CASRN:70225-14-8 DTXSID:DTXSID2072049</p>
 <p>Piperidinium perfluorooctanesulfonate CASRN:71463-74-6 DTXSID:DTXSID0072352</p>	 <p>Perfluorooctanesulfonate CASRN:45298-90-6 DTXSID:DTXSID80108992</p>	 <p>Tetraethylammonium perfluorooctanesulfonate CASRN:111873-33-7 DTXSID:DTXSID40584995</p>	 <p>Sodium perfluorooctanesulfonate CASRN:4021-47-0 DTXSID:DTXSID50635462</p>	 <p>Magnesium bis(perfluorooctanesulfonate) CASRN:91036-71-4 DTXSID:DTXSID80881314</p>	 <p>N-Decyl-N,N-dimethyl-1-decanaminium perfluorooctanesulfonate CASRN:251099-16-8 DTXSID:DTXSID00882964</p>

# ***Mass and Formula Searching***

# Advanced Searches

## Mass Search

### Mass Search

± Min/Max

Adduct

Neutral



All Adducts



Choose adduct from dropdown

191.131

Da

±

5

Da

ppm

Search 

# Advanced Searches

## Mass Search

### Search Results

Searched by Mass: 191.131 +/- 5.0 ppm.

329 of 329 chemicals visible

Select all

Download

Send to Batch Search

Mass Difference

DTXSID

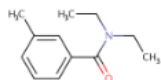
CASRN

TOXCAST

Mass Diff

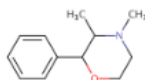
Multicomponent Chemicals

Filter by Name or CASRN



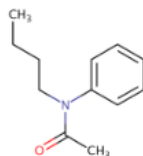
DEET

DTXSID: DTXSID2021995  
CASRN: 134-62-3  
TOXCAST: 12/768  
Mass Diff: 0.000014



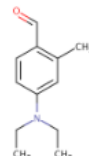
Phendimetrazine

DTXSID: DTXSID1023447  
CASRN: 634-03-7  
TOXCAST: -  
Mass Diff: 0.000014



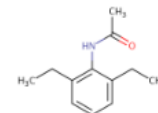
N-Butylacetanilide

DTXSID: DTXSID2042197  
CASRN: 91-49-6  
TOXCAST: -  
Mass Diff: 0.000014



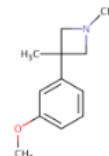
Benzaldehyde, 4-(diethylamino)-2-methyl-

DTXSID: DTXSID4059041  
CASRN: 92-14-8  
TOXCAST: -  
Mass Diff: 0.000014



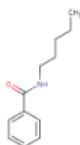
Acetanilide, 2',6'-diethyl-

DTXSID: DTXSID90168148  
CASRN: 16665-89-7  
TOXCAST: -  
Mass Diff: 0.000014



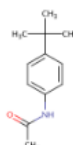
Azetidine, 1,3-dimethyl-3-(m-methoxyphenyl)-

DTXSID: DTXSID40173560  
CASRN: 19832-26-9  
TOXCAST: -  
Mass Diff: 0.000014



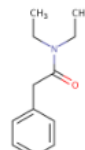
Benzamide, N-pentyl-

DTXSID: DTXSID20174196  
CASRN: 20308-43-4  
TOXCAST: -  
Mass Diff: 0.000014



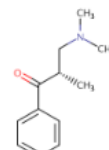
p-t-Butylacetanilide

DTXSID: DTXSID00174238  
CASRN: 20330-45-4  
TOXCAST: -  
Mass Diff: 0.000014



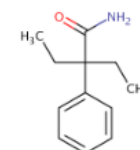
N,N-Diethylphenylacetamide

DTXSID: DTXSID00179048  
CASRN: 2431-96-1  
TOXCAST: -  
Mass Diff: 0.000014



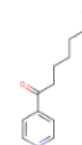
3-(Dimethylamino)-2-methylpropiofenone

DTXSID: DTXSID60180796  
CASRN: 26171-50-6  
TOXCAST: -  
Mass Diff: 0.000014



Butyramide, 2-ethyl-2-phenyl-

DTXSID: DTXSID60184653  
CASRN: 30568-39-9  
TOXCAST: -  
Mass Diff: 0.000014



1-Heptanone, 1-(4-pyridyl)-

DTXSID: DTXSID40186594  
CASRN: 32941-30-3  
TOXCAST: -  
Mass Diff: 0.000014

# MS-Ready Structures for Formula Search

## Molecular Formula Search

☒ MS Ready Formula  ☐ Exact Formula 



### Formula

Please use the format of the following example: C<sub>6</sub>H<sub>8</sub>O<sub>2</sub> or C<sub>6</sub>H(8-10)O(0-2)

Search 



- **EXACT Formula:** C<sub>10</sub>H<sub>16</sub>N<sub>2</sub>O<sub>8</sub>: 3 Hits

MS Ready Formula  ☒ Exact Formula 

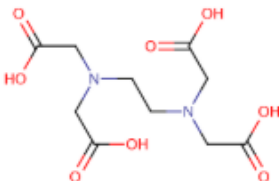
Formula

C<sub>10</sub>H<sub>16</sub>N<sub>2</sub>O<sub>8</sub>

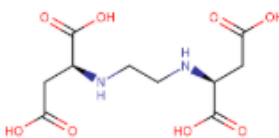
Select all Download ▾ Send to Batch Search Default ▾ ⬆

DTXSID × PubChem × CPDAT × ▾

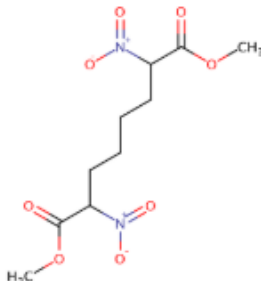
3 of 3 chemi



Ethylenediaminetetraacetic acid  
DTXSID: DTXSID6022977  
PubChem: 158  
CPDAT: 387



N,N'-Ethylenedi-L-aspartic acid  
DTXSID: DTXSID1051852  
PubChem: 25  
CPDAT: 8



Dimethyl 2,7-dinitrooctanedioate  
DTXSID: DTXSID20498864  
PubChem: 5  
CPDAT: 0

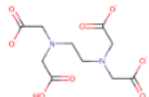
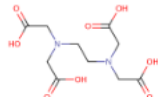
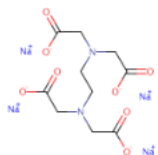
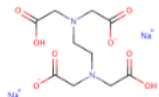
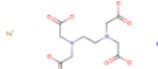
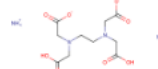
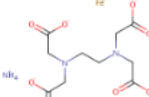
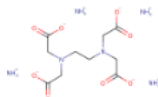
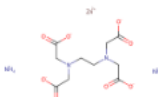
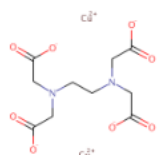
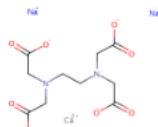
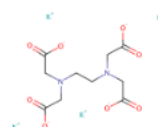
# MS-Ready Mappings

- **Same Input Formula: C<sub>10</sub>H<sub>16</sub>N<sub>2</sub>O<sub>8</sub>**
- **MS Ready Formula Search: 125 Chemicals**

125 chemicals

Select all Download Send to Batch Search Default DTXSID PubChem CPDAT

Hide chemicals that are: Filter by Name or CASR

 <p>Trisodium ethylenediaminetetraacetate DTXSID: DTXSID7020556 PubChem: 33 CPDAT: 82</p>	 <p>Ethylenediaminetetraacetic acid DTXSID: DTXSID6022977 PubChem: 158 CPDAT: 387</p>	 <p>Ethylenediaminetetraacetic acid tetrasod... DTXSID: DTXSID3026350 PubChem: 57 CPDAT: 1227</p>	 <p>Ethylenediaminetetraacetic acid, disodiu... DTXSID: DTXSID9027073 PubChem: 56 CPDAT: 1359</p>	 <p>Ethylenediaminetetraacetic acid ferric so... DTXSID: DTXSID5027774 PubChem: 53 CPDAT: 62</p>	 <p>Diammonium dihydrogen ethylenediami... DTXSID: DTXSID9027813 PubChem: 12 CPDAT: 17</p>
 <p>Ferrate(1-), [[N,N'-1,2-ethanediy]bis[N-]]... DTXSID: DTXSID9027815 PubChem: 24 CPDAT: 20</p>	 <p>Tetraammonium ethylenediaminetetraac... DTXSID: DTXSID8027820 PubChem: 11 CPDAT: 12</p>	 <p>Zincate(2-), [[N,N'-1,2-ethanediy]bis[N-]]... DTXSID: DTXSID8028343 PubChem: 5 CPDAT: 10</p>	 <p>EDTA, copper salt DTXSID: DTXSID0034564 PubChem: 8 CPDAT: 10</p>	 <p>Calcium disodium ethylenediaminetetra... DTXSID: DTXSID2036409 PubChem: 42 CPDAT: 29</p>	 <p>Tetrapotassium ethylenediaminetetra... DTXSID: DTXSID3036442 PubChem: 25 CPDAT: 36</p>

- 125 chemicals returned in total
  - 8 of the 125 are **single component** chemicals
  - 3 of the 8 are **isotope-labeled**
  - 3 are **neutral compounds** and 2 are **charged**
- Multiple components, stereo, isotopes and charge all collapsed and mapped through MS-Ready

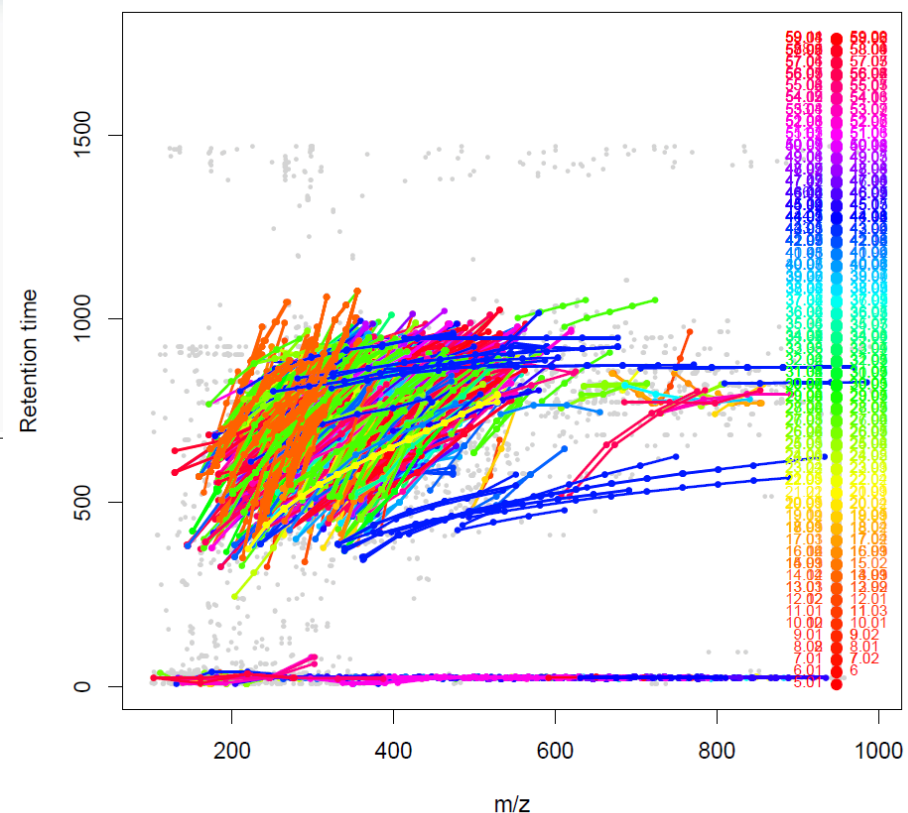
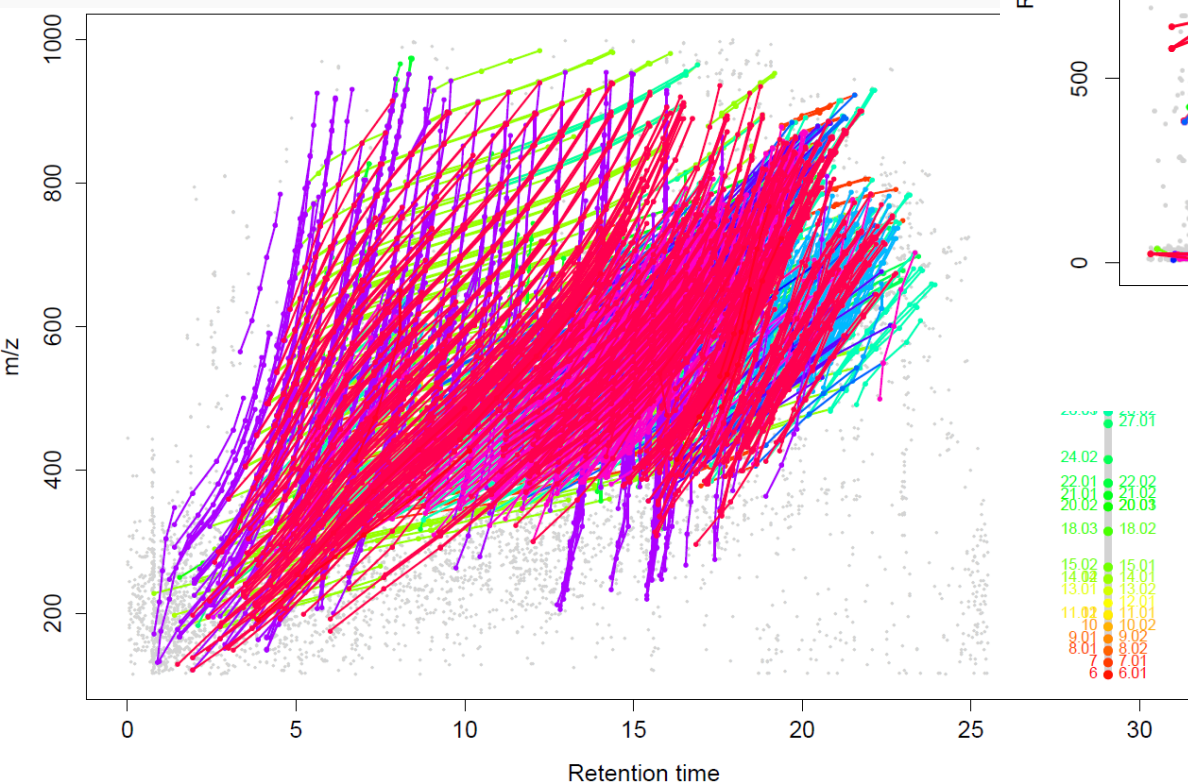
# ***“UVCB” Chemicals***

## 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.

# UVCBs challenge in non-target analysis

- Complex mixtures (UVCBs) are a **huge** and **very challenging** part of the unknowns in many environmental samples



Homologue screening plots from  
Swiss Wastewater (Schymanski *et al*  
2014, left) and Novi Sad (right)

**solutions**

# Public TSCA Inventory on Dashboard 31,460 Chemicals (1/24/2020)

## EPA|TSCA: TSCA Inventory, active non-confidential portion

☐ Identifier substring search

### List Details

**Description:** Section 8 (b) of the Toxic Substances Control Act (TSCA) requires EPA to compile, keep current and publish a list of each chemical substance that is manufactured or processed, including imports, in the United States for uses under TSCA. Information about what types of substances are on the TSCA inventory can be found here. The Toxic Substances Control Act (TSCA), as amended by the Frank R. Lautenberg Chemical Safety for the 21st Century Act, requires EPA to designate chemical substances on the TSCA Chemical Substance Inventory as either "active" or "inactive" in U.S. commerce. To accomplish this, EPA finalized a rule requiring industry reporting of chemicals manufactured (including imported) or processed in the U.S.. This reporting is used to identify which chemical substances on the TSCA Inventory are active in U.S. commerce and help inform the prioritization of chemicals for risk evaluation. The list contained in the dashboard includes the active TSCA inventory based on notifications through Feb. 7th 2018 and substances reported from Feb 8, 2018 – March 30, 2018 that have been unambiguously mapped to DSSTox using CASRN and chemical names. The curation of the non-confidential portion of active TSCA inventory is an ongoing process involving trained chemists to validate the correctness of DSSTox structural and identifier data. The content of the list will change over time as the non-confidential active TSCA inventory is updated and more substances are curated. (Updated January 5th 2020)

**Number of Chemicals:** 31460

2250 of 31460 chemicals loaded

Select all

Download

Send to Batch Search

Default

↑

CASRN

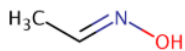
DTXSID

▼

Hide chemicals that are:

Filter by Name or CASRN

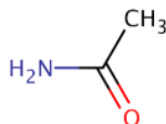
≡



Acetaldehyde oxime

CASRN:107-29-9

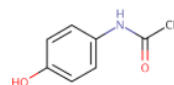
DTXSID:DTXSID2020004



Acetamide

CASRN:60-35-5

DTXSID:DTXSID7020005



Acetaminophen

CASRN:103-90-2

DTXSID:DTXSID2020006



Acetonitrile

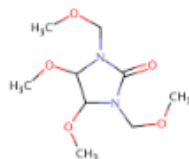
CASRN:75-05-8

DTXSID:DTXSID7020009

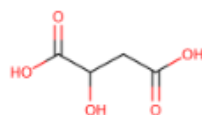


# Many Chemicals are “Complex”

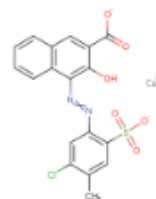
## >14000 chemicals are UVCBs



2-Imidazolidinone, 4,5-dimethoxy-1,3-bis(methoxymethyl)-  
DTXSID: DTXSID0027569  
PubChem: 24  
CASRN: 4356-80-9



Malic acid  
DTXSID: DTXSID0027640  
PubChem: 273  
CASRN: 6915-15-7



C.I. Pigment Red 48, calcium salt (1:1)  
DTXSID: DTXSID0027642  
PubChem: 0  
CASRN: 7023-81-2

0 related chemical  
structures with this  
substance

Lard, oil  
DTXSID: DTXSID0027690  
PubChem: 0  
CASRN: 8016-28-2

0 related chemical  
structures with this  
substance

Tall-oil pitch  
DTXSID: DTXSID0027692  
PubChem: 0  
CASRN: 8016-81-7

0 related chemical  
structures with this  
substance

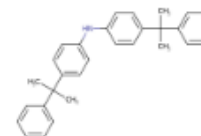
Palm kernel oil  
DTXSID: DTXSID0027694  
PubChem: 0  
CASRN: 8023-79-8

0 related chemical  
structures with this  
substance

Tallow, hydrogenated  
DTXSID: DTXSID0027696  
PubChem: 0  
CASRN: 8030-12-4

0 related chemical  
structures with this  
substance

Quaternary ammonium compounds, tri...  
DTXSID: DTXSID0027698  
PubChem: 0  
CASRN: 8030-78-2



4-(2-Phenylpropan-2-yl)-N-[4-(2-phenyl...  
DTXSID: DTXSID0027721  
PubChem: 50  
CASRN: 10081-67-1

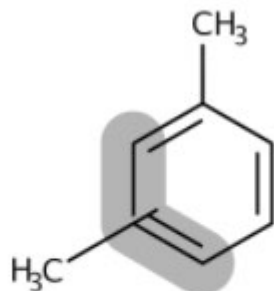
1 related chemical  
structure with this  
substance

Isomethyltetrahydrophthalic anhydride  
DTXSID: DTXSID0027729  
PubChem: 0  
CASRN: 11070-44-3

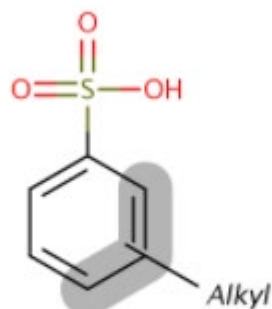


# “Markush Structures”

[https://en.wikipedia.org/wiki/Markush\\_structure](https://en.wikipedia.org/wiki/Markush_structure)



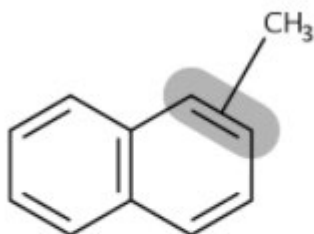
Xylenes  
1330-20-7



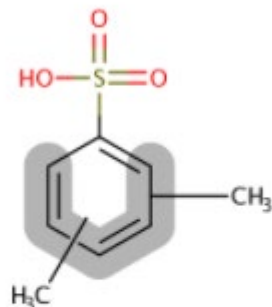
(C10-C16) Alkylbenzenesulfonic acid  
68584-22-5



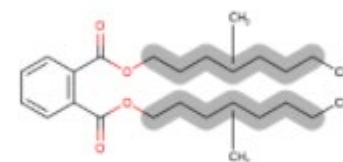
n-Nonylphenol  
25154-52-3



Methyl-naphthalene  
1321-94-4

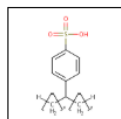


Sodium xylenesulfonate  
1300-72-7



Diisononyl phthalate  
28553-12-0

# How to represent complexity?



Alkylbenzenesulfonate, linear

42615-29-2 | DTXSID3020041

Searched by DSSTox Substance Id.

15 of 25 chemicals selected

Deselect all

Download

Send to Batch Search

Relationship

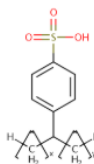
CASRN

DTXSID

Unselected

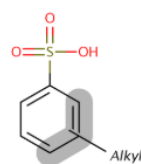
Filter by Name or CASRN

Searched Chemical



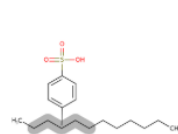
Alkylbenzenesulfonate, linear  
CASRN:42615-29-2  
DTXSID:DTXSID3020041

Component



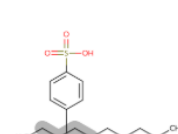
(C10-C16) Alkylbenzenesulfonic acid  
CASRN:68584-22-5  
DTXSID:DTXSID2028723

Component



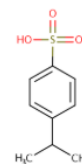
C12-linear alkyl benzene sulfonate  
CASRN:NOCAS\_891641  
DTXSID:DTXSID90891641

Component



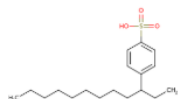
C10-linear alkylbenzenesulfonate  
CASRN:NOCAS\_891689  
DTXSID:DTXSID70891689

Markush Child



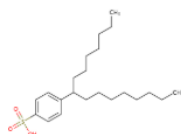
4-Isopropylbenzenesulfonic acid  
CASRN:16066-35-6  
DTXSID:DTXSID1044932

Markush Child



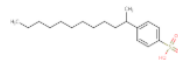
4-(3-Dodecyl)benzenesulfonic acid  
CASRN:18777-54-3  
DTXSID:DTXSID7058670

Markush Child



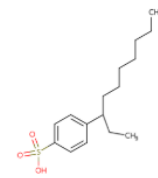
4-(1-Heptylnonyl)benzenesulfonic acid  
CASRN:80233-94-9  
DTXSID:DTXSID40273953

Markush Child



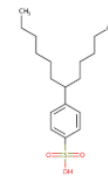
2-Phenyldodecane-p-sulfonate  
CASRN:18777-53-2  
DTXSID:DTXSID40274021

Markush Child



4-(Decan-3-yl)benzene-1-sulfonic acid  
CASRN:65186-00-7  
DTXSID:DTXSID20859618

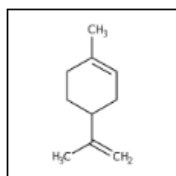
Markush Child



4-(Dodecan-6-yl)benzene-1-sulfonic acid  
CASRN:23003-92-1  
DTXSID:DTXSID30860093

# ***In the Dashboard Abstract Sifter***


# Literature Searching



Limonene

138-86-3 | DTXSID2029612

Searched by Approved Name.

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

Select a Query Term ▼

Retrieve Articles 

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

Optionally, edit the query before retrieving.

("138-86-3" OR "Limonene") AND (food AND (exposure OR near-field OR far-field OR nhanes OR Environmental Monitoring OR Environmental Exposure OR exposome))

70 of 70 articles loaded...



# Literature Searching

To find articles quickly, enter terms to sift abstracts. 

<input type="checkbox"/>	limonene ↓	food	exposure	Total	PMID	Year	Title
<input type="checkbox"/>	17	2	2	21	2024047	1991	The human relevance of the renal tumor-inducing pote...
<input type="checkbox"/>	11	2	3	16	23424676	2013	Mechanism of bacterial inactivation by (+)-limonene an...
<input type="checkbox"/>	10	1	3	14	23573938	2013	Safety evaluation and risk assessment of d-Limonene.
<input type="checkbox"/>	10	5	0	15	12633519	2003	Development of a questionnaire and a database for as...
<input type="checkbox"/>	9	1	1	11	18809464	2008	Odour of limonene affects feeding behaviour in the blo...

## The human relevance of the renal tumor-inducing potential of d- limonene in male rats: implications for risk assessment.

The monoterpene d-**limonene** is a naturally occurring chemical which is the major component in oil of orange. Currently, d-**limonene** is widely used as a flavor and fragrance and is listed to be generally recognized as safe (GRAS) in **food** by the Food and Drug Administration (21 CFR 182.60 in the Code of Federal Regulations). Recently, however, d-**limonene** has been shown to cause a male rat-specific kidney toxicity referred to as hyaline droplet nephropathy. Furthermore, chronic **exposure** to d-**limonene** causes a significant incidence of renal tubular tumors exclusively in male rats. Although d-**limonene** is not carcinogenic in female rats or male and female mice given much higher dosages, the male rat-specific nephrocarcinogenicity of d-**limonene** may raise some concern regarding the safety of d-**limonene** for human consumption. A considerable body of scientific data has indicated that the renal toxicity of d-**limonene** results from the accumulation of a protein, alpha 2u-globulin, in male rat kidney proximal tubule lysosomes. This protein is synthesized exclusively by adult male rats. Other species, including humans, synthesize proteins that share significant homology with alpha 2u-globulin. However, none of these proteins, including the mouse equivalent of alpha 2u-globulin, can produce this toxicity, indicating a unique specificity for alpha 2u-globulin. With chronic **exposure** to d-**limonene**, the hyaline droplet nephropathy progresses and the kidney shows tubular cell necrosis, granular cast formation at the corticomedullary junction, and compensatory cell proliferation. Both d-**limonene** and cis-d-**limonene**-1,2-oxide (the major metabolite involved in this toxicity) are negative in in vitro mutagenicity screens. Therefore, the toxicity-related renal cell proliferation is believed to be integrally involved in the carcinogenicity of d-**limonene** as persistent elevations in renal cell proliferation may increase fixation of spontaneously altered DNA or serve to promote spontaneously initiated cells. The scientific data base demonstrates that the tumorigenic activity of d-**limonene** in male rats is not relevant to humans. The three major lines of evidence supporting the human safety of d-**limonene** are (1) the male rat specificity of the nephrotoxicity and carcinogenicity; (2) the pivotal role that alpha 2u-globulin plays in the toxicity, as evidenced by the complete lack of toxicity in other species despite the presence of structurally similar proteins; and (3) the lack of genotoxicity of both d-**limonene** and d-**limonene**-1,2-oxide, supporting the concept of a nongenotoxic mechanism, namely, sustained renal cell proliferation.(ABSTRACT TRUNCATED AT 400 WORDS)



F1000Research

F1000Research 2017, 6(Chem Inf Sci):2164 Last updated: 02 OCT 2019



SOFTWARE TOOL ARTICLE

## Abstract Sifter: a comprehensive front-end system to PubMed [version 1; peer review: 2 approved]



Nancy Baker <sup>1</sup>, Thomas Knudsen<sup>2</sup>, Antony Williams <sup>2</sup>

<sup>1</sup>Leidos, Research Triangle Park, NC, USA

<sup>2</sup>National Center for Computational Toxicology, U.S. Environmental Protection Agency, Research Triangle Park, NC, USA

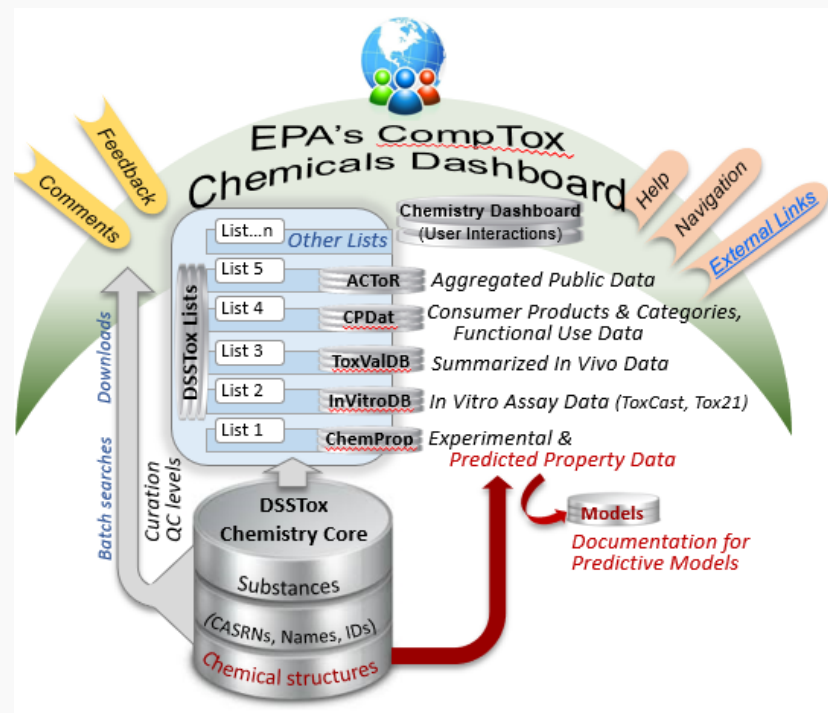
**v1** **First published:** 21 Dec 2017, 6(Chem Inf Sci):2164 (  
<https://doi.org/10.12688/f1000research.12865.1>)  
**Latest published:** 21 Dec 2017, 6(Chem Inf Sci):2164 (  
<https://doi.org/10.12688/f1000research.12865.1>)

Open Peer Review

Reviewer Status  

# Conclusion

- Dashboard access to data for ~875,000 chemicals (~895k in the Spring Release)
- MS-Ready data facilitates structure identification
- Related metadata facilitates candidate ranking
- Relationship mappings and chemical lists of great utility
- Curation and mutual sharing of chemical lists is important (e.g. NORMAN)





# Acknowledgements



## **EPA ORD**

Ann Richard  
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James McCord  
Seth Newton  
Katherine Phillips  
Tom Purucker  
Jon Sobus  
Mark Strynar  
Elin Ulrich  
Joach Pleil

## **TEAMS**

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Curation Team

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## **Collaborators**

Emma Schymanski  
NORMAN Network  
Andrew McEachran  
Jerry Zweigenbaum




# MANY presentations online

<https://tinyurl.com/w5hqs55>

Antony Williams

help? ✕

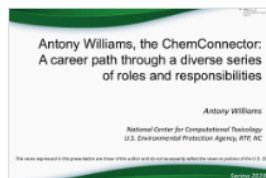
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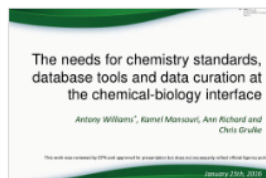
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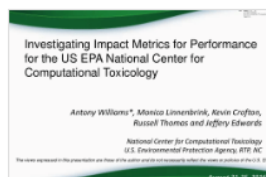
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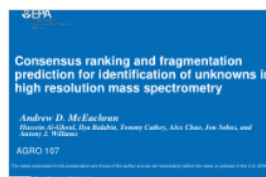
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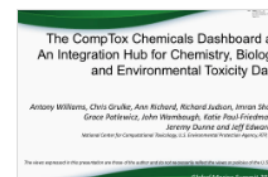
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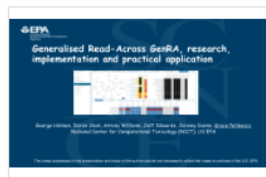
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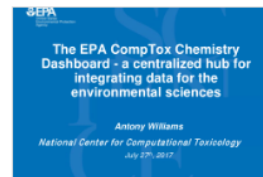
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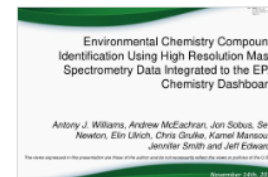
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Williams et al. *J Cheminform* (2017) 9:61  
DOI 10.1186/s13321-017-0247-6


 Journal of Cheminformatics

**DATABASE**

**Open Access**

### The CompTox Chemistry Dashboard: a community data resource for environmental chemistry



Antony J. Williams<sup>1\*</sup> , Christopher M. Grulke<sup>1</sup>, Jeff Edwards<sup>1</sup>, Andrew D. McEachran<sup>2</sup>, Kamel Mansouri<sup>1,2,4</sup>, Nancy C. Baker<sup>3</sup>, Grace Patlewicz<sup>1</sup>, Imran Shah<sup>1</sup>, John F. Wambaugh<sup>1</sup>, Richard S. Judson<sup>1</sup> and Ann M. Richard<sup>1</sup>

<https://doi.org/10.1186/s13321-017-0247-6>