



# Chemistry Data Management, Cheminformatics and the EPA's DSSTox Database

Antony J. Williams and Charles Lowe

Center for Computational Toxicology and Exposure

# Relevant definitions

- DSSTox is the **database** of chemical substances, structures, identifiers and intrinsic properties
- ChemReg is the chemical registration **application** used to register substances, lists and perform curation
- The CompTox Chemicals Dashboard is the **application** providing public access to a snapshot of DSSTox data and other data streams

# Historical Lineage

- 2000: DSSTox was conceived by Ann Richard
- 2004: Basic web interface went public with 7,000 substances
- 2011: Tox21 library added 8,500 substances managed in DSSTox
- 2013: DSSTox reached 24,000 substances and manual curation was unsustainable
- 2014: MySQL database expanded with public data resources to 740k substances with 5 QC levels. ChemReg introduced
- 2016: CompTox Chemicals Dashboard release. 560k chemicals
- 2016-2024: Data releases on an ongoing basis: 1.21M chemicals

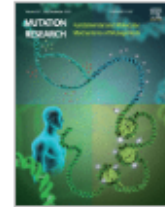
# Two Decades of Development

The Proposal: <https://pubmed.ncbi.nlm.nih.gov/11804603/>



Mutation Research/Fundamental and Molecular  
Mechanisms of Mutagenesis

Volume 499, Issue 1, 29 January 2002, Pages 27-52



Mutation Research Frontiers

## Distributed structure-searchable toxicity (DSSTox) public database network: a proposal

Ann M. Richard<sup>a</sup>  , ClarLynda R. Williams<sup>a b</sup>

# DSSTox Has Been Stable for Years



Computational Toxicology

Volume 12, November 2019, 100096



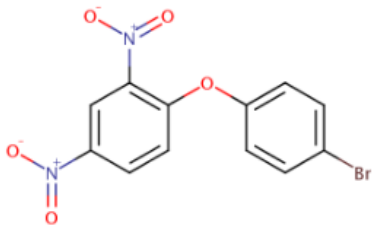
EPA's DSSTox database: History of development of a curated chemistry resource supporting computational toxicology research

[Christopher M. Grulke](#)<sup>a</sup>, [Antony J. Williams](#)<sup>a</sup>, [Inthirany Thillanadarajah](#)<sup>b</sup>, [Ann M. Richard](#)<sup>a</sup>  

# ChemReg: Registration and Curation

View/Edit a Single Record   Structure Search   Browse/Curate Records   Export DSSTox   Chemotypes   [Login](#)

CAS-RN matched  
<b>null</b>  
You are viewing the record associated with DTXSID0022270  
CASRN: 17589-66-1



Systematic Name: 1-(4-Bromophenoxy)-2,4-dinitrobenzene  
MolFormula: C12H7BrN2O5  
InChI Key: BJGBENCKKXEWGB-UHFFFAOYSA-N  
Smiles: [\[O-\]\[N+\]](#)  
[\(=O\)C1=CC\(=C\(OC2=CC=C\(Br\)C=C2\)C=C1\)](#)  
[\[N+\]\(O\)=O](#)  
PubChem ID: [221811](#)  
Chempid ID: [192492](#)

Substance ID: DTXSID0022270  
CAS: 17589-66-1  
Name: 4-Bromo-2',4'-dinitrodiphenyl ether  
Substance Type: Single Compound  
QC Level: [?](#) DSSTox\_Low  
Data Source: Public

Compound ID: DTXCID702270  
Chemical Shown: Tested Chemical

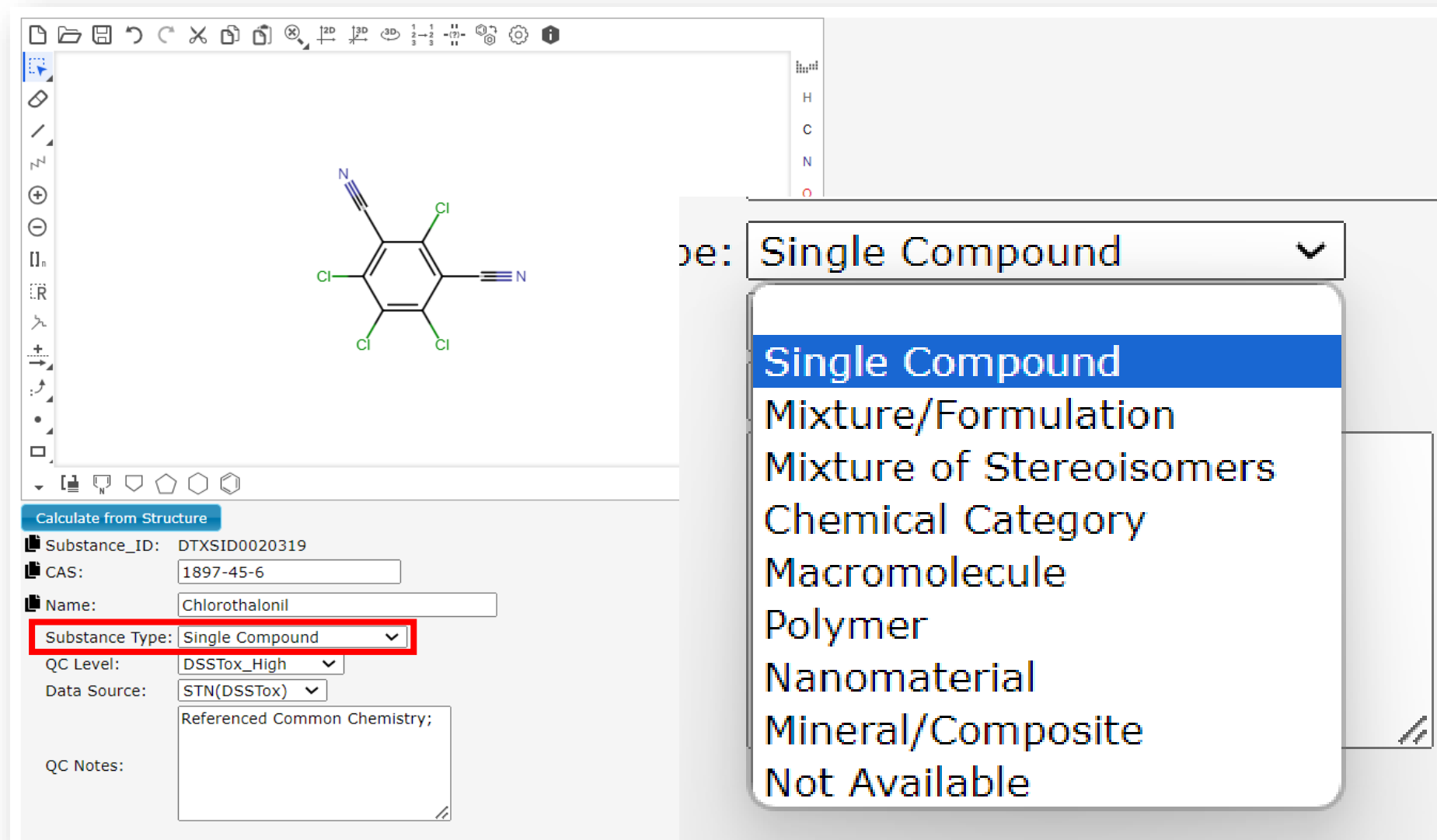
Internal QC Notes:

QC Notes:

Source of CAS-Compound: Public  
Double Stereo:   
Chiral Stereo:   
Chemical Form: Organic

- ▶ Associated Lists (10)
- ▶ Synonyms (0)
- ▶ Other Cas (0)
- ▶ Successor Substances (0)
- ▶ Predecessor Substances (0)

# Different Types of Chemical Substances



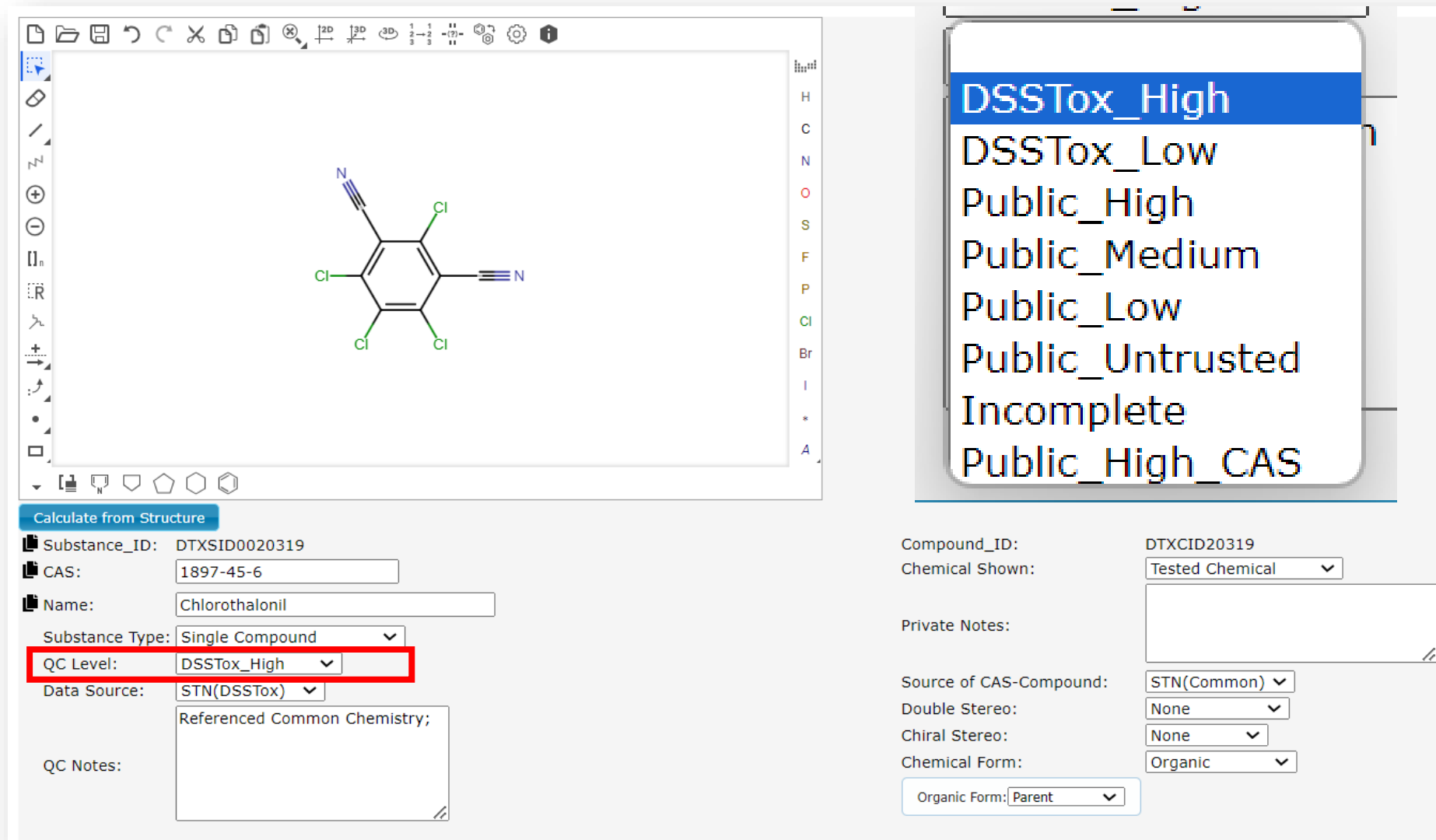
The image shows a screenshot of a chemical software interface. The main window displays the chemical structure of Chlorothalonil, a hexachlorocyclohexadiene derivative with two cyano groups. Below the structure, there is a form with the following fields:

- Substance\_ID: DTXSID0020319
- CAS: 1897-45-6
- Name: Chlorothalonil
- Substance Type: Single Compound (highlighted with a red box)
- QC Level: DSSTox\_High
- Data Source: STN(DSSTox)
- QC Notes: Referenced Common Chemistry;

On the right side, a dropdown menu is open, showing the following options:

- Single Compound (selected)
- Mixture/Formulation
- Mixture of Stereoisomers
- Chemical Category
- Macromolecule
- Polymer
- Nanomaterial
- Mineral/Composite
- Not Available

# QC Level Details



The image displays a chemical software interface. On the left, a chemical structure of Chlorothalonil is shown, consisting of a benzene ring with two cyano groups and four chlorine atoms. Below the structure, a form contains the following information:

- Substance\_ID: DTXSID0020319
- CAS: 1897-45-6
- Name: Chlorothalonil
- Substance Type: Single Compound
- QC Level: DSSTox\_High (highlighted with a red box)
- Data Source: STN(DSSTox)
- QC Notes: Referenced Common Chemistry;

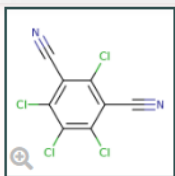
On the right, a dropdown menu is open, showing a list of QC levels. The top option, DSSTox\_High, is highlighted in blue. The other options are DSSTox\_Low, Public\_High, Public\_Medium, Public\_Low, Public\_Untrusted, Incomplete, and Public\_High\_CAS.

Below the dropdown, the following details are visible:

- Compound\_ID: DTXCID20319
- Chemical Shown: Tested Chemical
- Private Notes: (empty text area)
- Source of CAS-Compound: STN(Common)
- Double Stereo: None
- Chiral Stereo: None
- Chemical Form: Organic
- Organic Form: Parent



# QC Levels in the Dashboard

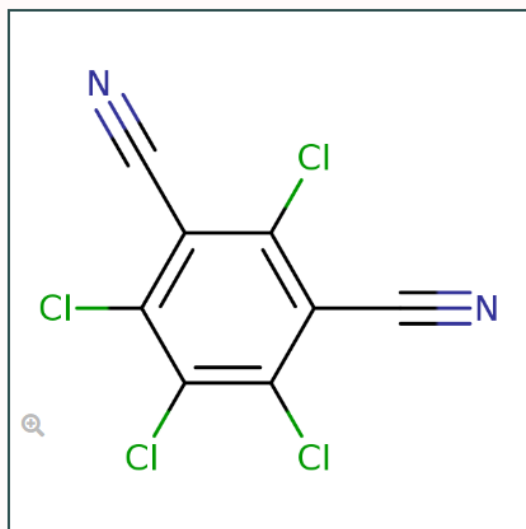


## Chlorothalonil

1897-45-6 | DTXSID0020319

Searched by Approved Name

### Chemical Details



Wikipedia

Quality Control Notes

Intrinsic Properties

Structural Identifiers

Linked Substances

Presence in Lists

Record Information



**Citation:** U.S. Environmental Protection Agency. Comptox Chemicals Dashboard.

<https://comptoxstaging.rtpnc.epa.gov/dashboard/chemical/details/DTXSID0020319> (accessed April 14, 2024) Chlorothalonil

#### Data Quality:

Level 1: Expert curated, highest confidence in accuracy and consistency of unique chemical identifiers

Level 2: Expert curated, unique chemical identifiers using multiple sources

Level 3: Programmatically curated from high quality EPA source, unique chemical identifiers have no conflicts in ChemID and PubChem

Level 4: Programmatically curated from ChemID, unique chemical identifiers have no conflicts in PubChem

Level 5: Programmatically curated from ACToR or PubChem, unique chemical identifiers with low confidence, single public source

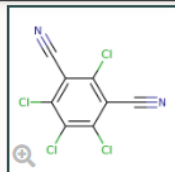
# Synonyms

▼ Synonyms (79)

<input type="checkbox"/>	Synonym	Source	Quality
<input checked="" type="checkbox"/>	TPN	DSSTox	Ambiguous
<input checked="" type="checkbox"/>	1,3-Benzenedicarbonitrile, 2,4,5,6-tetr	CommonChemistry	Valid Source
<input checked="" type="checkbox"/>	1,3-Benzenedicarbonitrile, 2,4,5,6-te	CommonChemistry	Valid Source
<input checked="" type="checkbox"/>	1,3-Dicyanotetrachlorobenzene	CommonChemistry	Valid Source
<input checked="" type="checkbox"/>	2,4,5,6-Tetrachloro-1,3-benzenedicarb	CommonChemistry	Valid Source
<input checked="" type="checkbox"/>	Clorthalonil	ChemID	Unique
<input checked="" type="checkbox"/>	Tetrachlorisofthalonitril	ChemID	Unique
<input checked="" type="checkbox"/>	UNII-J718M71A7A	ChemID	Unique
<input checked="" type="checkbox"/>	m-TCPN	ChEBI	Unique
<input checked="" type="checkbox"/>	m-Tetrachlorophthalonitrile	ChEBI	Unique
<input checked="" type="checkbox"/>	meta-TCPN	ChEBI	Unique
<input checked="" type="checkbox"/>	meta-Tetrachlorophthalodinitrile	ChEBI	Unique
<input checked="" type="checkbox"/>	Tetrachloroisophthalonitrile	Other	Expert Validated
<input checked="" type="checkbox"/>	2,4,5,6-Tetrachloro-1,3-benzenedicarb	Other	Expert Validated
<input checked="" type="checkbox"/>	SDS2787	Other	Unique
<input checked="" type="checkbox"/>	R44686	Other	Unique
<input checked="" type="checkbox"/>	217-588-1	Other	Unique
<input checked="" type="checkbox"/>	EC No.: 217-588-1	Other	Unique

Delete Selected Add Synonym

# Synonyms in the Dashboard



## Chlorothalonil

1897-45-6 | DTXSID0020319

Searched by Approved Name

### Synonyms

[EXPORT](#)

Synonym <span>↓↑</span>	Quality <span>↓↑</span>
<input type="text"/>	<input type="text"/>
<b>1,3-Benzenedicarbonitrile, 2,4,5,6-tetrachloro-</b>	<b>Valid</b>
<b>1897-45-6</b> <span>Active CAS-RN</span>	<b>Valid</b>
<b>2,4,5,6-Tetrachloro-1,3-benzenedicarbonitrile</b>	<b>Valid</b>
<b>2,4,5,6-Tetrachlorobenzene-1,3-dicarbonitrile</b>	<b>Valid</b>
<b>Chlorothalonil</b>	<b>Valid</b>
<b>Tetrachloroisophthalonitrile</b>	<b>Valid</b>
<i>1,3-Benzenedicarbonitrile, 2,4,5,6-tetrachloro-</i>	<i>Good</i>
<i>1,3-Dicyanotetrachlorobenzene</i>	<i>Good</i>
<i>2,4,5,6-Tetrachloro-1,3-benzenedicarbonitrile</i>	<i>Good</i>

# There Can Be *Multiple CAS RNs*

Substance\_ID: DTXSID0020319  
CAS: 1897-45-6  
Name: Chlorothalonil  
Substance Type: Single Compound  
QC Level: DSSTox\_High  
Data Source: STN(DSSTox)  
QC Notes: Referenced Common Chemistry;

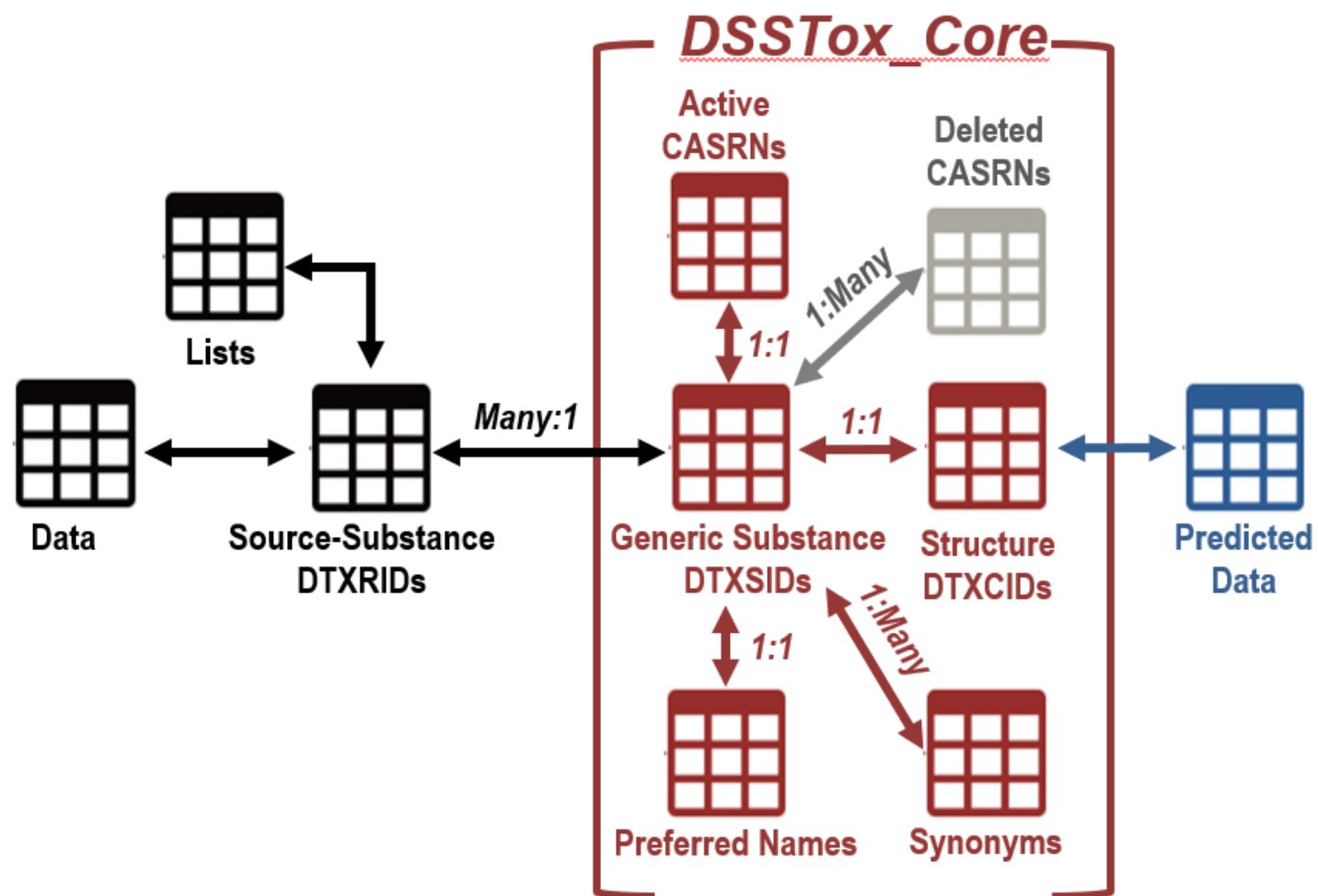
Compound\_ID: DTXCID20319  
Chemical Shown: Tested Chemical  
Private Notes:  
Source of CAS-Compound: STN(Common)  
Double Stereo: None  
Chiral Stereo: None  
Chemical Form: Organic  
Organic Form: Parent

▶ Synonyms (79)  
▼ Other Cas (5)

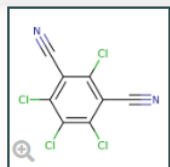
<input type="checkbox"/>	CAS-RN	Relationship	Source	Comments
<input checked="" type="checkbox"/>	101963-73-9	Deleted	SRS	
<input checked="" type="checkbox"/>	216082-57-4	Deleted	SRS	
<input checked="" type="checkbox"/>	342632-51-3	Deleted	SRS	
<input checked="" type="checkbox"/>	37223-69-1	Deleted	SRS	
<input checked="" type="checkbox"/>	462093-27-2	Deleted	SRS	

Delete Selected Add Other Cas

# The Data Model



# CAS RNs in the Dashboard



## Chlorothalonil

1897-45-6 | DTXSID0020319

Searched by Approved Name

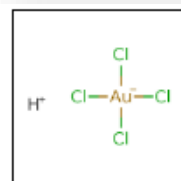
### Synonyms

Search Chemical Synonyms

EXPORT

Synonym ↓↑	Quality ↓↑
Repulse	Other
SDS2787	Other
Terraclactyl	Other
Tetrachlorisofthalonitril	Other
Tetrachloroisophthalonitrile	Other
TPN	Other
UNII-J718M71A7A	Other
101963-73-9 Deleted CAS-RN	Deleted
216082-57-4 Deleted CAS-RN	Deleted
342632-51-3 Deleted CAS-RN	Deleted
37223-69-1 Deleted CAS-RN	Deleted
462093-27-2 Deleted CAS-RN	Deleted

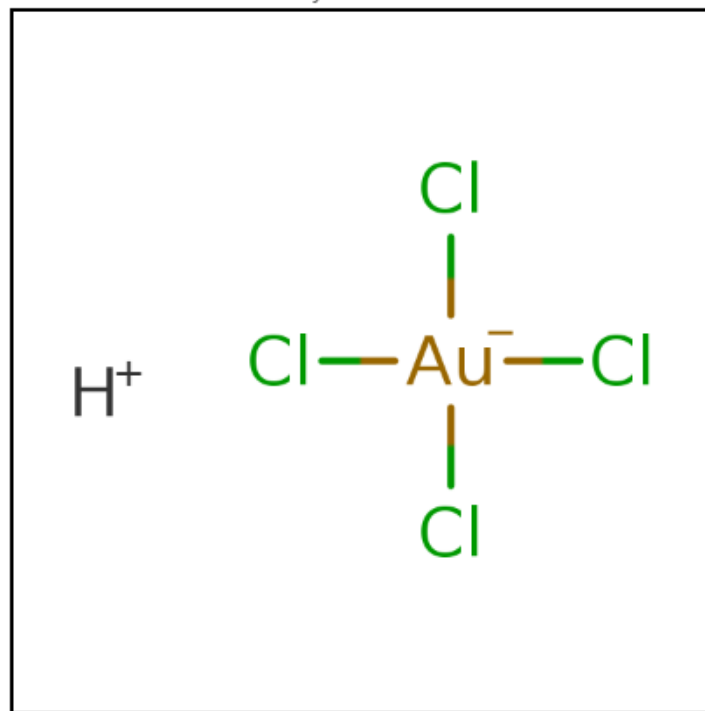
# One Substance – One Active CASRN



Tetrachloroauric acid

16903-35-8 | DTXSID701014499

Searched by CAS-RN.



## Wikipedia

Chloroauric acid is an inorganic compound with the chemical formula  $\text{H}[\text{AuCl}_4]$ . It forms hydro...

[Read more](#)


## Quality Control Notes

Coordination Compound

## Intrinsic Properties

 Molecular Formula:  $\text{AuCl}_4\text{H}$   Mol File  Find All Chemicals


 Average Mass: 339.77 g/mol  Isotope Mass Distribution


 Monoisotopic Mass: 337.849805 g/mol


# Other Databases have looser models

PubChem


**Structure not available** [16903-35-8](#)  
Substance SID: 470414174  
Data Source: [CymitQuimica](#) External ID: [CQ\\_16903-35-8](#)  
Data Source Category: Chemical Vendors  
Deposit Date: 2022-08-26 Last Modified Date: 2022-08-26


 [Gold\(III\)chloridesolution; KS-00000V50; 16903-35-8](#)  
Substance SID: 346440697 Compound CID: 166883  
Data Source: [King Scientific](#) External ID: KS-00000V50  
Data Source Category: Chemical Vendors; Legacy Depositors  
Deposit Date: 2017-10-13 Last Modified Date: 2021-08-04


 [Gold\(III\) chloride; Auric chloride Gold trichloride; 16903-35-8](#)  
Substance SID: 468741257 Compound CID: 26030  
Data Source: [J&H Chemical Co.,ltd](#) External ID: JH171429  
Data Source Category: Chemical Vendors  
Deposit Date: 2022-07-14 Last Modified Date: 2022-07-14


 [Chloroauric acid; gold\(3+\);hydron;tetrachloride; 16903-35-8](#)  
Substance SID: 442938174 Compound CID: 122706823  
Data Source: [Smolecule](#) External ID: S1797952  
Data Source Category: Chemical Vendors

PubChem

 [Chloroauric acid; ANW-41102; 16903-35-8](#)  
Substance SID: 160808603 Compound CID: 166883  
Data Source: [Anward](#) External ID: ANW-41102  
Data Source Category: Chemical Vendors; Legacy Depositors  
Deposit Date: 2013-02-18 Last Modified Date: 2023-12-17

 [Gold trichloride hydrochloride; 16903-35-8](#)  
Substance SID: 162094571 Compound CID: 10925836  
Data Source: [Chembase.cn](#) External ID: 106912  
Data Source Category: Chemical Vendors; Legacy Depositors  
Deposit Date: 2013-04-14 Last Modified Date: 2023-12-17

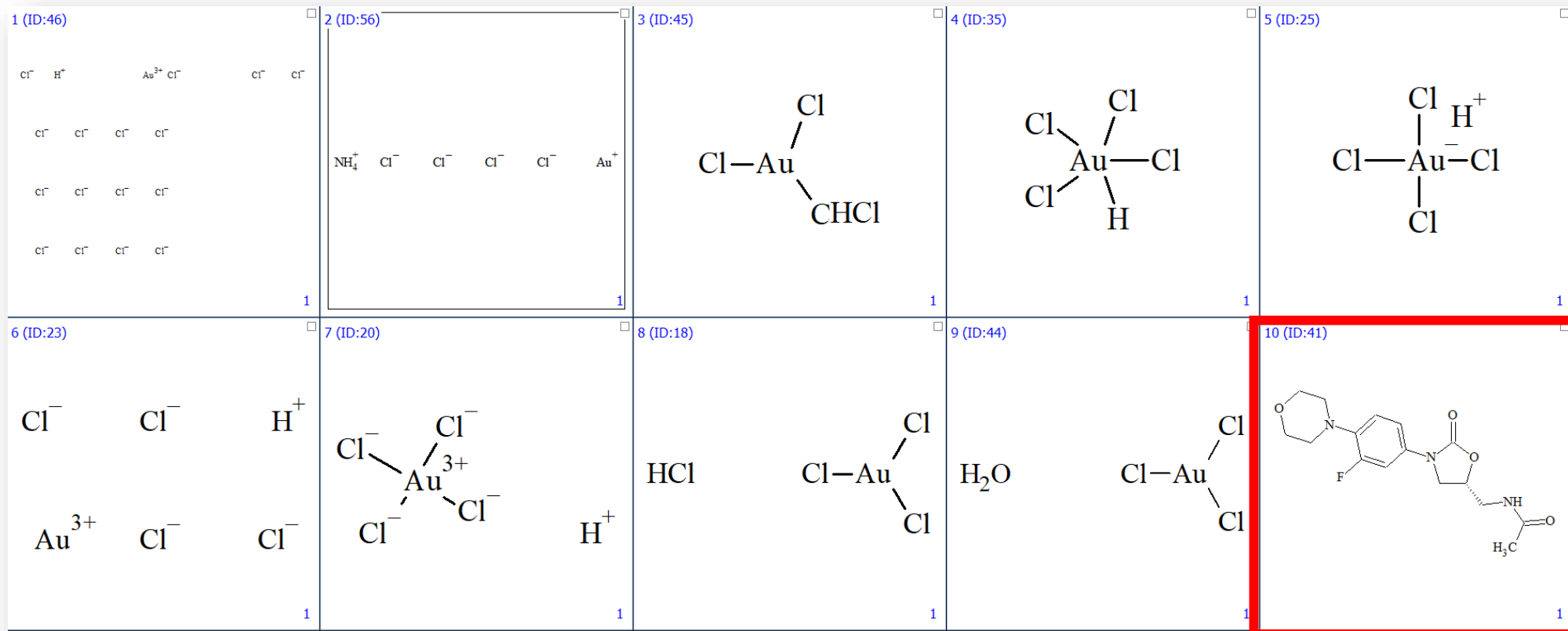
 [Aurate\(1-\), tetrachloro-, hydrogen, \(SP-4-1\)-; 16903-35-8](#)  
Substance SID: 176271341 Compound CID: 122706823  
Data Source: [EPA Substance Registry Services](#) External ID: 206094  
Data Source Category: Governmental Organizations  
Deposit Date: 2014-05-08 Last Modified Date: 2023-12-17

 [Chloroauric acid; RTR-030539; 16903-35-8](#)  
Substance SID: 204377739 Compound CID: 166883  
Data Source: [Tractus](#) External ID: RTR-030539  
Data Source Category: Chemical Vendors; Legacy Depositors  
Deposit Date: 2014-09-16 Last Modified Date: 2023-12-18

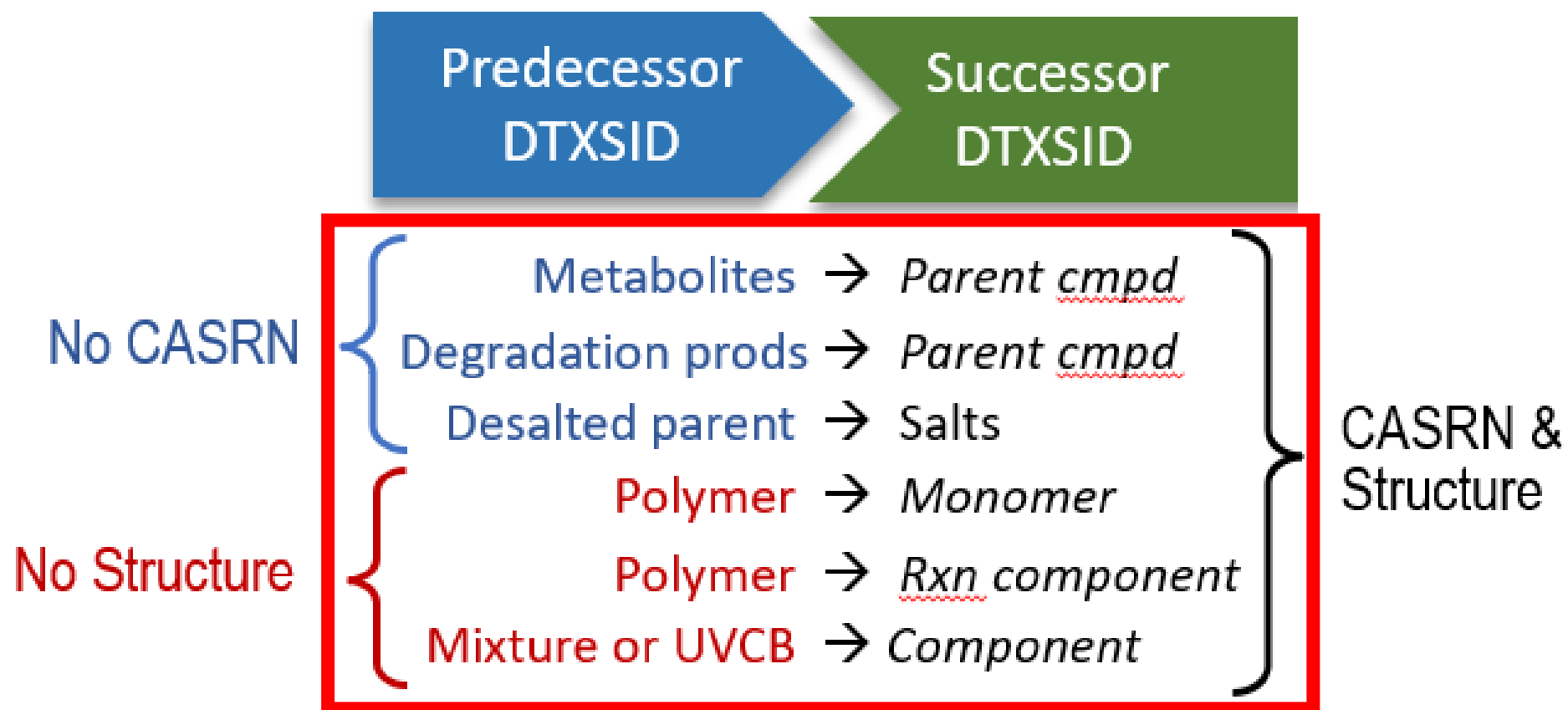


# Other Databases have looser models


## All of these in PubChem for 16903-35-8




# Predecessors and Successors





# Successors: Transformation Products



Water Research  
Volume 165, 15 November 2019, 114972

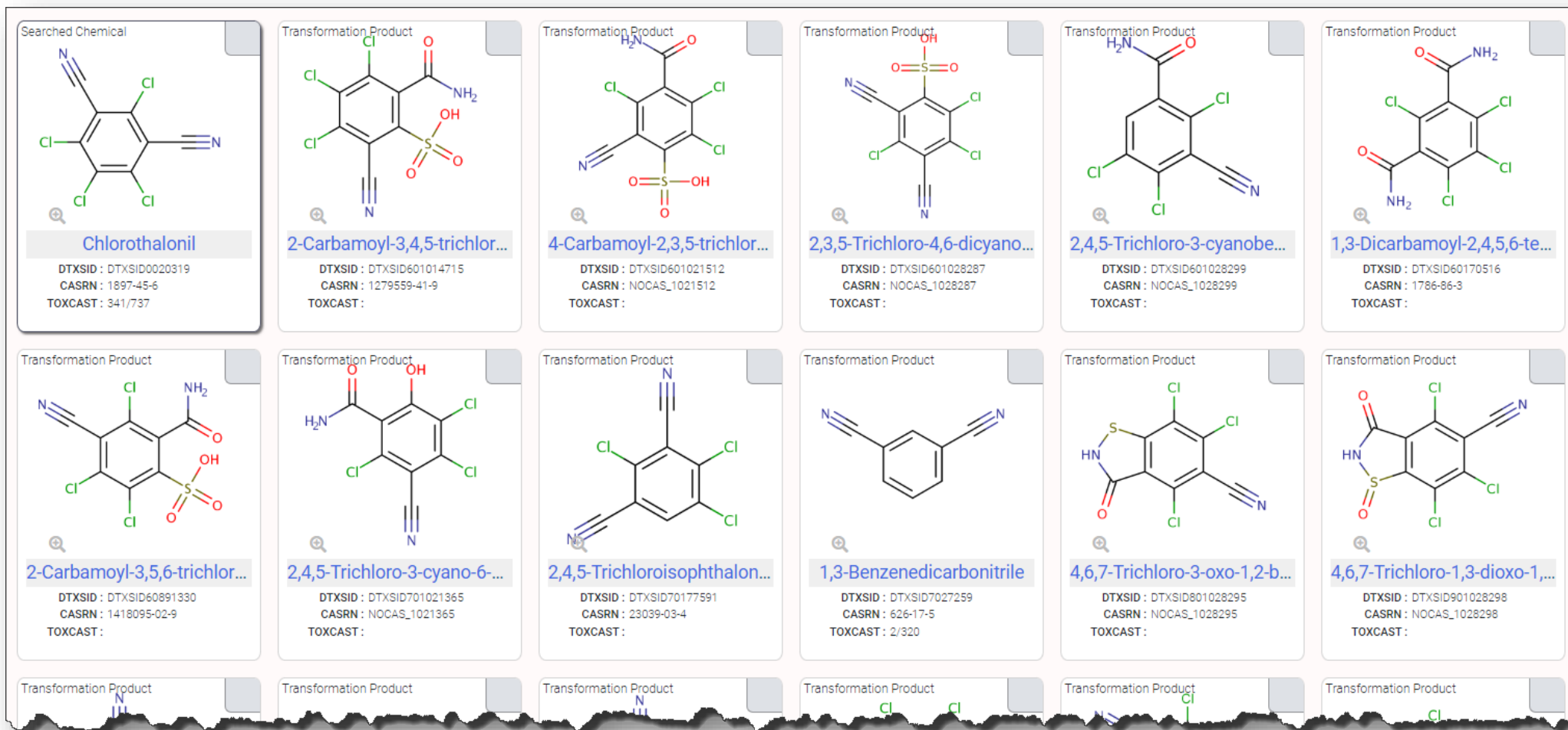


## New relevant pesticide transformation products in groundwater detected using target and suspect screening for agricultural and urban micropollutants with LC-HRMS


Karin Kiefer<sup>a, b</sup>, Adrian Müller<sup>a</sup>, Heinz Singer<sup>a</sup>, Juliane Hollender<sup>a, b</sup>  

1786-86-3	Transformation Product	STN(DSSTox)	✓	■		<a href="https://doi.org/10.1016/j.">https://doi.org/10.1016/j.</a>
19846-21-0	Transformation Product	STN(DSSTox)	✓	■		<a href="https://doi.org/10.1016/j.">https://doi.org/10.1016/j.</a>
23039-03-4	Transformation Product	STN(DSSTox)	✓	■		<a href="https://doi.org/10.1016/j.">https://doi.org/10.1016/j.</a>
28442-78-6	Transformation Product	STN(DSSTox)	✓	■		<a href="https://doi.org/10.1016/j.">https://doi.org/10.1016/j.</a>
56952-99-9	Transformation Product	STN(DSSTox)	✓	■		<a href="https://doi.org/10.1016/j.">https://doi.org/10.1016/j.</a>
61073-19-6	Transformation Product	Public	✓	■	2,3,4,6-Tetrachloro-5-cyanobenzamide	
115044-73-0	Transformation Product	STN(DSSTox)	✓	■		<a href="https://doi.org/10.1016/j.">https://doi.org/10.1016/j.</a>
19861-59-7	Transformation Product	STN(DSSTox)	✓	■		<a href="https://doi.org/10.1016/j.">https://doi.org/10.1016/j.</a>
1279559-41-9	Transformation Product	STN(DSSTox)	✓	■		<a href="https://doi.org/10.1016/j.">https://doi.org/10.1016/j.</a>

# Successors: Transformation Products



# Monomer mappings to polymers

<p>Searched Chemical</p>  <p><b>Tetrafluoroethylene</b> DTXSID : DTXSID6021325 CASRN : 116-14-3 TOXCAST :</p>	<p>Predecessor: Component</p> <p>2 related chemical structures with this substance</p> <p><b>Perfluoro-3-[(trifluoroeth...</b> DTXSID : DTXSID40880383 CASRN : 26655-00-5 TOXCAST :</p>	<p>Predecessor: Component</p> <p>2 related chemical structures with this substance</p> <p><b>Perfluoro-3,6-dioxa-4-met...</b> DTXSID : DTXSID90897643 CASRN : 31175-20-9 TOXCAST :</p>	<p>Predecessor: Component</p> <p>5 related chemical structures with this substance</p> <p><b>1-Butanol, 4-(ethenyloxy), ...</b> DTXSID : DTXSID90882650 CASRN : 235775-81-2 TOXCAST :</p>	<p>Predecessor: Component</p> <p>4 related chemical structures with this substance</p> <p><b>3-Cyclohexene-1-carboxyli...</b> DTXSID : DTXSID801019973 CASRN : 392286-82-7 TOXCAST :</p>
<p>Predecessor: Component</p> <p>2 related chemical structures with this substance</p> <p><b>Perfluorosulfonic acid, PT...</b> DTXSID : DTXSID30882013 CASRN : 66796-30-3 TOXCAST :</p>	<p>Predecessor: Component</p> <p>3 related chemical structures with this substance</p> <p><b>1-Propene, 1,1,2,3,3,3-hex...</b> DTXSID : DTXSID20882688 CASRN : 235775-93-6 TOXCAST :</p>	<p>Predecessor: Component</p> <p>2 related chemical structures with this substance</p> <p><b>Hexafluoropropene tetrafl...</b> DTXSID : DTXSID70880371 CASRN : 25067-11-2 TOXCAST :</p>	<p>Predecessor: Component</p> <p>4 related chemical structures with this substance</p> <p><b>2-Propanone, 1,1,1,3,3,3-h...</b> DTXSID : DTXSID40882680 CASRN : 125128-66-7 TOXCAST :</p>	<p>Predecessor: Component</p> <p>3 related chemical structures with this substance</p> <p><b>Tetrafluoroethylene-vinyl a...</b> DTXSID : DTXSID90882736 CASRN : 216660-17-2 TOXCAST :</p>
<p>Predecessor: Component</p>	<p>Predecessor: Component</p>	<p>Predecessor: Component</p>	<p>Predecessor: Component</p>	<p>Monomer</p>

# Polymers mapped to multiple monomers

## 2-Propanone, 1,1,1,3,3,3-hexafluoro-, polymer with 1,1-difluoroethene, t...

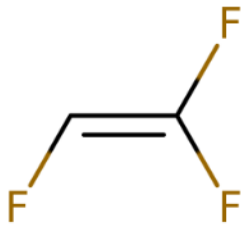
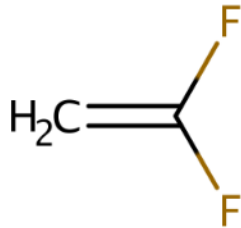
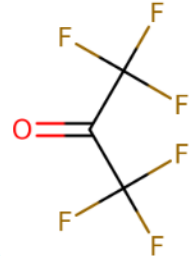
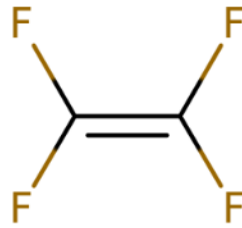
125128-66-7 | DTXSID40882680

Searched by DTXSID40882680.

### Related Substances ⓘ

Search Results SEND 5 TO BATCH SEARCH TILE INFO FILTER EXPORT PREFERRED VIEW

Showing 5 of 5 chemicals

<p>Searched Chemical</p> <p>4 related chemical structures with this substance</p> <p><b>2-Propanone, 1,1,1,3,3,3-h...</b></p> <p>DTXSID : DTXSID40882680 CASRN : 125128-66-7 TOXCAST :</p>	<p>Monomer</p>  <p><b>1,1,2-Trifluoroethene</b></p> <p>DTXSID : DTXSID4059887 CASRN : 359-11-5 TOXCAST :</p>	<p>Monomer</p>  <p><b>Vinylidene fluoride</b></p> <p>DTXSID : DTXSID3021439 CASRN : 75-38-7 TOXCAST :</p>	<p>Monomer</p>  <p><b>Hexafluoroacetone</b></p> <p>DTXSID : DTXSID9043778 CASRN : 684-16-2 TOXCAST :</p>	<p>Monomer</p>  <p><b>Tetrafluoroethylene</b></p> <p>DTXSID : DTXSID6021325 CASRN : 116-14-3 TOXCAST :</p>
--	---	---	--	--

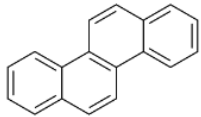
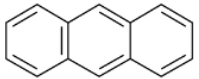
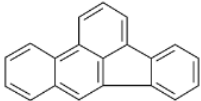
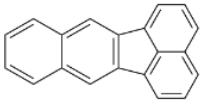
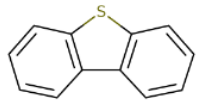
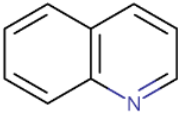
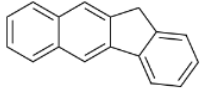
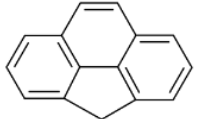
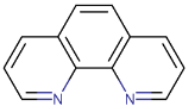
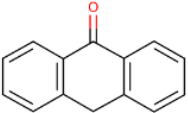
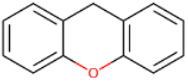
# Complex Substances: PAHs

**Polycyclic aromatic hydrocarbons**  
130498-29-2 | DTXSID3044043  
Searched by Synonym

Related Substances ⓘ

Search Results

Showing 73 of 73 chemicals

<p>Searched Chemical</p> <p>72 related chemical structures with this substance</p> <p><b>Polycyclic aromatic hydro...</b></p> <p>DTXSID : DTXSID3044043 CASRN : 130498-29-2 TOXCAST :</p>	<p>Component</p>  <p><b>Chrysene</b></p> <p>DTXSID : DTXSID0022432 CASRN : 218-01-9 TOXCAST : 7/257</p>	<p>Component</p>  <p><b>Anthracene</b></p> <p>DTXSID : DTXSID0023878 CASRN : 120-12-7 TOXCAST : 38/651</p>	<p>Component</p>  <p><b>Benzo(b)fluoranthene</b></p> <p>DTXSID : DTXSID0023907 CASRN : 205-99-2 TOXCAST : 160/624</p>	<p>Component</p>  <p><b>Benzo(k)fluoranthene</b></p> <p>DTXSID : DTXSID0023909 CASRN : 207-08-9 TOXCAST : 58/267</p>	<p>Component</p>  <p><b>Dibenzothiophene</b></p> <p>DTXSID : DTXSID0047741 CASRN : 132-65-0 TOXCAST : 15/460</p>
<p>Component</p>  <p><b>Quinoline</b></p> <p>DTXSID : DTXSID1021798 CASRN : 91-22-5 TOXCAST : 15/581</p>	<p>Component</p>  <p><b>11H-Benzo[b]fluorene</b></p> <p>DTXSID : DTXSID1022477 CASRN : 243-17-4 TOXCAST :</p>	<p>Component</p>  <p><b>4H-Cyclopenta(def)phenanthrene...</b></p> <p>DTXSID : DTXSID1024887 CASRN : 203-64-5 TOXCAST : 16/253</p>	<p>Component</p>  <p><b>1,10-Phenanthroline</b></p> <p>DTXSID : DTXSID1025857 CASRN : 66-71-7 TOXCAST : 115/357</p>	<p>Component</p>  <p><b>Anthrone</b></p> <p>DTXSID : DTXSID1049431 CASRN : 90-44-8 TOXCAST : 21/234</p>	<p>Component</p>  <p><b>9H-Xanthene</b></p> <p>DTXSID : DTXSID1059070 CASRN : 92-83-1 TOXCAST :</p>

# Complex Substance Support

## nano-silver\_na\_citrate\_29\_nanometers\_nanocomposix\_na\_2

NOCAS\_1029237 | DTXSID001029237

Searched by DTXSID001029237.

### Chemical Details

#### Quality Control Notes

This nano scaled material is composed of a Silver core with no information on the shell and citrate coating. 29 nanometers was reported for the particle size (diameter). This material was obtained from NanoComposix, with product/lot number unreported, designation 2.

### Related Substances ?

Search Results SEND 3 TO BATCH SEARCH TILE INFO FILTER EXPORT PREFERRED VIEW

Showing 3 of 3 chemicals

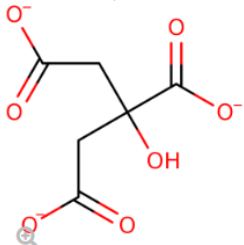
Searched Chemical

2 related chemical structures with this substance

[nano-silver\\_na\\_citrate<sub>29</sub>na...](#)

DTXSID : DTXSID001029237  
CASRN : NOCAS\_1029237  
TOXCAST :

Predecessor: Component



Citrate

DTXSID : DTXSID30155037  
CASRN : 126-44-3  
TOXCAST :

Predecessor: Component

Ag

Silver

DTXSID : DTXSID4024305  
CASRN : 7440-22-4  
TOXCAST :



# Complex Substance Support

## AFFF 3% Formulation Analysis Paper

NOCAS\_1353514 | DTXSID301353514

Searched by Approved Name.

### Chemical Details

#### Quality Control Notes

The formulation mapped in the related substances is an example of a 3% AFFF formulation reported in the article "Chemical Characterization of a Legacy Aqueous Film-Forming Foam Sample and Developmental Toxicity in Zebrafish (*Danio rerio*)" by Annunziato et al (<https://doi.org/10.1289/EHP6470>). A sample of legacy AFFF(3% application formulation, manufactured before 2001) was provided by the Massachusetts Department of Environmental Protection. High resolution mass spectrometry (HRMS) was used to identify PFAS and nonfluorinated compounds ,and a commercial laboratory measured 24 PFAS by a modified U.S.EPA Method 537.1.









# Complex Substance Support : AFFFs

## AFFF 3% Formulation Analysis Paper

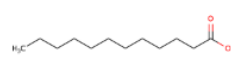
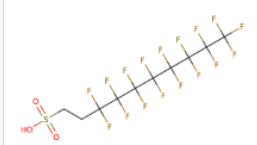
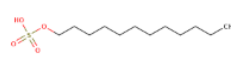


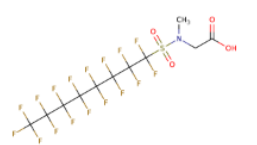
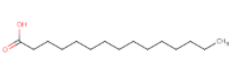
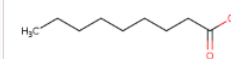
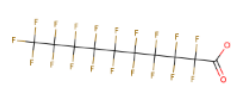

NOCAS\_1353514 | DTXSID301353514

Searched by Approved Name.

### Related Substances

  Search Results  SEND 40 TO BATCH SEARCH  TILE INFO  FILTER  EXPORT  PREFERRED VIEW 

Showing 40 of 40 chemicals

<p>Searched Chemical</p> <p>38 related chemical structures with this substance</p> <p><b>AFFF 3% Formulation Ana...</b></p> <p>DTXSID : DTXSID301353514 CASRN : NOCAS_1353514 TOXCAST :</p>	<p>Predecessor: Component</p>  <p><b>Dodecanoic acid</b></p> <p>DTXSID : DTXSID5021590 CASRN : 143-07-7 TOXCAST : 25/352</p>	<p>Predecessor: Component</p> <p>0 related chemical structures with this substance</p> <p><b>Hydrocaffeic acid polymer</b></p> <p>DTXSID : DTXSID001347528 CASRN : 71693-95-3 TOXCAST :</p>	<p>Predecessor: Component</p>  <p><b>8:2 Fluorotelomer sulfonic...</b></p> <p>DTXSID : DTXSID00192353 CASRN : 39108-34-4 TOXCAST : 26/258</p>	<p>Predecessor: Component</p>  <p><b>Lauryl sulfate</b></p> <p>DTXSID : DTXSID0042088 CASRN : 151-41-7 TOXCAST :</p>	<p>Predecessor: Component</p>  <p><b>Oleic acid</b></p> <p>DTXSID : DTXSID1025809 CASRN : 112-80-1 TOXCAST : 30/362</p>
<p>Predecessor: Component</p>  <p><b>Perfluoroheptanoic acid</b></p> <p>DTXSID : DTXSID1037303 CASRN : 375-85-9 TOXCAST : 38/675</p>	<p>Predecessor: Component</p>  <p><b>2-(N-Methylperfluoroocta...</b></p> <p>DTXSID : DTXSID10624392 CASRN : 2355-31-9 TOXCAST :</p>	<p>Predecessor: Component</p>  <p><b>Pentadecanoic acid</b></p> <p>DTXSID : DTXSID2021652 CASRN : 1002-84-2 TOXCAST : 8/234</p>	<p>Predecessor: Component</p>  <p><b>Nonanoic acid</b></p> <p>DTXSID : DTXSID3021641 CASRN : 112-05-0 TOXCAST : 7/590</p>	<p>Predecessor: Component</p>  <p><b>Perfluorodecanoic acid</b></p> <p>DTXSID : DTXSID3031860 CASRN : 335-76-2 TOXCAST : 269/705</p>	<p>Predecessor: Component</p>  <p><b>Perfluorohexanoic acid</b></p> <p>DTXSID : DTXSID3031862 CASRN : 307-24-4 TOXCAST : 24/701</p>

# Markush structures capture groups of related chemical compounds

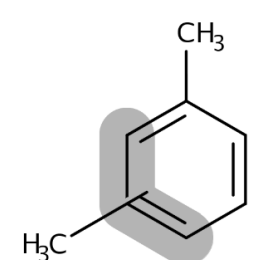
CompTox Chemicals Dashboard v2.3.0 Home Search Lists About Tools

**Polychlorinated biphenyls**  
1336-36-3 | DTXSID5024267  
Searched by Expert Validated Synonym.

**Chemical Details**

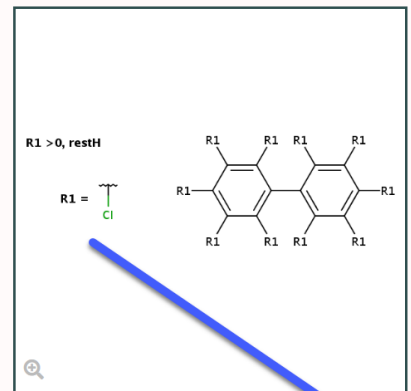
Chemical Details  
Executive Summary  
Physchem Prop.  
Env. Fate/Transport  
Hazard Data  
Safety > GHS Data  
ADME > IVIVE  
Exposure  
Bioactivity

**Xylenes**



**Chemical Details**

R1 >= 0, restH  
R1 = Cl



Wikipedia  
Quality Control Notes

Searched Chemical

Polychlorinated biphenyls  
DTXSID : DTXSID5024267  
CASRN : 1336-36-3  
TOXCASST :

Markush Child

2,3,4',5-Tetrachlorobiphenyl  
DTXSID : DTXSID4074223  
CASRN : 74472-34-7  
TOXCASST :

Markush Child

2,4'-Dichlorobiphenyl  
DTXSID : DTXSID0022511  
CASRN : 34883-43-7  
TOXCASST :

Markush Child

2,2',4,4'-Tetrachlorobiphenyl  
DTXSID : DTXSID0022513  
CASRN : 2437-79-8  
TOXCASST :

Markush Child

4,4'-Dichlorobiphenyl  
DTXSID : DTXSID0022515  
CASRN : 2050-68-2  
TOXCASST :

Markush Child

2,3,3',4,4',5-Hexachlorobiphenyl  
DTXSID : DTXSID0052706  
CASRN : 38380-08-4  
TOXCASST :

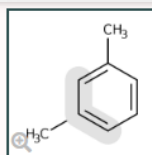
Markush Child

2,2',6,6'-Tetrachlorobiphenyl  
DTXSID : DTXSID0065983  
CASRN : 15968-05-5  
TOXCASST :

Markush Child

2,4,5-Trichlorobiphenyl  
DTXSID : DTXSID0073405  
CASRN : 15862-07-4  
TOXCASST :

# Complex Substances: Xylene Structures



## Xylenes

1330-20-7 | DTXSID2021446

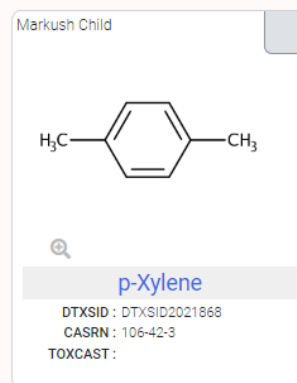
Searched by DTXSID2021446.

### Related Substances ?

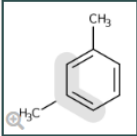
Search Results SEND 4 TO BATCH SEARCH TILE INFO FILTER 2 EXPORT PREFERRED VIEW

Showing 4 of 12 chemicals

Filtering out chemicals that are: No Structures, Unselected



# Complex Substances: Xylene Substances



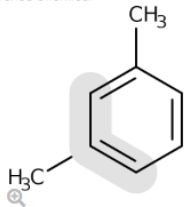
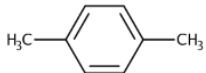
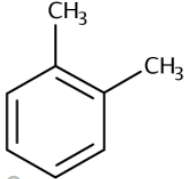
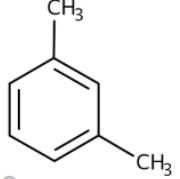
## Xylenes

1330-20-7 | DTXSID2021446  
Searched by DTXSID2021446.

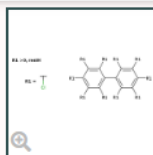
**Related Substances** ⓘ

Search Results SEND 11 TO BATCH SEARCH TILE INFO FILTER 1 EXPORT PREFERRED VIEW

Showing 11 of 12 chemicals  
Filtering out chemicals that are: Unselected

<p>Searched Chemical</p>  <p><b>Xylenes</b></p> <p>DTXSID : DTXSID2021446 CASRN : 1330-20-7 TOXCAST : 1/234</p>	<p>Predecessor: Component</p> <p>4 related chemical structures with this substance</p> <p><b>Xylenes; defined mixture 2</b></p> <p>DTXSID : DTXSID7021447 CASRN : NOCAS_21447 TOXCAST :</p>	<p>Predecessor: Component</p> <p>5 related chemical structures with this substance</p> <p><b>Total Petroleum Hydrocar...</b></p> <p>DTXSID : DTXSID30891529 CASRN : NOCAS_891529 TOXCAST :</p>	<p>Predecessor: Component</p> <p>3 related chemical structures with this substance</p> <p><b>Vorlex NA 087</b></p> <p>DTXSID : DTXSID801033977 CASRN : 82975-08-4 TOXCAST :</p>	<p>Predecessor: Component</p> <p>4 related chemical structures with this substance</p> <p><b>Xylenes; defined mixture 1</b></p> <p>DTXSID : DTXSID9021421 CASRN : NOCAS_21421 TOXCAST :</p>	<p>Predecessor: Component</p> <p>3 related chemical structures with this substance</p> <p><b>Dilan</b></p> <p>DTXSID : DTXSID9040346 CASRN : 8027-00-7 TOXCAST :</p>
<p>Component</p> <p>2 related chemical structures with this substance</p> <p><b>Aromatic hydrocarbons, C...</b></p> <p>DTXSID : DTXSID601027322 CASRN : 91995-18-5 TOXCAST :</p>	<p>Component</p> <p>1 related chemical structure with this substance</p> <p><b>Aromatic hydrocarbons, C...</b></p> <p>DTXSID : DTXSID501027331 CASRN : 93571-75-6 TOXCAST :</p>	<p>Markush Child</p>  <p><b>p-Xylene</b></p> <p>DTXSID : DTXSID2021868 CASRN : 106-42-3</p>	<p>Markush Child</p>  <p><b>o-Xylene</b></p> <p>DTXSID : DTXSID3021807 CASRN : 95-47-6</p>	<p>Markush Child</p>  <p><b>m-Xylene</b></p> <p>DTXSID : DTXSID6026298 CASRN : 108-38-3</p>	

# Complex Substances: PCBs



## Polychlorinated biphenyls

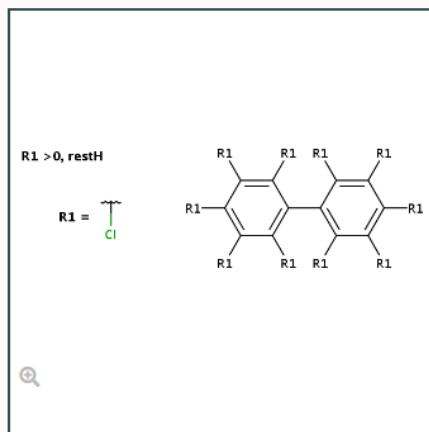
1336-36-3 | DTXSID5024267

Searched by Expert Validated Synonym

PCBs

DTXSID5024267

### Chemical Details



### Wikipedia

**Polychlorinated biphenyls (PCBs)** are highly carcinogenic chemical compounds, formerly used in industrial and consumer products, whose production was banned in the United States by the Toxic Substances Control Act in 1976 and internationally by the Stockholm Convention on Persistent Organic Pollutants in 2001.

PCBs are organochlorine compounds with the formula  $C_{12}H_{10-x}Cl_x$ ; they were once widely used in the manufacture of carbonless

[Read more](#)

### Quality Control Notes

biphenyl with multiple (unknown number) chlorines attached at unknown locations

# Complex Substances: PCBs – 209 “Children”

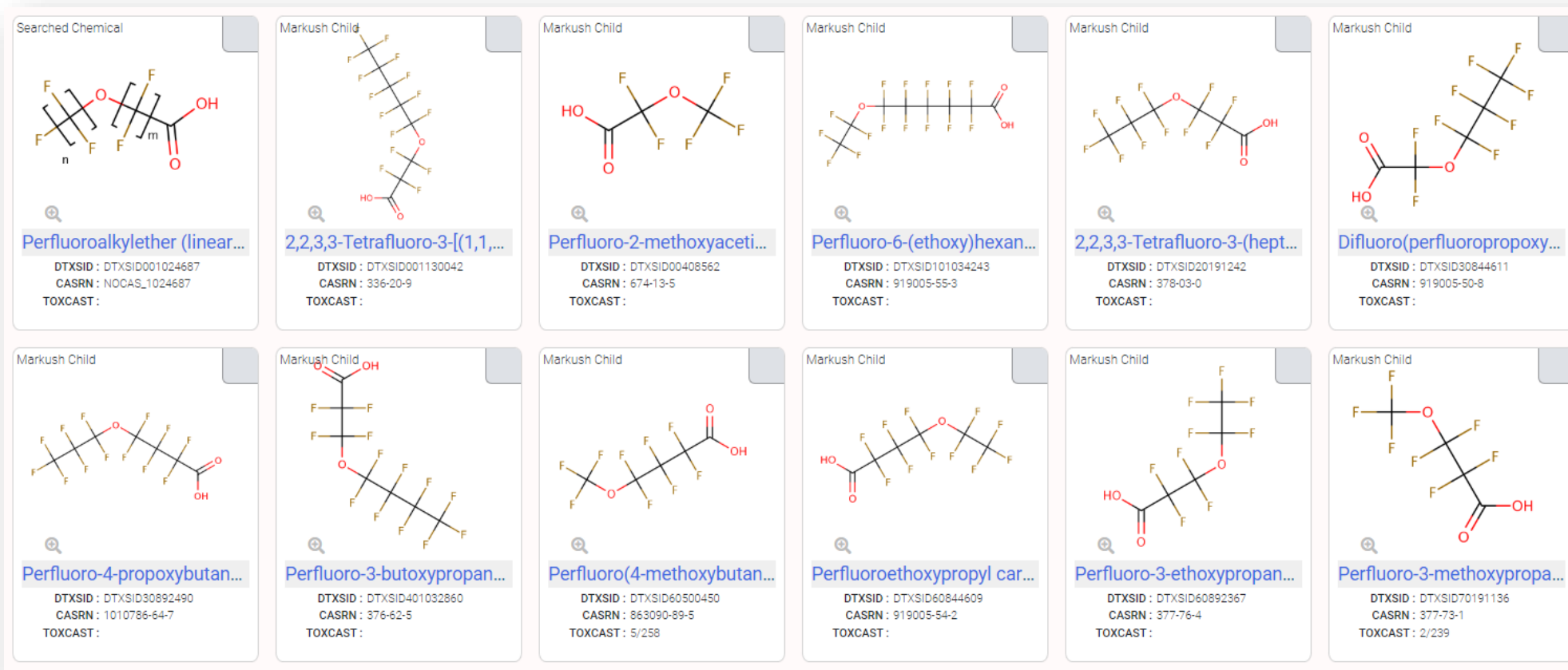


# Complex Substances: PFAS classes

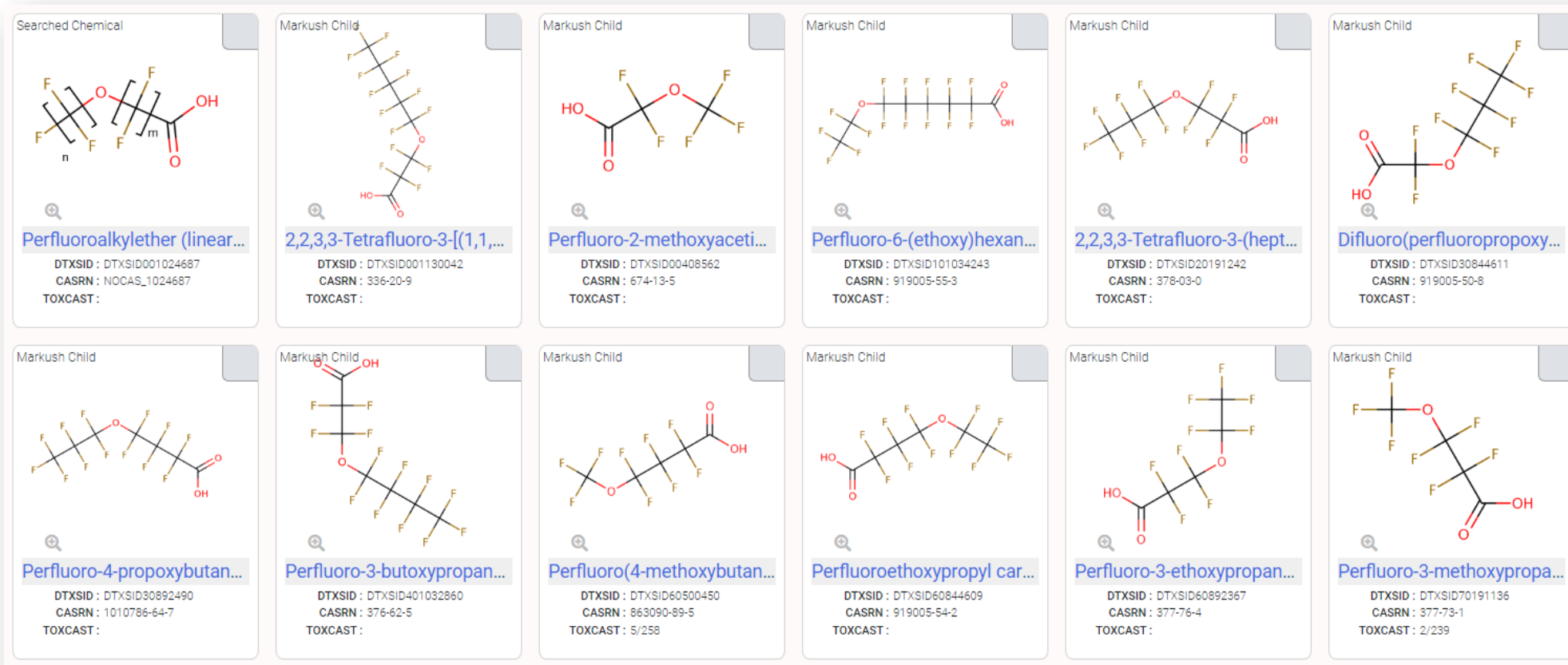
<p><b>N-diHOPAmHOB-FASA</b> DTXSID : DTXSID001010234 CASRN : NOCAS_1010234 TOXCAST :</p>	<p><b>CMAmB-FA</b> DTXSID : DTXSID001010246 CASRN : NOCAS_1010246 TOXCAST :</p>	<p><b>N-SPAmP-FASAA</b> DTXSID : DTXSID001010258 CASRN : NOCAS_1010258 TOXCAST :</p>	<p><b>N-CMAmP-FASAA</b> DTXSID : DTXSID001010260 CASRN : NOCAS_1010260 TOXCAST :</p>	<p><b>Perfluoroalkyl (linear) alkyl ether</b> DTXSID : DTXSID001015365 CASRN : NOCAS_1015365 TOXCAST :</p>	<p><b>Perfluoroalkylether (linear)</b> DTXSID : DTXSID001024687 CASRN : NOCAS_1024687 TOXCAST :</p>
<p><b>Poly[2-(perfluorooctyl)ethyl] ether</b> DTXSID : DTXSID001029613 CASRN : 74049-08-4 TOXCAST :</p>	<p><b>(Perfluoroethyl)hexane</b> DTXSID : DTXSID001032668 CASRN : 1287702-49-1 TOXCAST :</p>	<p><b>26-(Perfluorooctyl)octamethyl ether</b> DTXSID : DTXSID001034002 CASRN : 88243-17-8 TOXCAST :</p>	<p><b>(1H,1H,2H,2H-Perfluorodecyl) ether</b> DTXSID : DTXSID001096947 CASRN : 161045-59-6 TOXCAST :</p>	<p><b>(Perfluoroalkyl)methyl perfluoroether</b> DTXSID : DTXSID001336248 CASRN : NOCAS_1336248 TOXCAST :</p>	<p><b>Perfluoroalkanesulfonyl fluoride</b> DTXSID : DTXSID001336262 CASRN : NOCAS_1336262 TOXCAST :</p>



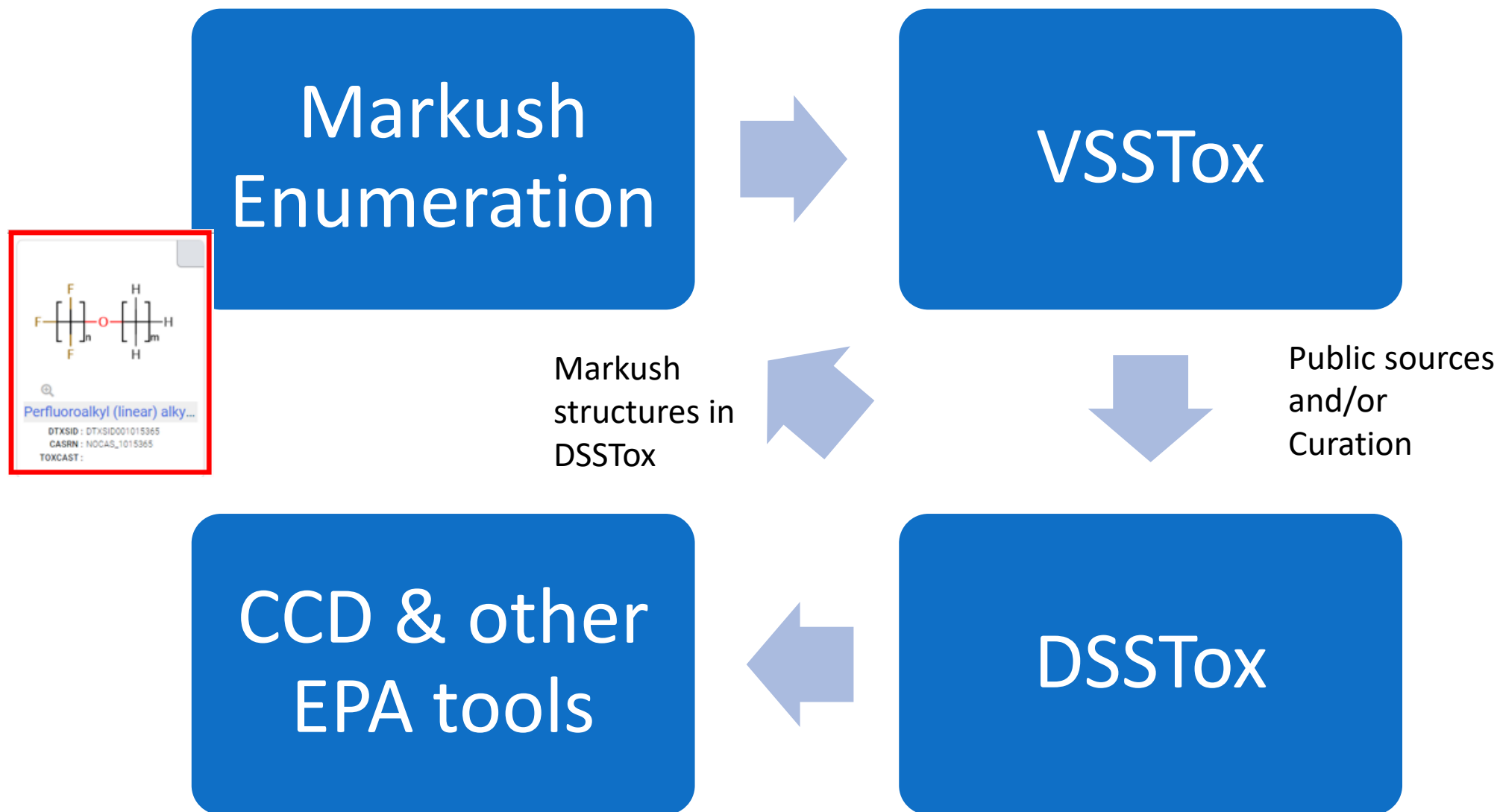
# “Enumerated” PFAS Markush structures



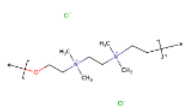
# 22 found in DSSTox, but 400 enumerated “Children”



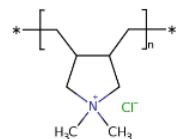
# VSSTox will capture “Virtual Children”



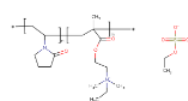
# Complex Substances: QACs/Quats



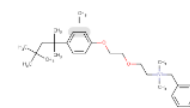
Polyquaternium-42  
CASRN:31512-74-0  
DTXSID:DTXSID8034829



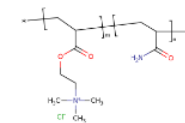
Polyquaternium 6  
CASRN:26062-79-3  
DTXSID:DTXSID8035714



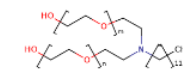
Polyquaternium 11  
CASRN:53633-54-8  
DTXSID:DTXSID0041303



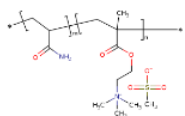
Methylbenzethonium  
CASRN:62741-89-3  
DTXSID:DTXSID3047976



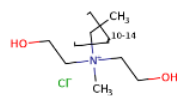
Polyquaternium 33  
CASRN:69418-26-4  
DTXSID:DTXSID3049592



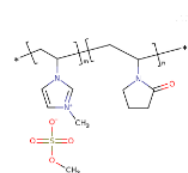
Amines, coco alkyl, ethoxylated (C12, C14)  
CASRN:61791-14-8  
DTXSID:DTXSID7050456



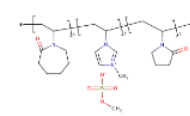
Polyquaternium 5  
CASRN:26006-22-4  
DTXSID:DTXSID6051279



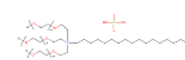
Alkyl dihydroxyethyl methyl ammonium ...  
CASRN:70750-47-9  
DTXSID:DTXSID60103465



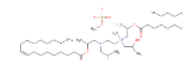
Polyquaternium 44  
CASRN:150599-70-5  
DTXSID:DTXSID90108827



Polyquaternium 46  
CASRN:174761-16-1  
DTXSID:DTXSID30169896



Quaternium-52  
CASRN:58069-11-7  
DTXSID:DTXSID20206789



Quaternium 82  
CASRN:65059-61-2  
DTXSID:DTXSID00894461

# Chemical Lists

- Individual chemicals can be associated with specific lists for which they are members.

Source Identifier	Inventory Code
Chlorothalonil	CPDBAS
Chlorothalonil	IRISTR
Chlorothalonil	NTPGTZ
Chlorothalonil	NTPBSI
Chlorothalonil	EPAPAI
Chlorothalonil	TCNCGC
Chlorothalonil	TCNCGC
Chlorothalonil	EPAICE

# Chemical Lists on the Dashboard

**Presence in Lists**

Federal

- TOXCAST\_PhaseI - EPA ToxCast Screening Library (Phase I subset)
- TOXCASST\_PhaseII - EPA ToxCast Screening Library (Phase II Subset)
- TOXCAST\_PhaseIII - EPA ToxCast Screening Library (Phase II Subset)
- TOXCAST\_ph1v2 - EPA ToxCast Screening Library (ph1v2 Subset)
- CHEMINV: EPA Chemical Inventory for ToxCast
- ENDOCRINE: EDSP21 Tier 1 Screening Chemicals: List 1
- ENDOCRINE: EDSP Universe of Chemicals
- ECOTOX: Ecotoxicology knowledgebase
- WATER|EPA: Drinking Water Standard and Health Advisories Table
- NIOSH: International Chemical Safety Cards
- MASSPECDB: National Environmental Methods Index
- EPA: IRIS Chemicals
- TOXCAST: EPA ToxCast Screening Assay In Vitro DB Version 3
- EPA: High Production Volume List
- EPA: Mechanism of Action (MoA) for aquatic toxicity
- CHEMINV: ToxCast/Tox21 Chemical inventory available as DMSO solutions (20181123)
- TOX21SL: Tox21 Screening Library
- EPA|PESTICIDES Office of Pesticide Programs Information Network

US State

- California Office of Environmental Health Hazard Assessment

International

- FOOD: EFSA OpenFoodTox
- NORMAN: KEMI List of Substances on the Market

# List creation in DSSTox

**ChemReg: Chemical Registration for DSSTox**

View/Edit a Single Record   Structure Search   Browse/Curate Records   Export DSSTox   Chemotypes   **Manage Chemical Lists**   Manage Property Data   Add Deleted Casrns   QlikViz Dashboards   Welcome, awilli04   Logout

Welcome awilli04

Please provide basic information on this list of chemicals

List Abbreviation (6-8 Characters)

List Name (~100-250 Characters)

Short Description (Up to 250 Characters)

Long Description (Lots of Characters)

List Type Category

NCCT Contact

Source Contact

Source Contact Email

Source Reference

Source DOI (eg: http://dx.doi.org/10.1000/182)

Source Website

Date Source Updated:

Intended Accessibility:

List Type:

# Lists in the Dashboard

## 40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities

Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey

Start typing or paste text to search.

Type-ahead search

Identifier substring search

### List Details

Description: Extremely Hazardous Substance List and Threshold Planning Quantities; Emergency Planning and Release Notification Requirements; Final Rule. (52 FR 13378) This FR notice contains the EHS list of chemicals as published in 1987. This list has been revised over time and should not be used for current compliance purposes. The current EHS list can be found at [40 CFR 355](#).

Number of Chemicals: 354

Search Results

SEND 354 TO BATCH SEARCH

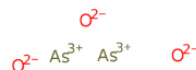
TILE INFO

FILTER

EXPORT

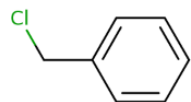
PREFERRED VIEW

Showing 354 of 354 chemicals



Arsenic oxide (As2O3)

DTXSID : DTXSID0020103



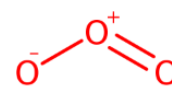
Benzyl chloride

DTXSID : DTXSID0020153



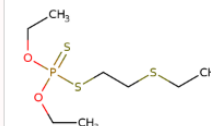
Ethylene oxide

DTXSID : DTXSID0020600



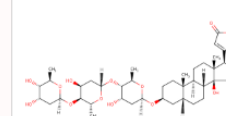
Ozone

DTXSID : DTXSID0021098



Disulfoton

DTXSID : DTXSID0022018



Digitoxin

DTXSID : DTXSID0022933



# Lists in the Dashboard

CompTox Chemicals Dashboard v2.4.0   Home   Search   Lists   About   Tools   Submit Comments   Search all data

## Chemical Lists ?

Search Chemical Lists   EXPORT   COPY URL

Showing 498 of 498 Records

List Acronym ↓↑	List Name ↓↑	# Chemicals ↓↑	Updated ↓↑	List Description
40CFR1164	40 CFR 116.4 Designation of Hazardous Substances (Above Ground Storage Tanks)	333	2022-05-16T14:02:1...	<p>Hazardous Substance List associated with the Federal Water Pollution Control Act, as amended by the Federal Water Pollution Control Act Amendments of 1972 (Pub. L. 92-500), and as further amended by the Clean Water Act of 1977 (Pub. L. 95-217), 33 U.S.C. 1251 et seq.; and as further amended by the Clean Water Act Amendments of 1978 (Pub. L. 95-676)The current list can be found at <a href="#">40 CFR 116.4 list</a>.</p> <p>Other lists of interest are:</p> <p><a href="#">List of constituents of motor fuels relevant to leaking underground storage tank sites</a> <a href="#">List of constituents of motor fuels relevant to leaking underground storage tank sites</a></p> <p><a href="#">Chemicals present in Underground Storage Tanks</a> <a href="#">Chemicals present in Underground Storage Tanks</a></p>
40CFR355	40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities	354	2022-05-19T09:38:...	<p>Extremely Hazardous Substance List and Threshold Planning Quantities; Emergency Planning and Release Notification Requirements; Final Rule, (52 FR 13378) This FR notice contains the EHS list of chemicals as published in 1987. This list has been revised over time and should not be used for current compliance purposes. The current EHS list can be found at <a href="#">40 CFR 355</a>.</p>
AEGLVALUES	AEGLs: Acute Exposure Guideline Levels	174	2021-06-15T12:41:37Z	<p>Acute Exposure Guideline Level (AEGLs) values are intended to protect most individuals in the general population, including those that might be particularly susceptible to the harmful effects of the chemicals. Acute exposure guideline levels (AEGLs) describe the human health effects from once-in-a-lifetime, or rare, exposure to airborne chemicals. Used by emergency responders when dealing with chemical spills or other catastrophic exposures, AEGLs are set through a collaborative effort of the public and private sectors worldwide.</p>

Rows: 498

# Work in Progress

- The ChemReg application is being rebuilt at present
- The data model will be extended as appropriate
- We are building in new efficiencies to allow us to register chemicals faster, add in relevant mappings but no loss in quality
- The VSSTox database is in development

# Acknowledgements

- DSSTox has been curated by many of team members. Our present team has five members: Indira, Saku, Hengguang, Vicente and James
- DSSTox is the legacy work of Ann Richard
- ChemReg is the legacy work of Chris Grulke
- Both are now supported by our colleagues in SCDCD