

EPA CompTox chemicals dashboard: An online resource for environmental chemists

Antony Williams, Chris Grulke, Jeremy Dunne and Jeff Edwards

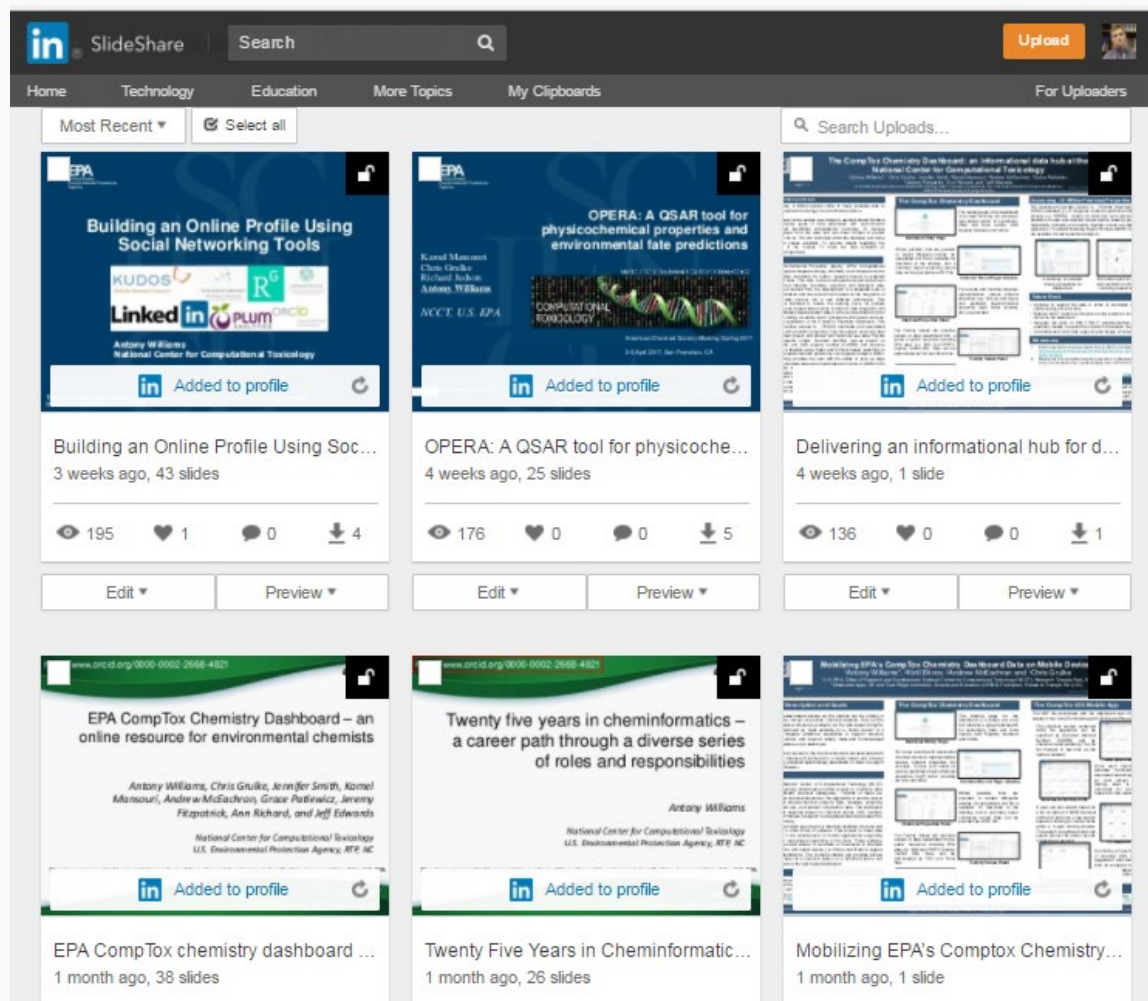
National Center for Computational Toxicology, U.S. Environmental Protection Agency, RTP, NC

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

*Spring 2019
ACS Spring Meeting, Orlando*

Limit notetaking if you wish

www.slideshare.net/AntonyWilliams



The screenshot displays the SlideShare website interface. At the top, there is a navigation bar with the SlideShare logo, a search bar, and an 'Upload' button. Below the navigation bar, there are tabs for 'Home', 'Technology', 'Education', 'More Topics', 'My Clipboards', and 'For Uploaders'. The main content area shows a grid of presentation thumbnails. Each thumbnail includes a title, a brief description, the number of slides, and engagement metrics (views, likes, comments, downloads). The presentations are:

- Building an Online Profile Using Social Networking Tools**: 43 slides, 195 views, 1 like, 0 comments, 4 downloads. Added to profile 3 weeks ago.
- OPERA: A QSAR tool for physicochemical properties and environmental fate predictions**: 25 slides, 176 views, 0 likes, 0 comments, 5 downloads. Added to profile 4 weeks ago.
- Delivering an informational hub for d...**: 1 slide, 136 views, 0 likes, 0 comments, 1 download. Added to profile 4 weeks ago.
- EPA CompTox Chemistry Dashboard – an online resource for environmental chemists**: 38 slides, 1 month ago.
- Twenty five years in cheminformatics – a career path through a diverse series of roles and responsibilities**: 26 slides, 1 month ago.
- Mobilizing EPA's CompTox Chemistry Dashboard Data on Mobile Devices**: 1 slide, 1 month ago.

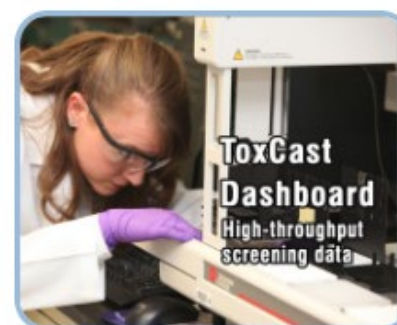
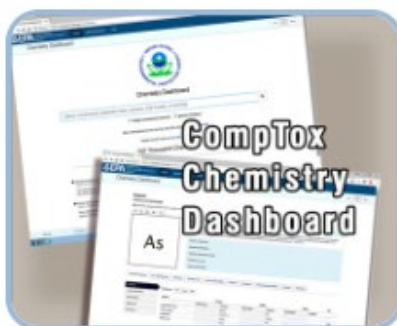
Each presentation thumbnail also features a 'Added to profile' button and a 'Preview' button.

Environmental Topics

Laws & Regulations

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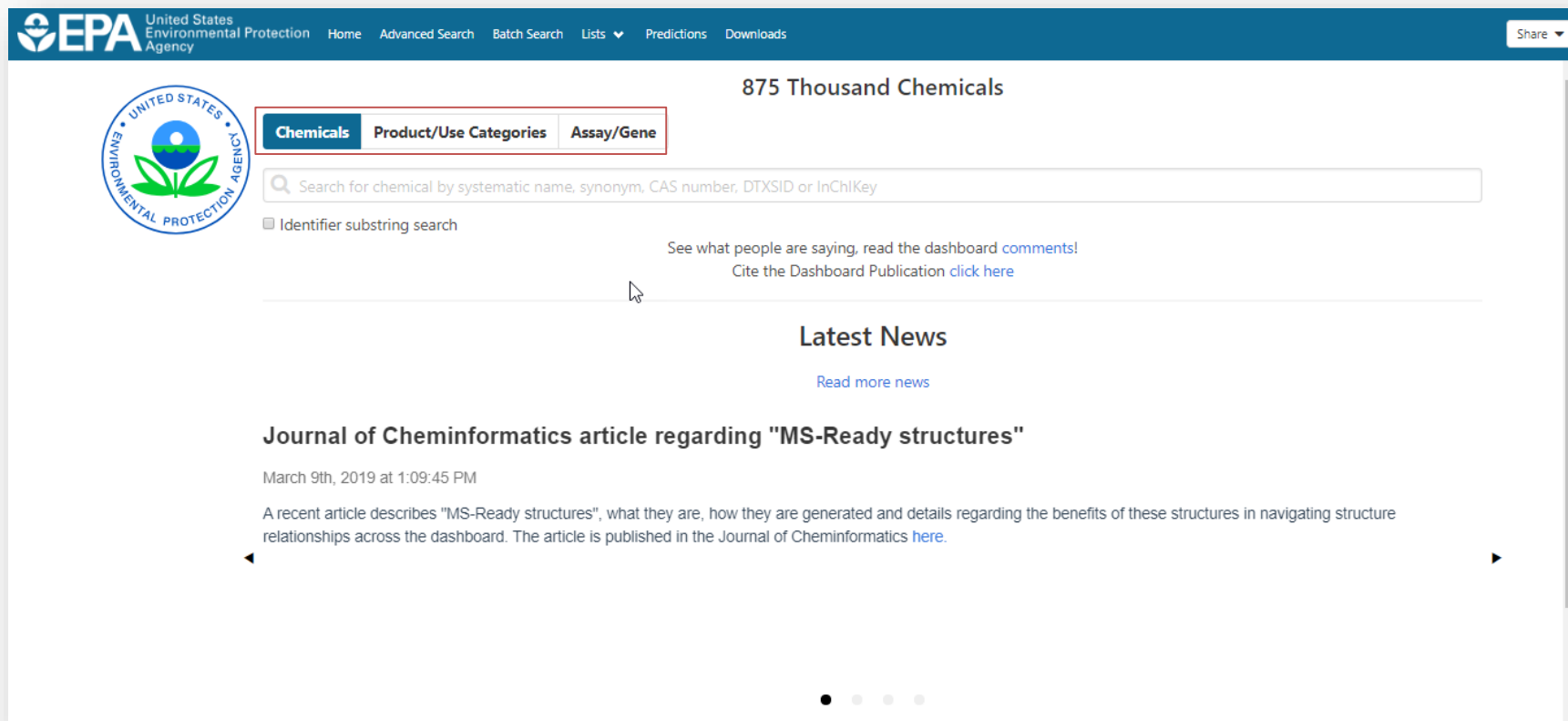
Hotlines

- **A publicly accessible website** delivering access:
 - ~875,000 chemicals with related property data
 - Experimental and predicted physicochemical property data
 - Experimental Human and Ecological hazard data
 - Integration to “biological assay data” for 1000s of chemicals
 - Information regarding consumer products containing chemicals
 - Links to other agency websites and public data resources
 - “Literature” searches for chemicals using public resources
 - “Batch searching” for thousands of chemicals
 - Real time prediction of physchem and toxicity endpoints

CompTox Chemicals Dashboard

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

875k Chemical Substances



The screenshot shows the EPA CompTox Chemicals Dashboard. At the top is a blue navigation bar with the EPA logo, the text "United States Environmental Protection Agency", and links for Home, Advanced Search, Batch Search, Lists, Predictions, and Downloads. A "Share" button is in the top right. Below the navigation bar is a white header area with the EPA seal on the left and the text "875 Thousand Chemicals" on the right. Under the seal are three tabs: "Chemicals" (selected), "Product/Use Categories", and "Assay/Gene". Below the tabs is a search bar with the placeholder text "Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey". To the left of the search bar is a checkbox for "Identifier substring search". To the right of the search bar are two links: "See what people are saying, read the dashboard [comments!](#)" and "Cite the Dashboard Publication [click here](#)". Below this is a section titled "Latest News" with a link "Read more news". The first news item is titled "Journal of Cheminformatics article regarding 'MS-Ready structures'" and is dated "March 9th, 2019 at 1:09:45 PM". The text of the article states: "A recent article describes 'MS-Ready structures', what they are, how they are generated and details regarding the benefits of these structures in navigating structure relationships across the dashboard. The article is published in the Journal of Cheminformatics [here](#)." At the bottom of the dashboard are four small circular indicators.

United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Share

875 Thousand Chemicals

Chemicals Product/Use Categories Assay/Gene

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

Identifier substring search

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

Latest News

[Read more news](#)


Journal of Cheminformatics article regarding "MS-Ready structures"


March 9th, 2019 at 1:09:45 PM

A recent article describes "MS-Ready structures", what they are, how they are generated and details regarding the benefits of these structures in navigating structure relationships across the dashboard. The article is published in the Journal of Cheminformatics [here](#).


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

EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Copy Share Submit Comment

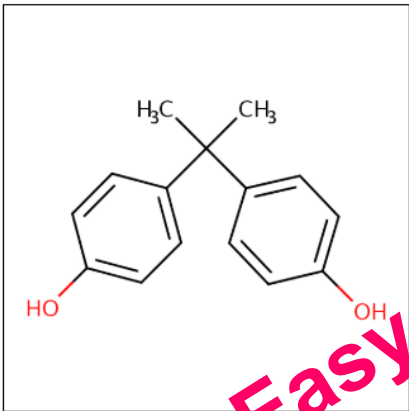
Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

DETAILS

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






Chemical structure of Bisphenol A (BPA) is shown, featuring two hydroxyphenyl groups connected by a central carbon atom bonded to two methyl groups.



Wikipedia


Bisphenol A (BPA) is an organic synthetic compound with the chemical formula $(\text{C}_6\text{H}_4)_2\text{C}(\text{C}_6\text{H}_4\text{OH})_2$ 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

Let's Not Do the Easy Searches For One Chemical

THE POWER OF BATCH SEARCHING

Batch Access to Underlying Data

https://comptox.epa.gov/dashboard/dsstoxdb/batch_search

Batch Search ?












Step One: Select Input

Please enter one identifier per line



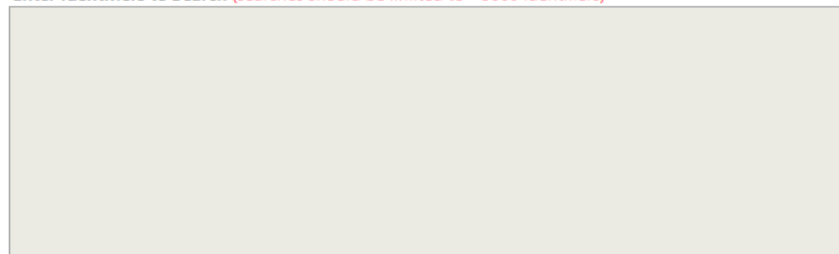
Select Input Type(s)

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

 Display All Chemicals










*** Download Chemical Data

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



A large, empty rectangular text input area for entering identifiers.

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 

This search is based on what we refer to as "Mass Spec (MS) Ready" structures. All chemicals within the database are treated in a manner such that all are desalted, mixtures are separated, and stereochemistry is removed as Mass Spectrometry detects the major components of a salt or mixture and is insensitive to stereochemistry. As an example, a search for the monoisotopic mass of phenol will return phenol, sodium phenolate and calcium phenoxide. See the publication for more details: <https://doi.org/10.1186/s13321-018-0299-2>.

 Display All Chemicals










... Download Chemical Data


Enter Identifiers to Search (search)

CAS Numbers...



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 

 Display All Chemicals

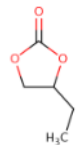
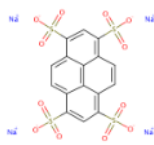
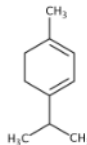
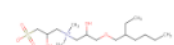

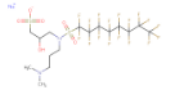
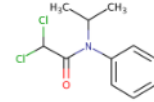
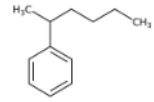
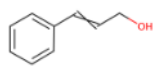
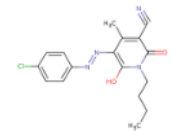
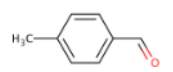
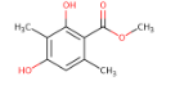
... Download Chemical Data

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

34396-03-7
56863-02-6
38640-62-9
762-04-9
14576-08-0
116-02-9
4395-65-7
12225-18-2
27757-95-5
12236-62-3

Display Chemicals










Select all Download Send to Batch Search Default CASRN TOXCAST PubMed 22 chemicals Hide chemicals that are: Filter by Name or CASRN


 <p>Butylene carbonate CASRN: 4437-85-8 TOXCAST: 2/398 PubMed: 1</p>	 <p>1,3,6,8-Pyrenetetrakisulfonic acid, tetrasod... CASRN: 59572-10-0 TOXCAST: 0/249 PubMed: 10</p>	 <p>alpha-Terpinene CASRN: 99-86-5 TOXCAST: 15/574 PubMed: 137</p>	 <p>1-Propanaminium, 3-[[[2-ethylhexyl)oxy]... CASRN: 108797-85-9 TOXCAST: - PubMed: 0</p>	 <p>1-Propanaminium, N-(carboxymethyl)-N... CASRN: 59272-84-3 TOXCAST: - PubMed: 0</p>	 <p>Sodium 3-[[[3-(dimethylamino)propyl]](p... CASRN: 94133-90-1 TOXCAST: - PubMed: 0</p>
 <p>2,2-Dichloro-N-isopropylacetanilide CASRN: 39105-95-8 TOXCAST: - PubMed: 0</p>	 <p>2-Phenylhexane CASRN: 6031-02-3 TOXCAST: - PubMed: 0</p>	 <p>3-Phenyl-2-propen-1-ol CASRN: 104-54-1 TOXCAST: 18/422 PubMed: 106</p>	 <p>3-Pyridinecarbonitrile, 1-butyl-5-[[[4-chlo... CASRN: 69808-32-8 TOXCAST: - PubMed: 0</p>	 <p>4-Methylbenzaldehyde CASRN: 104-87-0 TOXCAST: 3/250 PubMed: 2</p>	 <p>Methyl 2,4-dihydroxy-3,6-dimethylbenz... CASRN: 4707-47-5 TOXCAST: 30/427 PubMed: 0</p>

CAS Numbers...



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 

 Display All Chemicals

... Download Chemical Data

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

34396-03-7
56863-02-6
38640-62-9
762-04-9
14576-08-0
116-02-9
4395-65-7
12225-18-2
27757-95-5
12236-62-3

Select Output Format:

 Download as...

TSV







CSV

Excel






SDF

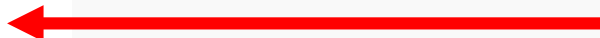
Chemical Identifiers

Chemical Identifiers

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

Structures

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



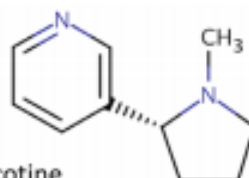
Open Science for Identifying “Known Unknown” Chemicals

Emma L. Schymanski^{*,†} and Antony J. Williams^{*,‡}



Nicotine

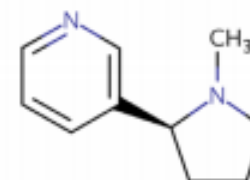
CN1CCC[C@H]1C1=CN=CC=C1
DTXSID1020930 | SNICXCGAKADSCV
54-11-5 | **162.1157** | 0.929 | **72**
Tox: **yes** | Expo: **yes** | Bioassay: **yes**



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**

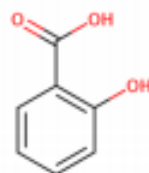
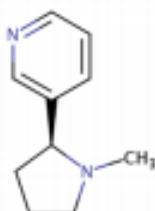
LEGEND: Name, SMILES
DTXSID | InChIKey 1st Block
CAS | Monoiso. Mass | logP | Sources
Data on: Toxicity | Exposure | Bioassays



HCl

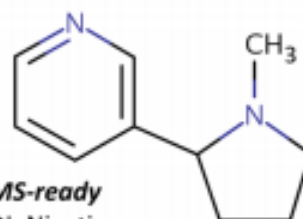
Nicotine hydrochloride

Cl.CN1CCC[C@H]1C1=CN=CC=C1
DTXSID602093 | HDJBTCJIMNXEW
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=CC(=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**



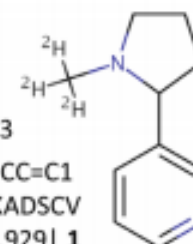
MS-ready

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 Structures”

<https://doi.org/10.1186/s13321-018-0299-2>

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^{1,2*}, Kamel Mansouri^{1,2,3}, Chris Grulke², Emma L. Schymanski⁴, Christoph Ruttkies⁵ and Antony J. Williams^{2*}

MS-Ready SMILES

A	B	C	D	E	F	G	H
INPUT	FOUND_BY	DTXSID	PREFERRED_NAME	MS_READY_SMILES			
59572-10-0	CAS-RN	DTXSID904	1,3,6,8-Pyrenetetrasulfonic acid, tetrasodium	s	OS(=O)(=O)C1=CC(=C2C=CC3=C(C=C		
104-54-1	CAS-RN	DTXSID904	3-Phenyl-2-propen-1-ol		OCC=CC1=CC=CC=C1		
4395-65-7	CAS-RN	DTXSID904	C.I. Solvent Blue 68		NC1=C2C(=O)C3=C(C=CC=C3)C(=O)C		
12225-18-2	CAS-RN	DTXSID904	C.I. Pigment Yellow 97		COC1=CC(Cl)=C(OC)C=C1NC(=O)C(N		
14576-08-0	CAS-RN	DTXSID904	Cyclohexene, 4-(1-methoxy-1-methylethyl)-1-h		COC(C)(C)C1CCC(C)=CC1		
4707-47-5	CAS-RN	DTXSID904	Methyl 2,4-dihydroxy-3,6-dimethylbenzoate		COC(=O)C1=C(O)C(C)=C(O)C=C1C		
34396-03-7	CAS-RN	DTXSID904	Silane, trimethoxy(2,4,4-trimethylpentyl)-		CO[Si](CC(C)CC(C)(C)C)(OC)OC		
2475-46-9	CAS-RN	DTXSID904	1-(Methylamino)-4-(2-hydroxyethylamino)anthr		CNC1=CC=C(NCCO)C2=C1C(=O)C1=C		
94133-90-1	CAS-RN	DTXSID904	Sodium 3-[[3-(dimethylamino)propyl][(perfluoro		CN(C)CCCN(CC(O)CS(O)(=O)=O)S(=O		
762-04-9	CAS-RN	DTXSID904	Diethyl phosphite		CCOP(=O)OCC		


Intrinsic And Predicted Properties

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



TEST and OPERA Predictions

Predicted

 Download Predicted Data ▼

Source	Result	Calculation Details	QMRF
EPISUITE	9.93e-4	Not Available	Not Available
NICEATM	2.16e-4	Not Available	Available
TEST	4.41e-4	TEST Report	Not Available
OPERA	1.42e-4	OPERA Model Report [Inside AD]	Available

Transparency for prediction models



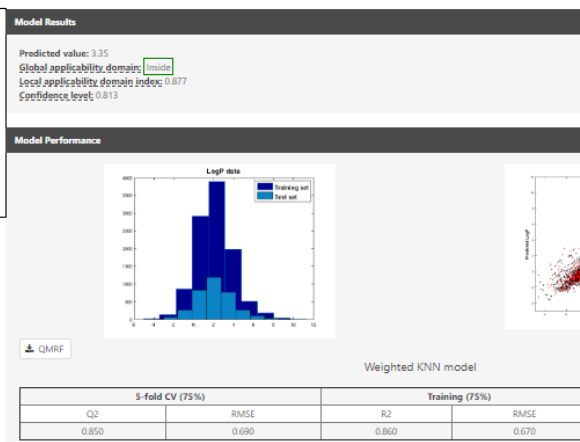
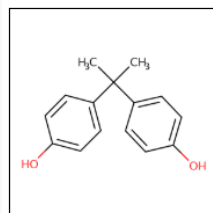
Predicted

Download Predicted Data ▼

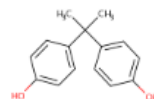
Source	Result	Calculation Details	QMRF
EPISUITE	3.64	Not Available	Not Available
NICEATM	2.40	Not Available	Available
ACD/Labs Consensus	3.63	Not Available	Not Available
ACD/Labs	3.43	Not Available	Not Available
OPERA	3.35	OPERA Model Report [Inside AD]	Available

OPERA Models: LogP: Octanol-Water

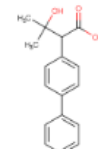
Bisphenol A
80-05-7 | DTXSID7020182



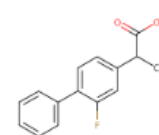
Nearest Neighbors from the Training Set



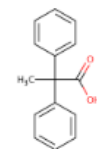
Bisphenol A
Measured: 3.32
Predicted: 3.35076



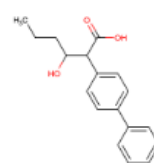
BUTANOIC ACID 2-(4-BIPHENYL)-3-
HYDROXY-3-METHY
Measured: 3.25
Predicted: 3.39062



Flurbiprofen
Measured: 4.16
Predicted: 3.94445



2,2-Diphenylacetic acid
Measured: 2.69
Predicted: 2.84603



3-OH-2-(4-BIPHENYL)-HEXANOIC ACID
Measured: 3.75
Predicted: 3.70322

TEST Real-Time Predictions

EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Search: Atrazine

100%

Select properties to predict

T.E.S.T.


- ☒ Toxicological properties
 - ☒ 96 hour fathead minnow LC50
 - ☒ 48 hour D. magna LC50
 - ☒ 48 hour T. pyriformis IGC50
 - ☒ Oral rat LD50
 - ☒ Bioaccumulation factor
 - ☒ Developmental toxicity
 - ☒ Ames mutagenicity
 - ☒ Estrogen Receptor RBA
 - ☒ Estrogen Receptor Binding
- ☒ Physical properties
 - ☒ Normal boiling point
 - ☒ Melting point
 - ☒ Flash point
 - ☒ Vapor pressure
 - ☒ Density
 - ☒ Surface tension
 - ☒ Thermal conductivity
 - ☒ Viscosity
 - ☒ Water solubility

Calculate

Chemical structure of Atrazine: CC1=NC2=C(N1)N=CN=C2C3=CC=CC=C3

Chiral

TEST Real-Time Predictions with detailed calculation reports

 EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Share Search all data

Provider: T.E.S.T.

Download Summary

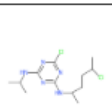
Property	Experimental Value	Consensus	Hierarchical clustering	Single model	Group contribution	Nearest neighbor
96 hour fathead minnow LC50		4.951 -Log10(mol/L) 3.425 mg/L	5.198 -Log10(mol/L) 1.943 mg/L	5.257 -Log10(mol/L) 1.693 mg/L	5.287 -Log10(mol/L) 1.581 mg/L	4.064 -Log10(mol/L) 26.452 mg/L
48 hour D. magna LC50		4.430 -Log10(mol/L) 11.374 mg/L	4.764 -Log10(mol/L) 5.269 mg/L	5.006 -Log10(mol/L) 3.020 mg/L	4.430 -Log10(mol/L) 11.386 mg/L	3.521 -Log10(mol/L) 92.353 mg/L
48 hour T. pyriformis IGC50			5.272 -Log10(mol/L) 1.639 mg/L			
Oral rat LD50		1.989 -Log10(mol/kg) 3141.571 mg/kg	1.867 -Log10(mol/kg) 4157.591 mg/kg			2.111 -Log10(mol/kg) 2373.843 mg/kg
Bioaccumulation factor		1.321 Log10 20.956	1.209 Log10 16.192	1.585 Log10 38.452	1.517 Log10 32.923	0.974 Log10 9.409
Developmental toxicity		true	true	true		
Ames mutagenicity		false	false			false
Estrogen Receptor RBA						
Estrogen Receptor Binding		false	false	false	false	
Normal boiling point		357.4 °C	334.0 °C		432.8 °C	305.5 °C
Melting point		111.3 °C	98.3 °C		99.1 °C	136.7 °C
Flash point		219.9 °C	272.7 °C		211.4 °C	175.7 °C
Vapor pressure		-6.849 Log10(mmHg) 1.417*10 ⁻⁷ mmHg	-6.471 Log10(mmHg) 3.382*10 ⁻⁷ mmHg		-7.617 Log10(mmHg) 2.415*10 ⁻⁸ mmHg	-6.458 Log10(mmHg) 3.486*10 ⁻⁷ mmHg
Density		1.211 g/cm ³	1.157 g/cm ³		1.278 g/cm ³	1.197 g/cm ³

TEST Real-Time Predictions with detailed calculation reports

Predicted Vapor pressure at 25°C for C1C=1N=C(N=C(N1)NC(C)CCC(Cl)C)NC(C)C from Consensus method

Prediction results		
Endpoint	Experimental value	Predicted value
Vapor pressure at 25°C Log10(mmHg)	N/A	-6.85
Vapor pressure at 25°C mmHg	N/A	1.42E-07

Individual Predictions	
Method	Predicted value Log10(mmHg)
Hierarchical clustering	-6.47
Group contribution	-7.62
Nearest neighbor	-6.46

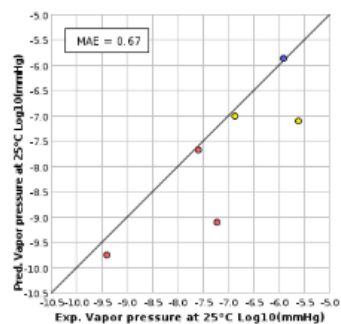


Predictions for the test chemical and for the most similar chemicals in the external test set

If the predicted value matches the experimental values for similar chemicals in the test set (and the similar chemicals are in the test set)

CAS	Structure	Similarity Coefficient	Experimental value Log10(mmHg)	Predicted value Log10(mmHg)
<chem>C1C=1N=C(N=C(N1)NC(C)CCC(Cl)C)NC(C)C</chem> (test chemical)			N/A	-6.85
7287-19-6		0.83	-5.91	-5.86
130339-07-0		0.77	-5.62	-7.11
21725-46-2		0.76	-6.86	-7.01
120928-09-8		0.58	-7.59	-7.67
101200-48-0		0.56	-9.41	-9.76
119738-06-6		0.55	-7.23	-9.11

Prediction results (colors defined in table below)




Chemicals	MAE*
Entire set	0.47
Similarity coefficient ≥ 0.5	0.67

*Mean absolute error in Log10(mmHg)

TEST/OPERA Batch Download


DTXSID	C	D	E	F	G	H	I	J	K	L	A
DTXSID904	PREFERR	BIOCONCE	BOILING_F	48HR_DAP	DENSITY_C	DEVTOX_T	96HR_FATI	FLASH_PC	MELTING_I		
DTXSID904	Methyl 2,4-	4.30527	294.167	2.259E-05	1.253	0.673	9.29E-05	136.111	96.637		
DTXSID904	3-Phenyl-2-	7.2277	254.617	0.0003532	1.059	0.795	6.653E-05	124.886	57.333		
DTXSID904	alpha-Terpir	584.62	174.7	9.772E-06	0.86	0.78	1.462E-05	49.96	-39.21		
DTXSID904	3,3,5-Trimet	20.2302	197.088	0.0005224	0.885	0.974	0.0003819	76.508	21.347		
DTXSID904	Diethyl phos	0.796159	142.81	-	1.028	0.941	-	58.069	-42.817		
DTXSID904	4-Methylber	-	221.904	0.0001233	1.066	0.517	8.65E-05	87.033	23.053		
DTXSID904	Butylene ca-	-	167.924	-	1.114	0.447	-	96.795	0.641	-	
DTXSID904	Silane, trim	183.231	187.37	-	0.86	0.343	-	72.907	-60.671		
DTXSID904	Linoleic diet	5.87489	430.153	2.443E-05	0.96	0.454	4.875E-06	255.997	40.201		
DTXSID904	Cyclohexen	46.3447	197.405	4.613E-05	0.892	0.74	0.0001194	73.597	-10.519		
DTXSID904	C.I. Solvent	34.914	493.758	2.944E-06	1.36	0.87	1.104E-06	262.584	211.867		
DTXSID904	C.I. Pigmen	3.02691	-	-	1.43	1.074	-	423.613	249.017		
DTXSID904	C.I. Pigmen	3.2961	-	-	1.686	0.778	-	-	275.574		
DTXSID904	1-(Methylan	14.8936	434.621	5.129E-05	1.38	0.859	9.12E-06	292.795	212.665		
DTXSID904	Isoamyl sal	21.6272	285.877	3.681E-05	1.105	0.744	1.6E-05	117.032	44.513		
DTXSID904	3-Pyridine	-	167.613	3.451E-08	1.267	0.983	-	317.894	182.082		


Metadata

- ☐ Curation Level Details ⓘ 
- ☐ NHANES/Predicted Exposure ⓘ
- ☐ Data Sources ⓘ
- ☐ Include ToxVal Data Availability ⓘ
- ☐ Assay Hit Count ⓘ
- ☐ Number of PubMed Articles ⓘ
- ☐ PubChem Data Sources ⓘ
- ☐ CPDat Product Occurrence Count ⓘ
- ☐ IRIS ⓘ
- ☐ PPRTV ⓘ
- ☐ QC Notes ⓘ

Curation Level Details

- We have full time curators checking data

 **Record Information**

 **Citation:** U.S. Environmental Protection Agency. Chemistry Dashboard.
<https://comptox.epa.gov/dashboard/DTXSID3031654> (accessed Mar 17th, 2019), Microcystin LR

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

Metadata

- ☐ Curation Level Details 
- ☐ NHANES/Predicted Exposure 
- ☐ Data Sources 
- ☐ Include ToxVal Data Availability  
- ☐ Assay Hit Count 
- ☐ Number of PubMed Articles 
- ☐ PubChem Data Sources 
- ☐ CPDat Product Occurrence Count 
- ☐ IRIS 
- ☐ PPRTV 
- ☐ QC Notes 

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

Access to Chemical Hazard Data

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

EXPOSURE

BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES


SYNONYMS



LITERATURE


LINKS











COMMENTS

Hazard













DataType
 Toxicity Value

 Human  Eco

 Download Columns

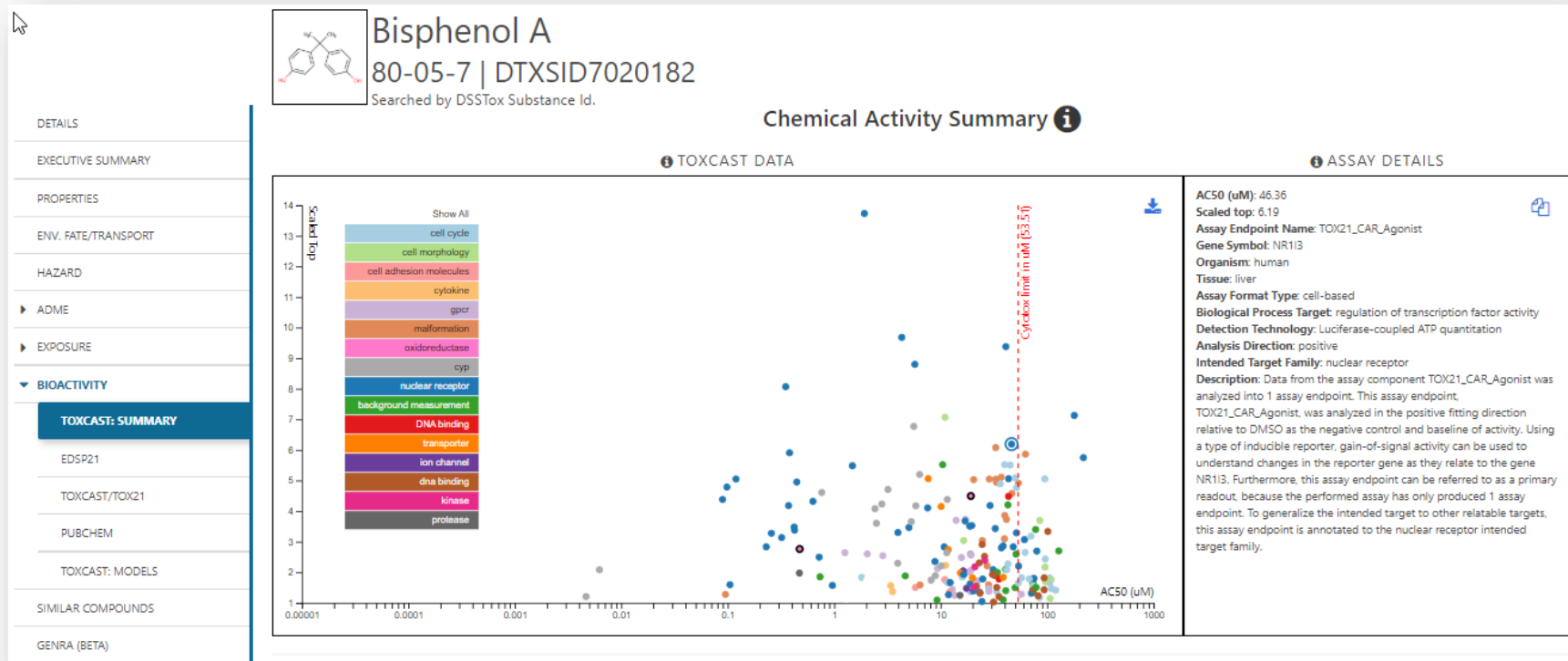
More	Priority	Type	Subtype	Risk assessment class	Value	Units	Study type	Exposure route	Species	Subsource	Source
	7	MEQ	Short-term Critical Air	short-term	500	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEQ	Short-term Marginal Air	short-term	100	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEQ	Short-term Negligible Air	short-term	15	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEQ	Soil Negligible Soil	chronic	106000	mg/kg	-	soil	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEQ	Long-Term, SL/d Negligible Water	chronic	7	mg/L	-	oral	-	TG 230 Military Exposure Guidelines Table	DOD
	6	RfD	-	chronic	0.05	mg/kg-day	-	oral	rat	Wignall	Wignall
	5	RfD	-	chronic	0.05	mg/kg-day	-	-	-	MSC Table 5	Pennsylvania DEP ToxValues
	4	RfD	-	chronic	0.05	mg/kg-day	chronic	oral	rat	IRIS	Chiu
	3	RfD	-	chronic	0.6	mg/kg-day	-	oral	rat	EPA/ORNL/OLEM	HEAST
	1	RfD	-	chronic	0.05	mg/kg-day	-	oral	-	EPA NCEA	IRIS

Metadata












- ☐ Curation Level Details 
- ☐ NHANES/Predicted Exposure 
- ☐ Data Sources 
- ☐ Include ToxVal Data Availability 
- ☐ Assay Hit Count  
- ☐ Number of PubMed Articles 
- ☐ PubChem Data Sources 
- ☐ CPDat Product Occurrence Count 
- ☐ IRIS 
- ☐ PPRTV 
- ☐ QC Notes 

In Vitro Bioassay Screening

ToxCast and Tox21




Metadata

- ☐ Curation Level Details 
- ☐ NHANES/Predicted Exposure 
- ☐ Data Sources 
- ☐ Include ToxVal Data Availability 
- ☐ Assay Hit Count 
- ☐ Number of PubMed Articles 
- ☐ PubChem Data Sources 
- ☐ CPDat Product Occurrence Count 
- ☐ IRIS 
- ☐ PPRTV 
- ☐ QC Notes 



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

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

▶ ADME

▼ EXPOSURE

PRODUCT & USE CATEGORIES

CHEMICAL WEIGHT FRACTION

CHEMICAL FUNCTIONAL USE

TOXICS RELEASE INVENTORY

MONITORING DATA

EXPOSURE PREDICTIONS

PRODUCTION VOLUME

▼ BIOACTIVITY













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Columns ▼ 10 ▼

Product or Use Categorization	Categorization type	Number of Unique Products
manufacturing, metals	CPCat Cassette	17
adhesive	CPCat Cassette	17
paint	CPCat Cassette	16
manufacturing, machines	CPCat Cassette	12
manufacturing, plastics	CPCat Cassette	11
building_material, flooring	CPCat Cassette	8
surface_treatment, metals	CPCat Cassette	8
construction	CPCat Cassette	8
stabilizer	CPCat Cassette	7
manufacturing, chemical	CPCat Cassette	6

First << < 1 2 3 4 5 6 7 8 9 10 > >> Last

Metadata

- ☐ Curation Level Details 
- ☐ NHANES/Predicted Exposure 
- ☐ Data Sources 
- ☐ Include ToxVal Data Availability 
- ☐ Assay Hit Count 
- ☐ Number of PubMed Articles 
- ☐ PubChem Data Sources 
- ☐ CPDat Product Occurrence Count 
- ☐ IRIS  
- ☐ PPRTV 
- ☐ QC Notes 



United States
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Atrazine
1912-24-9 | DTXSID9020112
Searched by Approved Name.

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

► ADME

► EXPOSURE

► BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

▼ LITERATURE

GOOGLE SCHOLAR

PUBMED ABSTRACT SIFTER

PUBCHEM ARTICLES

PUBCHEM PATENTS

PPRTV

IRIS

LINKS

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Atrazine

CASRN 1912-24-9

- [IRIS Summary \(PDF\)](#) (15 pp, 126 K)
- [Reregistration Eligibility Decision \(RED\)](#) (PDF) (323 pp, 1.86 M)
- Status:** EPA [announced in a 2004 Federal Register Notice](#) that chemicals used as pesticides would not be re-assessed by the IRIS Program. This entry in the IRIS database is preserved at the request of EPA program and regional offices. Additional toxicological information may be found under "Other EPA Information."

[CONTACT US](#)

IRIS Toxicity Values

Other EPA Information

Noncancer Assessment

[Reference Dose for Oral Exposure \(RfD\) \(PDF\)](#) (13 pp, 129 K) last updated: 10/01/2009

System	RfD (mg/kg-day)	Basis	PoD	Composite UF
Other	3.5 x 10 ⁻⁴	Decreased body weight gain	NOAEL: 3.5 mg/kg-day	100

Chemical Structure for Atrazine











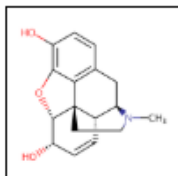
Synonyms

Integrated Data in Excel Sheet

DTXSID	PREFERRED_NAME	QC_LEVEL	TOXVAL	DTOXCAST	TOXCAST	#PUBMED	ARTIRIS_LINK	QC_NOTES
DTXSID2026494	Dichlorodiphenylsilane	DSSTox_Low	Y	4.29	9/210	3	-	-
DTXSID5026621	Trichlorophenylsilane	DSSTox_Low	Y	-	-	-	-	-
DTXSID6026797	1,3,5-Trimethylbenzene	DSSTox_Low	Y	1.07	7/657	53	Y	-
DTXSID7026811	Benzenethiol	DSSTox_Low	Y	9.2	37/402	201	-	-
DTXSID6026872	Butyl isocyanate	DSSTox_Low	Y	0.95	2/211	21	-	-
DTXSID7026940	Ethyl silicon trichloride	DSSTox_Low	-	-	-	-	-	-
DTXSID3027033	Silane, dichloroethenylmethyl	DSSTox_Low	Y	-	-	1	-	-
DTXSID2027204	Methyl isothiocyanate	DSSTox_Low	Y	5.85	46/786	60	-	-
DTXSID5027273	Carbon monoxide	DSSTox_Low	Y	-	-	18454	-	-
DTXSID9027289	Diketene	DSSTox_Low	Y	-	-	22	-	-
DTXSID3027291	Tetramethyl orthosilicate	DSSTox_Low	Y	3.79	8/211	53	-	-
DTXSID0027355	Chlorodimethylsilane	DSSTox_Low	-	-	-	-	-	-
DTXSID3027407	Ethyl dichlorophosphate	DSSTox_Low	Y	2.93	11/376	-	-	-
DTXSID0027482	Trimethoxysilane	DSSTox_Low	Y	-	-	58	-	-
DTXSID4027529	2,2-Dimethylpropanoyl chloric	DSSTox_Low	Y	0.95	2/211	7	-	-
DTXSID7027627	Propylene dinitrate	DSSTox_Low	Y	-	-	14	-	-
DTXSID6027684	Kerosine	DSSTox_High	Y	-	-	712	-	A complex combi
DTXSID3027746	Pentacarbonyl iron	DSSTox_High	Y	-	-	155	-	-
DTXSID5029269	Trichloro(octyl)silane	DSSTox_Low	Y	-	-	7	-	-
DTXSID4029301	Trichlorosilane	DSSTox_Low	Y	-	-	46	-	-
DTXSID6029672	Sulfur dioxide	DSSTox_Low	Y	-	-	4646	-	-
DTXSID5029685	Nitric acid	DSSTox_Low	Y	-	-	1193	-	-

Enhanced Data Sheets

- ☐ MetFrag Input File (Beta) 
- ☐ ToxPrint single fingerprints 
- ☐ Abstract Sifter Input File (Beta)  
- ☐ Synonyms and Identifiers 
- ☐ Related Substance relationships 
- ☐ ToxPrint fingerprints (ChemoTyper format - CSV/TSV only) 
- ☐ Associated ToxCast Assays 




Morphine

57-27-2 | DTXSID9023336

Searched by Approved Name.

Abstract Sifter

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.

"57-27-2" OR "Morphine"

Literature Searching

Child (Infant through adolescent)

Dust and Exposure


Food and Exposure

Water and Exposure

Algae

Disaster / Emergency



 Optionally, edit the query before retrieving.

("57-27-2" OR "Morphine") AND ((water OR groundwater OR drinking water) AND Environmental Exposure)




Literature Searching

37 of 37 articles loaded...

To find articles quickly, enter terms to sift abstracts. 

<input type="checkbox"/>	wastewater	Spectrometry ↓	EPA	Total	PMID	Year	Title	Authors	Journal	Rev
<input type="checkbox"/>	4	2	0	6	29274731	2017	Simultaneous analysis of opioid analgesics and thei...	Krizman-Matic; Kostanjevecki; Ahel; Terzic	Journal of chromatography. A	
<input type="checkbox"/>	0	1	0	1	25768972	2015	Evaluating external contamination of polybrominate...	Poon; Aleksa; Carnevale; Kapur; Goodyer; Koren	Therapeutic drug monitoring	
<input type="checkbox"/>	0	1	0	1	22544551	2012	Spatial distribution of illicit drugs in surface waters o...	Vazquez-Roig; Andreu; Blasco; Morillas; Picó	Environmental science and pollution research inter...	
<input type="checkbox"/>	1	1	0	2	20801487	2010	Analysis of illicit and illicit drugs in waste, surface an...	Berset; Brenneisen; Mathieu	Chemosphere	
<input type="checkbox"/>	1	1	0	2	17935751	2007	Illicit drugs, a novel group of environmental contami...	Zuccato; Castiglioni; Bagnati; Chiabrando; Grassi; ...	Water research	
<input type="checkbox"/>	2	1	1	4	17607391	2007	Using environmental analytical data to estimate lev...	Bones; Thomas; Paull	Journal of environmental monitoring : JEM	
<input type="checkbox"/>	3	1	2	6	17180984	2006	Simultaneous determination of psychoactive drugs ...	Hummel; Löffler; Fink; Ternes	Environmental science & technology	
<input type="checkbox"/>	6	0	0	6	30583189	2018	Assessment of drugs of abuse in a wastewater trea...	Kumar; Tschärke; O'Brien; Mueller; Wilkins; Padhye	The Science of the total environment	
<input type="checkbox"/>	0	0	3	3	30488421	2018	Effect of enriched environment during adolescence ...	Mohammadian; Najafi; Miladi-Gorji	Developmental psychobiology	
<input type="checkbox"/>	3	0	0	3	29574368	2018	Estimation of the consumption of illicit drugs during ...	Foppe; Hammond-Weinberger; Subedi	The Science of the total environment	
<input type="checkbox"/>	1	0	0	1	28787791	2017	Evaluation of in-sewer transformation of selected illi...	Gao; Banks; Li; Jiang; Lai; Mueller; Thai	The Science of the total environment	
<input type="checkbox"/>	9	0	0	9	28472697	2017	Occurrence and fate of illicit drugs and pharmaceuti...	Causanilles; Ruepert; Ibáñez; Emke; Hernández; d...	The Science of the total environment	
<input type="checkbox"/>	0	0	0	0	28010888	2016	Dose-dependent effects of morphine on lipopolysac...	Mottaz; Schönenberger; Fischer; Eggen; Schirmer; ...	Environmental pollution (Barking, Essex : 1987)	
<input type="checkbox"/>	0	0	0	0	27746311	2016	Effects of voluntary exercise on the viability, prolifer...	Haydari; Safari; Zarbakhsh; Bandegi; Miladi-Gorji	Neuroscience letters	
<input type="checkbox"/>	0	0	0	0	27261879	2016	Genotoxic effects induced by the exposure to an en...	Parolini; Magni; Castiglioni; Binelli	Ecotoxicology and environmental safety	
<input type="checkbox"/>	3	0	0	3	27179320	2016	Temporal trends in drug use in Adelaide, South Aus...	Tschärke; Chen; Gerber; White	The Science of the total environment	



Open for Science




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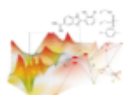
Check for updates

SOFTWARE TOOL ARTICLE

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


 Nancy Baker ¹, Thomas Knudsen², Antony Williams ²

 Author details

 This article is included in the [Chemical Information Science](#) gateway.


Abstract

The Abstract Sifter is a Microsoft Excel based application that enhances existing search capabilities of PubMed. The Abstract Sifter assists researchers to search effectively, triage results, and keep track of articles of interest. The tool implements an innovative "sifter" functionality for relevance ranking, giving the researcher a way to find articles of interest quickly. The tool also gives




METRICS

629





VIEWS


118





DOWNLOADS


 Get PDF

 Get XML









 Cite

 Export

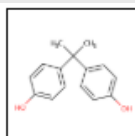
 Track

 Email

Enhanced Data Sheets

- ☐ MetFrag Input File (Beta) 
- ☐ ToxPrint single fingerprints 
- ☐ Abstract Sifter Input File (Beta) 
- ☐ Synonyms and Identifiers  
- ☐ Related Substance relationships 
- ☐ ToxPrint fingerprints (ChemoTyper format - CSV/TSV only) 
- ☐ Associated ToxCast Assays 

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 Active CAS RN	Valid
BPA	Valid
4,4'-Propane-2,2-diylidiphenol	Valid
Phenol, 4,4'-(1-methylethylidene)bis-	Valid
4-06-00-06717 Beilstein Registry Number	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

Enhanced Data Sheets

- ☐ MetFrag Input File (Beta) 
- ☐ ToxPrint single fingerprints 
- ☐ Abstract Sifter Input File (Beta) 
- ☐ Synonyms and Identifiers 
- ☐ Related Substance relationships  
- ☐ ToxPrint fingerprints (ChemoTyper format - CSV/TSV only) 
- ☐ Associated ToxCast Assays 

Transformation Products

Chlorothalonil

1897-45-6 | DTXSID0020319

Searched by DSSTox Substance Id.

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

EXPOSURE

BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

LITERATURE

LINKS

COMMENTS

8 chemicals

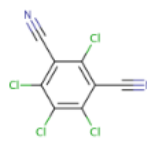
Download / Send

Sort by: Relationship

Show info: DTXSID CASRN Select all

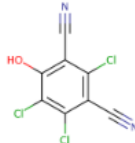
Filter by: Name or CASRN Hide

Searched Chemical



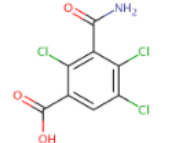
Chlorothalonil
DTXSID: DTXSID0020319
CASRN: 1897-45-6

Transformation Product



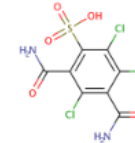
4-Hydroxy-2,5,6-trichloroisophthalonitrile
DTXSID: DTXSID00182588
CASRN: 28343-81-5

Transformation Product



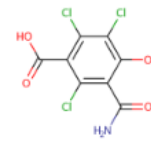
3-Carbamoyl-2,4,5-trichlorobenzoic acid
DTXSID: DTXSID10597537
CASRN: 142733-37-7

Transformation Product



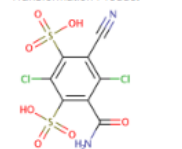
2,4-dicarbamoyl-3,5,6-trichlorobenzene-1-sulfonic acid
DTXSID: DTXSID30891327
CASRN: NOCAS_891327

Transformation Product



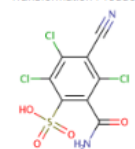
3-carbamoyl-2,5,6-trichloro-4-hydroxybenzoic acid
DTXSID: DTXSID00891328
CASRN: NOCAS_891328

Transformation Product



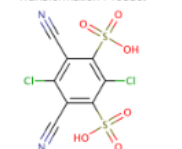
4-carbamoyl-2,5-dichloro-6-cyanobenzene-1-sulfonic acid
DTXSID: DTXSID00891329
CASRN: NOCAS_891329

Transformation Product



2-carbamoyl-3,5,6-trichloro-4-cyanobenzene-1-sulfonic acid
DTXSID: DTXSID00891330
CASRN: NOCAS_891330

Transformation Product



2,5-dichloro-4,6-dicyanobenzene-1,3-disulfonic acid
DTXSID: DTXSID20891331
CASRN: NOCAS_891331

Related Substance Relationships

Enhanced Data Sheets

- ☐ MetFrag Input File (Beta)
- ☐ ToxPrint single fingerprints
- ☐ Abstract Sifter Input File (Beta)
- ☐ Synonyms and Identifiers
- ☒ Related Substance relationships
- ☐ ToxPrint fingerprints (ChemoTyper)
- ☐ Associated ToxCast Assays

- ☐ EPA: National-Scale Air
- ☐ EPA: PPRTV Chemical R
- ☐ EPA: Provisional Adviso
- ☐ EPA: Safer Choice Chem

Selecting this checkbox provides a separate Excel worksheet containing the relationship between two chemicals. The output file includes the DTXSIDs and names/CASRN between the input list and the related chemical. Relationships include, for example, polymer, components, salt form, transformation product and other relationships.

	A	B	C	D	E	
1	INPUT	DTXSID	PREFERRED_NAME	HAS_RELATIONSHIP_WITH	RELATED_DTXSID	RELATED_PREFERRED_NAME
2	xylenes	DTXSID2021446	Xylenes	Transformation Product	DTXSID40176394	N-Benzoylalanine
3	xylenes	DTXSID2021446	Xylenes	Component	DTXSID6026298	m-Xylene
4	xylenes	DTXSID2021446	Xylenes	Component	DTXSID3021807	o-Xylene
5	xylenes	DTXSID2021446	Xylenes	Component	DTXSID2021868	p-Xylene
6	xylenes	DTXSID2021446	Xylenes	Predecessor: Component	DTXSID9021421	Xylenes; defined mixture 1
7	xylenes	DTXSID2021446	Xylenes	Predecessor: Component	DTXSID7021447	Xylenes; defined mixture 2
8	xylenes	DTXSID2021446	Xylenes	Predecessor: Component	DTXSID30891529	Total Petroleum Hydrocarbons
9	xylenes	DTXSID2021446	Xylenes	Markush Child	DTXSID3021807	o-Xylene
10	xylenes	DTXSID2021446	Xylenes	Markush Child	DTXSID6026298	m-Xylene
11	xylenes	DTXSID2021446	Xylenes	Markush Child	DTXSID2021868	p-Xylene

CASRN Checking


	96949-21-2	NO_MATCH	-	-
	29066-34-0	Deleted CAS-RN	DTXSID9041817	dl-Men
	8039-6 ⁺ 6	Deleted CAS-RN	DTXSID70897323	Ethoxyl
	76925-99-0	Deleted CAS-RN	DTXSID1044487	Methyl
	111-88-9	Checksum Failed	-	-
is[[1	187273-40-6	Checksum Failed	-	-
	24213-24-5	Checksum Failed	-	-
nd 1,2	25640-14-0	Checksum Failed	-	-
hanec	68601-19-5	Checksum Failed	-	-
opyl 2-	67990-40-3	CAS-RN	DTXSID90987412	N,N-Di
	68440-90-4	CAS-RN	DTXSID9098434	Siloxan
	68425-44-5	CAS-RN	DTXSID9098305	Amides
	68132-78-5	CAS-RN	DTXSID9096995	Amines
	68071-95-4	CAS-RN	DTXSID9096575	Quateri

Batch Searching Formula/Mass










Batch Search


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 

 Display All Chemicals

+/- ppm

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

41.0265
56.02621
53.0265
58.0418
93.0578
113.9639
151.8754
69.9377
77.9872

This search is based on what we refer to as "Mass Spec (MS) Ready" structures. All chemicals within the database are treated in a manner such that all are desalted, mixtures are separated, and stereochemistry is removed as Mass Spectrometry detects the major components of a salt or mixture and is insensitive to stereochemistry. As an example, a search for the monoisotopic mass of phenol will return phenol, sodium phenolate and calcium phenoxide. See the publication for more details: <https://doi.org/10.1186/s13321-018-0299-2>.

Searching batches using MS-Ready Formula (or mass) searching

	A	B	C	D	E	F	G
1	INPUT	DTXSID	CASRN	PREFERRED NAME	MOL FORMULA	MONOISOTOPIC MASS	DATA SOURCES
2	C14H22N2O3	DTXSID2022628	29122-68-7	Atenolol	C14H22N2O3	266.163042576	46
3	C14H22N2O3	DTXSID0021179	6673-35-4	Practolol	C14H22N2O3	266.163042576	32
4	C14H22N2O3	DTXSID4048854	841-73-6	Bucolome	C14H22N2O3	266.163042576	20
5	C14H22N2O3	DTXSID1045407	13171-25-0	Trimetazidine dihydrochloride	C14H24Cl2N2O3	338.116398	19
6	C14H22N2O3	DTXSID0045753	56715-13-0	R-(+)-Atenolol	C14H22N2O3	266.163042576	19
7	C14H22N2O3	DTXSID2048531	5011-34-7	Trimetazidine	C14H22N2O3	266.163042576	14
8	C14H22N2O3	DTXSID10239405	93379-54-5	Esatenolol	C14H22N2O3	266.163042576	12
9	C14H22N2O3	DTXSID50200634	52662-27-8	N-(2-Diethylaminoethyl)-2-(4-hydroxyphenoxy)acetamide	C14H22N2O3	266.163042576	7
10	C14H22N2O3	DTXSID4020111	51706-40-2	dl-Atenolol hydrochloride	C14H23ClN2O3	302.1397203	6
11	C14H22N2O3	DTXSID1068693	51963-82-7	Benzenamine, 2,5-diethoxy-4-(4-morpholinyl)-	C14H22N2O3	266.163042576	5
12	C18H34N2O6S	DTXSID3023215	154-21-2	Lincomycin	C18H34N2O6S	406.213757997	35
13	C18H34N2O6S	DTXSID7047803	859-18-7	Lincomycin hydrochloride	C18H35ClN2O6S	442.1904357	22
14	C18H34N2O6S	DTXSID20849438	1398534-62-7	PUBCHEM_71432748	C18H35ClN2O6S	442.1904357	1
15	C10H12N2O	DTXSID1047576	486-56-6	Cotinine	C10H12N2O	176.094963014	40
16	C10H12N2O	DTXSID8075330	50-67-9	Serotonin	C10H12N2O	176.094963014	22
17	C10H12N2O	DTXSID8044412	2654-57-1	4-Methyl-1-phenylpyrazolidin-3-one	C10H12N2O	176.094963014	18
18	C10H12N2O	DTXSID80165186	153-98-0	Serotonin hydrochloride	C10H13ClN2O	212.0716407	11
19	C10H12N2O	DTXSID2048870	29493-77-4	(4R,5S)-4-methyl-5-phenyl-4,5-dihydro-1,3-oxazol-2-amine	C10H12N2O	176.094963014	10
20	C10H12N2O	DTXSID10196105	443-31-2	6-Hydroxytryptamine	C10H12N2O	176.094963014	9
21	C10H12N2O	DTXSID90185693	31822-84-1	1,4,5,6-Tetrahydro-5-phenoxy pyrimidine	C10H12N2O	176.094963014	7
22	C10H12N2O	DTXSID40178777	2403-66-9	2-Benzimidazolepropanol	C10H12N2O	176.094963014	7
23	C10H12N2O	DTXSID80157026	13140-86-8	N-Cyclopropyl-N'-phenylurea	C10H12N2O	176.094963014	6
24	C10H12N2O	DTXSID30205607	570-14-9	4-Hydroxytryptamine	C10H12N2O	176.094963014	6
25	C14H18N4O3	DTXSID5023900	17804-35-2	Benomyl	C14H18N4O3	290.137890456	68
26	C14H18N4O3	DTXSID3023712	738-70-5	Trimethoprim	C14H18N4O3	290.137890456	51
27	C14H18N4O3	DTXSID40209671	60834-30-2	Trimethoprim hydrochloride	C14H19ClN4O3	326.1145682	8
28	C14H18N4O3	DTXSID70204210	55687-49-5	Benzenemethanol, 4-((2,4-diamino-5-pyrimidinyl)methyl)-2-	C14H18N4O3	290.137890456	5
29	C14H18N4O3	DTXSID20152671	120075-57-2	6-Methoxy-4-(3-(N,N-dimethylamino)propylamino)-5,8-quin	C14H18N4O3	290.137890456	4
30	C14H18N4O3	DTXSID30213742	63931-79-3	1H-1,2,4-Benzotriazepine-3-carboxylic acid, 4,5-dihydro-4-	C14H18N4O3	290.137890456	3
31	C14H18N4O3	DTXSID30219608	69449-07-6	2,4-Pyrimidinediamine, 5-((3,4,5-trimethoxyphenyl)methyl)-	C14H20N4O4	308.14845514	3
32	C14H18N4O3	DTXSID20241155	94232-27-6	L-Aspartic acid, compound with 5-((3,4,5-trimethoxyphenyl	C18H25N5O7	423.175398165	3
33	C14H18N4O3	DTXSID80241156	94232-28-7	L-Glutamic acid, compound with 5-((3,4,5-trimethoxyphenyl	C19H27N5O7	437.191048229	3
34	C14H18N4O3	DTXSID20143781	101204-93-7	1H-Pyrido(2,3-e)-1,4-diazepine-2,3,5-trione, 4-(2-(diethylam	C14H18N4O3	290.137890456	3
35	C12H11N7	DTXSID6021373	396-01-0	Triamterene	C12H11N7	253.107593382	52
36	C12H11N7	DTXSID00204465	5587-93-9	Ampyrimine	C12H11N7	253.107593382	7
37	C12H11N7	DTXSID5064621	7300-26-7	Benzenamine, 4-azido-N-(4-azidophenyl)-	C12H9N7	251.091943318	4
38	C12H11N7	DTXSID00848025	90293-82-6	Sulfuric acid-6-phenylpteridine-2,4,7-triamine (1/1)	C12H13N7O4S	351.074973101	1
39	C12H11N7	DTXSID50575293	92310-83-3	(1E)-N-Phenyl-1,2-bis(1H-1,2,4-triazol-1-yl)ethan-1-imine	C12H11N7	253.107593382	1
40	C8H9NO2	DTXSID2020006	103-90-2	Acetaminophen	C8H9NO2	151.063328534	75
41	C8H9NO2	DTXSID6025567	134-20-3	Methyl 2-aminobenzoate	C8H9NO2	151.063328534	50

AN EXAMPLE APPLICATION



Trends in Environmental Analytical Chemistry

Volume 20, October 2018, e00059



Opioid occurrence in environmental water samples—A review

Marina Celia Campos-Mañas ^a, Imma Ferrer ^b  , E.Michael Thurman ^b, Ana Agüera ^a

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

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

Presence in Lists:

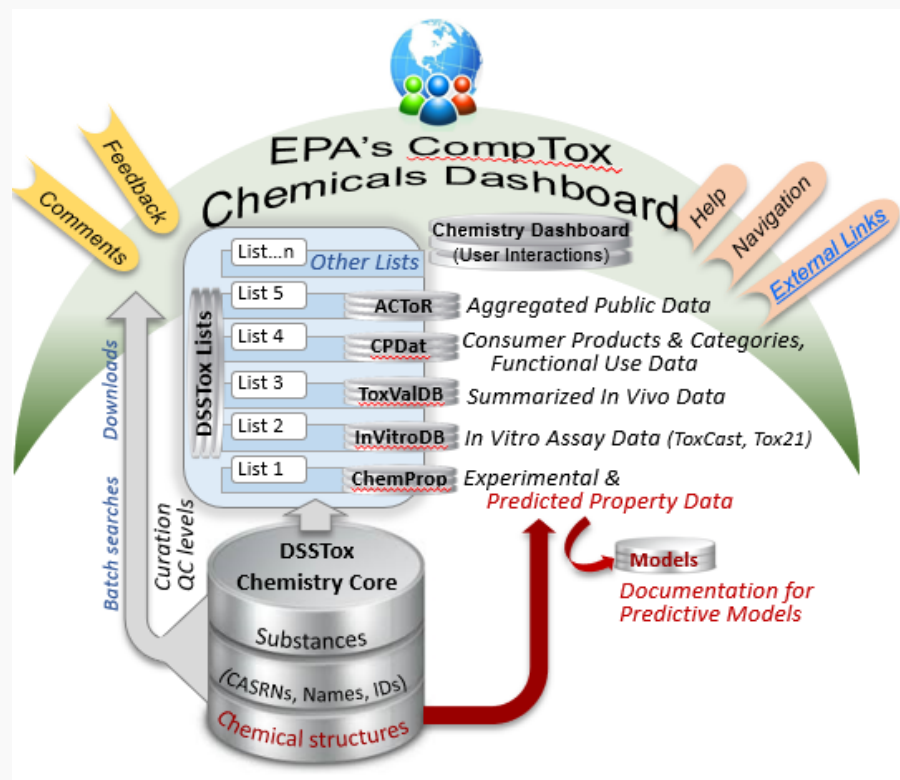
- ✓ ☐ [40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities](#)
- ☐ [AEGLS: Acute Exposure Guideline Levels](#)
- ☐ [ANDROGEN: Androgen Receptor Chemicals](#)
- ☐ [ARTICLE; Bench-Mark Dose Human Health Assessment List \(Wignall et al., 2014\)](#)
- ☐ [ATSDR: Minimal Risk Levels \(MRLs\) for Hazardous Substances](#)
- ☐ [ATSDR: Toxic Substances Portal Chemical List](#)
- ☐ [Barbara Wetmore's HHTK list](#)
- ☐ [California Office of Environmental Health Hazard Assessment](#)
- ☐ [CERAPP: Collaborative Estrogen Receptor Activity Prediction Project](#)
- ☐ [CHEMINV; ToxCast/Tox21 Chemical inventory available as DMSO solutions \(20181123\)](#)
- ☐ [CHEMINV: EPA Chemical Inventory for ToxCast](#)
- ☐ [CHEMINV: EPA ToxCast CHEMINV list of volatiles](#)

Batch Search in specific lists

<input type="checkbox"/>	INPUT	DTXSID	MASSBANKREF	NEMILIST	WRTMSD	NORMANPRI	SUSDAT
<input type="checkbox"/>	Buprenorph	DTXSID202	-	-	Y	-	Y
<input type="checkbox"/>	Codeine	DTXSID202	Y	Y	Y	Y	Y
<input type="checkbox"/>	Dextrometh	DTXSID302	Y	Y	Y	-	Y
<input type="checkbox"/>	Dihydrocod	DTXSID502	Y	-	Y	Y	Y
<input type="checkbox"/>	Dihydromor	DTXSID704	-	-	-	-	Y
<input type="checkbox"/>	Ethylmorph	DTXSID104	-	-	Y	-	Y
<input type="checkbox"/>	Fentanyl	DTXSID902	Y	-	Y	-	Y
<input checked="" type="checkbox"/>	Heroin	DTXSID604	Y	-	Y	Y	Y
<input checked="" type="checkbox"/>	Hydrocodor	DTXSID802	Y	Y	Y	Y	Y
<input type="checkbox"/>	Hydromorph	DTXSID802	-	-	Y	-	Y
<input type="checkbox"/>	Ketamine	DTXSID802	Y	-	Y	-	Y
<input checked="" type="checkbox"/>	Meperidine	DTXSID902	Y	-	Y	-	Y
<input type="checkbox"/>	Methadone	DTXSID702	Y	Y	Y	-	Y
<input checked="" type="checkbox"/>	Morphine	DTXSID902	Y	Y	Y	Y	Y
<input type="checkbox"/>	Morphinone	DTXSID501	-	-	-	-	Y
<input checked="" type="checkbox"/>	Naloxone	DTXSID802	-	-	Y	-	Y
<input type="checkbox"/>	Naltriben	-	-	-	-	-	-
<input type="checkbox"/>	Oxycodone	DTXSID502	Y	Y	Y	Y	Y
<input type="checkbox"/>	Oxymorpho	DTXSID502	-	-	Y	-	Y
<input type="checkbox"/>	Propoxyph	DTXSID102	Y	Y	Y	-	Y
<input type="checkbox"/>	Sufentanil	DTXSID602	-	-	Y	-	Y
<input type="checkbox"/>	Tramadol	DTXSID908	Y	Y	Y	Y	Y

Conclusion

- Dashboard access to data for ~875,000 chemicals
- Batch search capability for integrated search for thousands of chemicals across diverse data
- Future capabilities will include batch prediction
- Ongoing data expansion continues day to day
- We are committed to open API development for data access and predictions



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DATABASE

Open Access

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



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