

Accessing Environmental Chemistry Data via Data Dashboards

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

CompTox Chemicals Dashboard >906k chemicals



CompTox Chemicals Dashboard Home Search - List	s ▼ About ▼ Tools ▼	Submit Comments
	Welcome to the new EPA CompTox Chemicals Dashboard	_
The new Dashboard is a comp	ete rebuild and is replacing the CompTox Chemicals Dashboard released on July 12th 2020.	6
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Construction of the Owner of Constru-	Complox Chemicals Dashboard	
	Search 906,511 Chemicals	
Chemicals Products/Use Category	jories Assay/Gene	
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Bearch for chemical by systematic hame	Start turing to coardh	
	Start typing to search.	
	Latest News	
	Read More News	
10.000		



- Develop a "first-stop-shop" for environmental chemical data to support EPA and partner decision making:
 - Centralized location for relevant chemical data
 - Chemistry, exposure, hazard and dosimetry
 - Combination of existing data and predictive models
 - Publicly accessible, periodically updated, curated
- Easy access to data improves efficiency and ultimately accelerates chemical risk assessment

CompTox Chemicals Dashboard https://comptox.epa.gov/dashboard





BASIC Search





- Type ahead search using Names, synonyms and CASRNs
- Millions of identifiers
- Substring search

Search Results

Searched with 'Synonym Substring': Benzo(A)Pyrene

183 chemicals

Detailed Chemical Pages





• Chemical page: Wikipedia snippet when available, intrinsic properties, structural identifiers, linked substances

"Executive Summary"

Executive Summary

Quantitative Risk Assessment Values

🕑 IRIS values available 🗹

🖄 No PPRTV values

🔮 EPA RSL values available 🗹

🕑 Minimum RfD:0.0003 mg/kg-day (chronic,) 🗹

🕑 Minimum RfC:2e-06 mg/m3 (chronic,) 🗹

- Chronic toxicity PODs available C
- Subchronic Toxicology
 No subchronic toxicity data available
- Developmental Toxicology
 No developmental toxicity data available
- Acute Toxicology

No acute toxicity data available



- Overview of toxicityrelated info
 - Quantitative values
 - Physchem. and Fate & Transport
 - Adverse Outcome Pathway links
 - In vitro bioactivity summary plot

Experimental and Predicted Data



Summary	~	Q Search Chemical P
🛓 export 🔸		
Property	Experimental average	\equiv Predicted average \equiv
Polarizability	-	35.8 (1)
Henry's Law	4.57e-7 (1)	4.59e-7 (1)
Boiling Point	495 (3)	480 (4)
Flash Point	-	234 (2)
Melting Point	177 (8)	189 (3)
Molar Refractivity	-	90.3 (1)
Molar Volume	-	196 (1)
Surface Tension	-	53.9 (2)
Density	-	1.28 (2)
Vapor Pressure	5.49e-9 (1)	3.61e-9 (3)

- Physchem and Fate & Transport experimental and predicted data
- Data can be downloaded as Excel, TSV and CSV files

Chemical Hazard Data



ToxVal Database

- >50k chemicals
- >770k tox. values
- >30 sources of data
- ~5k journals cited
- ~70k citations

£	Export 🔻													
ore	Priority ↑	Source	≡ Туре	$\equiv \Big $ Subtype \equiv	Risk Assessment	≡ Qualifi er	Value 🗄	E Units	Study Type	${}^{\rm Exposur}_{\rm e\ Route}\equiv$	Critical effect 🛛 🚍	Species \equiv	Year	
	0		[ון
Ē	1	IRIS	LOAEL	12	chronic	=	9.10e-3	mg/m3	2	inhalation	reduced ovulation rate and ovary weight	2	223	
Ľ	1	IRIS	LOAEL		chronic	=	4.60e-3	mg/m3	÷	inhalation	reduced embryo/fetal survival	-	-	
ŀ	3	ECOTOX	NOEL	17	chronic growth	53 5	100	mg/kg f	Growth	Food	Weight	norway	2000	
È	3	ECOTOX	NOEL	121	chronic growth	120	25.0	ul/org	Growth	Topical,	Weight	house	1990	
ľ	3	ECOTOX	NOEL	-	chronic growth		50.0	mg/kg f	Growth	Food	Weight	norway	2000	
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È	3	ECOTOX	NOEL	-	chronic growth	572	100	mg/kg f	Growth	Food	Weight	norway	2000	
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Ē	3	ECOTOX	LOEL		chronic growth		100	mg/kg f	Growth	Food	Weight	norway	2000	
Ē	3	ECOTOX	LOEL	-	chronic growth	123	100	mg/kg f	Growth	Food	Weight	norway	2000	
B	3	ECOTOX	NOEL	12	chronic arowth		25.0	ul/org	Growth	Topical,	Weight	house	1990	

Safety Data





Sources of Exposure to Chemicals



Chemical Weight Fractions (CWF)

Q Search Chemical Weig	ght F	ractions												🛓 EXPO	रा र
Product Name	≡	Product Use Category	=	Categorization Subtype	=	Minimum Weight Fraction	Ξ	Maximum Weight Fraction	=	Data Type	=	Source	=	Product Coun	t =
	∇		∇		∇		∇		∇		∇		V	7	∇
48743 pah mixture		Not yet Categorized				-		-		reported		SIRI		1	^
asphalt cement penetration 60-7	70	Not yet Categorized				-		-		reported		SIRI		1	
base-neutral 4 1ml methylene ch	<u>1</u>	Not yet Categorized				-		-		reported		SIRI		1	. 1
base neutral calibration checkco.		Not yet Categorized				-		-		reported		SIRI		1	
benzo (a) pyrene_ 98%_ b1008-0	<u>)</u>	Not yet Categorized				-		-		reported		SIRI		1	
benzo (a) pyrene_ md-1956		Not yet Categorized				0.990		1.00		reported		SIRI		1	
blasocut 2000 cf art no 875		Not yet Categorized				0.00		1.00e-3		reported		SIRI		1	
blasocut 2000 universal_ 870		Not yet Categorized				-		-		reported		SIRI		1	
blasocut 2000 universal art_ 870		Not yet Categorized				0.00		1.00e-3		reported		SIRI		1	
blasocut 4000 strong_ 872		Not yet Categorized				-		-		reported		SIRI		1	
blasocut 4000 universal art_ 872		Not yet Categorized				0.00		1.00e-3		reported		SIRI		1	
clp-011a clp base/neutrals check		Not yet Categorized				-		-		reported		SIRI		1	-

What about PFAS?



9

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Chemical Details

Perfluorooctanesulfonic acid 1763-23-1 | DTXSID3031864 Searched by DTXSID3031864.

Details



Wikipedia

Perfluorooctanesulfonic acid (PFOS) (conjugate base perfluorooctanesulfonate) is an anthropogenic (human-made) fluorosurfactant, now regarded as a global pollutant. PFOS was the key ingredient in Scotchgard, a fabric protector made by 3M, and related stain repellents. In many contexts, PFOS refers to the parent sulfonic acid and its various salts of perfluorooctanesulfonate. These are all colorless or white, water soluble solids. Although of low acute toxicity, PFOS has

Read more



Are there Similar Compounds?





Relationships in the data



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Markush Chemicals



• PFOS is a member of linear perfluoroalkyl sulfonates

Perfluoroalkyl sulfonates NOCAS_892979 | DTXSID70892979 Searched by DSSTox Substance Id.



...and their Markush Children...



• Linear perfluoroalkyl sulfonates has children...





Bioactivity Data





Add to Export

RIS



ToxCast Chemical Landscape: Paving the Road to 21st Century Toxicology

Ann M. Richard^{*†}, Richard S. Judson[†], Keith A. Houck[†], Christopher M. Grulke[†], Patra Volarath[‡], Inthirany Thillainadarajah[§], Chihae Yang^{∥⊥}, James Rathman^{⊥#}, Matthew T. Martin[†], John F. Wambaugh[†], Thomas B. Knudsen[†], Jayaram Kancherla[⊽], Kamel Mansouri[⊽], Grace Patlewicz[†], Antony J. Williams[†], Stephen B. Little[†], Kevin M. Crofton[†], and Russell S. Thomas[†]

View Author Information $^{\sim}$

Cite this: Chem. Res. Toxicol. 2016, 29, 8, 1225–	Article Views	Altmetric	Citations	Share
251 Publication Date: July 1, 2016 ~	6687	36	244	
https://doi.org/10.1021/acs.chemrestox.6b00135	LEARN AI	TRICS	\bigcirc	

ToxCast/Tox21 Data





Full transparency in terms of data



Concentration Response data

Concentration Response Data

Analytical Data on Tox21 Browser 🗹

🛓 export 👻

	Name 1	■ Description	=	Endpoint Name	=	Active	=	Deta	Rep	All P	Gene	=	Intended Target 📃	Cell Line 📃	Cell For	=
		2	V		7		7					7	V			∇
		ACEA Pierrienses		ACEA AD appoint 90hr		leasti is			الاما	-	40		stavaidal		colline	
	ASSAT SOURCE. ACEA	ACLA DIOSCIETICES		ACEA_AR_agonist_boni		macuve			<u> </u>	-	AK		Steroidai	prostate	centine	
	ASSAY SOURCE: ACEA	ACEA Biosciences		ACEA_AR_agonist_AUC_viability		Active		E .	2	⊞	null		cytotoxicity	prostate	cell line	
	ASSAY SOURCE: ACEA	ACEA Biosciences		ACEA_AR_antagonist_80hr		Active		È	₩.	⊞	AR		steroidal	prostate	cell line	
	ASSAY SOURCE: ACEA	ACEA Biosciences		ACEA_AR_antagonist_AUC_viability		Active		=	2	⊞	null		cytotoxicity	prostate	cell line	
	ASSAY SOURCE: ACEA	ACEA Biosciences		ACEA_ER_80hr		Active		=	.~	⊞	ESR1		steroidal	breast	cell line	
	ASSAY SOURCE: ACEA	ACEA Biosciences		ACEA_ER_AUC_viability		Inactive		Ê	₩.	⊞	null		cytotoxicity	breast	cell line	
	ASSAY SOURCE: APR	Apredica		APR_HepG2_CellCycleArrest_1h_dn		Inactive		Ê	₩.	⊞	null		proliferation	liver	cell line	
	ASSAY SOURCE: APR	Apredica		APR_HepG2_CellCycleArrest_1h_up		Inactive		È	~	⊞	null		arrest	liver	cell line	
	ASSAY SOURCE: APR	Apredica		APR_HepG2_CellCycleArrest_24h_d	In	Inactive		Ľ	~	⊞	null		proliferation	liver	cell line	
	ASSAY SOURCE: APR	Apredica		APR_HepG2_CellCycleArrest_24h_u	ıp	Inactive		Ľ	<u>⊷</u>	⊞	null		arrest	liver	cell line	
	ASSAY SOURCE: APR	Apredica		APR_HepG2_CellCycleArrest_72h_d	In	Inactive			<u>⊷</u>	⊞	null		proliferation	liver	cell line	
	ASSAY SOURCE: APR	Apredica		APR_HepG2_CellCycleArrest_72h_u	ıр	Inactive		È	<u>⊷</u>	⊞	null		arrest	liver	cell line	
	ASSAY SOURCE: APR	Apredica		APR_HepG2_CellLoss_1h_dn		Inactive		È	~	⊞	null		cytotoxicity	liver	cell line	
	ASSAY SOURCE: APR	Apredica		APR_HepG2_CellLoss_1h_up		Inactive		Ľ	₩.	⊞	null		proliferation	liver	cell line	-
																•
Ro	ws: 1.398						Total	Rows: 1.3	98							

Full access to concentration-response curves





Use Models Derived from the Data



Screening Chemicals for Estrogen Receptor Bioactivity Using a Computational Model

Article Views

3796

Altmetric

27

LEARN ABOUT THESE METRICS

Citations

157

Patience Browne^{*†}, Richard S. Judson[‡], Warren M. Casey[§], Nicole C. Kleinstreuer^{II}, and Russell S. Thomas[‡]

View Author Information \sim

 Cite this: Environ. Sci. Technol. 2015, 49, 14, 8804– 8814
 Publication Date: June 12, 2015 v https://doi.org/10.1021/acs.est.5b02641

Vol. 124, No. 7 | Research

CERAPP: Collaborative Estrogen Receptor Activity Prediction Project

Kamel Mansouri, Ahmed Abdelaziz, Aleksandra Rybacka, Alessandra Roncaglioni, Alexander Tropsha, Alexandre Varnek, Alexey Zakharov, Andrew Worth, Ann M. Richard, Christopher M. Grulke, Daniela Trisciuzzi, Denis Fourches, Dragos Horvath, Emilio Benfenati, Eugene Muratov, Eva Bay Wedebye, Francesca Grisoni, Giuseppe F. Mangiatordi, <u>... See all authors</u> V

Published: 1 July 2016 https://doi.org/10.1289/ehp.1510267 Cited by: 76

Development and Validation of a Computational Model for Androgen Receptor Activity

Nicole C. Kleinstreuer^{*†}, Patricia Ceger[‡], Eric D. Watt[§], Matthew Martin[§], Keith Houck[§], Patience Browne^{II}, Russell S. Thomas[§], Warren M. Casey[†], David J. Dix[⊥], David Allen[‡], Srilatha Sakamuru[#], Menghang Xia[#], Ruili Huang[#], and Richard Judson[§]

View Author Information ~

♥ Cite this: Chem. Res. Toxicol. 2017, 30, 4, 946–964
Publication Date: November 18, 2016 ∨
https://doi.org/10.1021/acs.chemrestox.6b00347
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Vol. 128, No. 2 Research

CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity

Kamel Mansouri , Nicole Kleinstreuer, Ahmed M. Abdelaziz, Domenico Alberga, Vinicius M. Alves, Patrik L. Andersson, Carolina H. Andrade, Fang Bai, Ilya Balabin, Davide Ballabio, Emilio Benfenati, Barun Bhhatarai, Scott Boyer, Jingwen Chen, Viviana Consonni, Sherif Farag, Denis Fourches, Alfonso T. García-Sosa, Paola Gramatica, Francesca Grisoni, <u>... See all authors</u>

Published: 7 February 2020 | CID: 027002 | https://doi.org/10.1289/EHP5580 | Cited by: 2



Searching Literature and the Internet

Literature Searching



Literature - PubMed Abstract Sifter

Abstract Sifter Instructions

 Select PubMed starting point query
Hazard 🗸
Choose 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, enter any PubMed query or edit the query from step 1 ("50-32-8" OR "Benzo(a)pyrene") AND (NOAEL OR NOEL OR LOEL OR Rfd OR "reference dose" OR "reference concentration" OR "adverse effect level"[tiab] OR "cancer slope factor"[tiab])



- Real-time retrieval of data from PubMed ~30 million abstracts and growing)
- Choose from set of pre-defined queries
- Adjust and fine tune queries based on interests

Literature Searching



- "Sifting" of results using multiple terms
- Frequency counting terms
- Color highlighting of terms
- Download list to Excel
- Send list to PubMed for downloading ref. file
- Direct link via PubMed ID



What's the best way to search the internet for chemical data?



- We know how complex chemicals identifiers are...
 - CASRN(s)
 - Hundreds of names (maybe)
 - SMILES
 - InChIs
 - EINECS, EC numbers
- What can WE do to help you navigate the internet?

External Links – Also use Identifiers Names, CASRN, PubChem IDs, InChIs.



Benzo(a)pyrene 50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

General

- (a) EPA Substance Registry Service
- PubChem
- Chemspider
- () CPCat
- 🥖 DrugBank
- W Wikipedia
- Q MSDS Lookup
- ChEMBL
- toxPlanet
- ACS Reagent Chemicals
- 🌞 Wolfram Alpha
- 🔀 ECHA Infocard
- ChemAgora
- Consumer Product Information Database
- ChEBI
- NIST Chemistry Webbook
- **WEBWISER**
- PubChem Safety Sheet

PubChem: Chemical Vendors

Consumer Product Information Database

Toxicology

ACToR

- оң DrugPortal
- CCRIS
- ChemView
- CTD
- eChemPortal
- Gene-Tox
- HSDB
- ACToR PDF Report
- CREST
 National Air Toxics Assessment
- ChemView
- Chemical Checker
- BindingDB
- CalEPA OEHHA
- MIOSH IDLH Values
- LactMed
- ECOTOX

Publications

Toxline

- PPRTVWEB
- NH) PubMed
- IRIS Assessments
- 🖲 EPA HERO
- 🚾 NIOSH Skin Notation Profiles
- 💷 NIOSH Pocket Guide
- RSC Publications
- 🕌 BioCaddie DataMed
- Springer Materials
- Bielefeld Academic Search Engine
- CORE Literature Search
- G Google Books (Text Search)
- Google Patents (Text search)
- G Google Scholar (Text search)
- G Google Patents (Structure search)
- Google Books (Structure Search)
- G Google Scholar (Structure search)
- Federal Register

Analytical

RSC Analytical Abstracts

- 🗟 Tox21 Analytical Data
- 😬 MONA: MassBank North America
- imzCloud 🧆
- NIST IR Spectrum
- NIST MS Spectrum
- 🐗 MassBank
- NIST Antoine Constants
- IR Spectra on PubChem
- NIST Kovats Index values
- Protein DataBank
- 🍐 National Environmental Methods Index

Prediction

- 2D NMR HSQC/HMBC Prediction
- Carbon-13 NMR Prediction
- Proton NMR Prediction
- ChemRTP Predictor
- LSERD

United States Environmental Protection Agency

External Links



Links to ~90 websites providing access to additional data on the chemical of interest







Chemical Lists and Categories

A List of Lists of Chemicals

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



Q Search Chem	ical Lists			LEXPORT - COPY URL
			Showi	ng 36 of 319 Records
List Acronym 🖓	≡ List Name	# Chemicals	Updated	List Description
PFAS				Σ
EPAPFASDW537	PFAS EPA WATER: Existing EPA DW Method	19	2019-11-16	EPA has recently revised method 537.1 for the PFAS on this list to detect them in drinking water.
EPAPFASDWTREAT	PFAS EPA WATER: Drinking Water Treatment	9	2019-11-16	EPA is gathering and evaluating treatment effectiveness and cost data for removing these PFAS from drinking water systems.
EPAPFASINSOL	PFAS EPA: Chemical Inventory Insoluble in	43	2021-11-21	Per- and Polyfluoroalkyl Substances (PFASs) in EPA's expanded ToxCast chemical inventory that were determined to be insoluble in DMSO above 5mM concentration. These PFAS chemicals were successfully procured from commercial suppliers (with a small number provided by National Toxicology Program partners) but deemed unsuitable for testing due to limited DMSO solubility. For a complete list of solubilized PFAS in EPA's inventory, see https://comptox.epa.gov/dashboard/chemical-lists/EPAPFASINV
EPAPFASINV	PFAS EPA: ToxCast Chemical Inventory	430	2021-11-21	Per- and Polyfluoroalkyl Substances (PFAS) included in EPA's expanded ToxCast chemical inventory and available for testing. These PFAS chemicals were successfully procured from commercial suppliers (with a small number provided by National Toxicology Program partners) and were deemed suitable for testing (i.e., solubilized in DMSO above 5mM, and not gaseous or highly reactive). All or portions of this inventory are being made available to EPA researchers and collaborators to be analyzed and tested in various high-throughput screening (HTS) and high-throughput toxicity (HTT) assays.
				The https://comptox.epa.gov/dashboard/chemical-lists/EPAPFAS75S1 list is a prioritized subset of this larger chemical inventory.

The OECD List of PFAS

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

PFAS: Listed in OECD Global Database

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

Identifier substring search

List Details

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

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

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

Number of Chemicals: 4729

Search Results	~ <mark>~</mark>	SEND 4729 TO BATCH SEARCH	TILE INFO + FILTER +			Ł EXPORT +	
		s	howing 4729 of 4729 chemicals				
HHHHH		0 related chemical structures with this substance	~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~		HHHHH		
© 2-(N-Methylperfluoroocta	Q 1-lodo-4-(tridecafluorohex	Copolymer of 2,3,3,3-tetra DTXSID : DTXSID60882687	Q 1,1,1,2,2,3,3,4,4,5,5,6,6-Trid	🔍 🧜 Potassium perfluorooctan	و حر ا 3,4,4,5,5,6,6,7,7,8,8,9,9,10,		



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Example PFAS-UVCBs





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

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

PFAS List Paper Just Published



frontiers in Environmental Science	Toxicology, Pollution and the Environment
SECTION ABOUT ARTICLES RESEARCH TOPICS FOR	AUTHORS - EDITORIAL BOARD S A ARTICLE ALERTS
< Articles	THIS ARTICLE IS PART OF THE RESEARCH TOPIC Environmental Pollution and Toxicity of Emerging Per- and Poly View all Articles >
ORIGINAL RESEARCH article Assembly and curation of	lists of per- and
environmental science res	earch
Provisionally accepted The final version of the article will be published here soon pending final qualit	y checks Notify me
Matter Samano ⁴ , 💄 Inthirany Thillainadarajah ⁴ , Bryan Me	her Grulke ¹ , 💄 Charles N. Lowe ¹ , Gabriel Sinclair ³ , 💄 eyer ⁴ , 🌉 Grace Patlewicz ¹ and 🎆 Ann M. Richard ¹



Batch Searching

Batch Searching



- Singleton searches are great but...
- ...we generally want data on LOTS of chemicals!
- Typical questions
 - What are the structures for a set of chemical names? Set of CASRNs?
 - Can I get chemical lists in Excel files? As a list of SMILES strings? Can I get an SDF file?
 - Can I include predicted properties? OPERA? TEST?
 - Are "these chemicals" screened in Toxcast?
 - I need masses and formulae for a list of chemicals

Batch Search



Batch Search	
 Select Input Type(s) Substance Identifiers 	2 Enter Identifiers to Search (Please enter one identifier per line. Processing time increases with number of inputs.)
 Chemical Name CASRN InChIKey DSSTox Substance ID DSSTox Compound ID InChIKey Skeleton MS-Ready Formula(e) Exact Formula(e) Monoisotopic Mass 	DTXSID9020374 DTXSID9020827 DTXSID2022678 DTXSID4023381 DTXSID9044164 DTXSID7032004 DTXSID7032004 DTXSID4022361 DTXSID8021771
45% loaded	3 OF CHOOSE EXPORT OPTIONS
45 Chemicals Fo	ound from 110 Input(s)
REPLACE IDENTIFIERS WITH SELECTED CHEMICALS	
Structure DTXSID \equiv Preferred Name	\equiv CASRN \equiv Mono. Mass \equiv Mol. Formula \equiv
DTXSID2022678	90357-06-5 430.061041 <u>C18H14F4N2O4S</u>
DTXSID3020621 (R,R)-Fenvalerate	67614-33-9 419.128821 <u>C25H22CINO3</u>

Batch Search – Excel, CSV, SDF file



A DOWNLOAD EXPORT FILE

5

Batch Search



AutoSave 💽 🕅 🏷 ۲ 🖓 ۲ 🗸	CCD-Batch-Search_2022-03-27_05_36_52.xlsx ▼	♀ Search	Williams, Antony WA	⊡ - ⊡ X
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1 DTXSID PREFERRED_NAME	INCHIKEY CASRN SMILES MOLECULAR_FOR	RMULA AVERAGE_MONOISO SAFETY_D DATA_SC	NUMBER_IRIS_LINK ATMOSPH	BIOCONCE BIODEGRA BOILIN
2 DTXSID9020299 [Chlorobenzilate	RAPBNVD:510-15-6 CCOC(=0) C16H14Cl2O3	325.19 324.032 Y 15	4 16 Y 1.37E-11	477.542 4.6243 349.9
3 DTXSID6034712 Mesosulfuron-methyl	NIFKBBMC208465-21COC(=0)C C1/H21N509S2	503.5 503.0781 Y 9	5 10 1.79E-11	3.2453 4.26547 254.0
4 DIXSID/034/55 Foramsulturon		452.44 452.1114 Y 9	2.33E-11	3.84639 5.67465 265.
6 DTXSID1033004 17-Methyltestosterone	BRIVELINV 69227-76- CCCN1CC16H22N2OS	302.430 302.2240 f 14	1 42 1 38E 11	52 49 6 80035 353 7
7 DTXSID0020529 2 4-Dinitrotoluene	RMBERMI 121-14-2 CC1=C(C=(C7H6N2O4	182 135 182 0328 Y	3 379 Y 1.63E-11	9 12436 3 5609 299 8
8 DTXSID2034673 Jodosulfuron methyl este	r IUIFOMPK144550-36 [Na+].COCC14H13IN5NaO65	5 529 24 528 9529 Y	3 1 77F-11	3 51252 4 73647 265 (
9 DTXSID7024247 Pentachlorobenzene	CEOCDNV 608-93-5 CIC1=CC(CC6HCI5	250.32 247.8521 Y 17	0 84 Y 2.25E-13	5620.75 6.16855 277.0
10 DTXSID0034227 Icaridin	QLHULAH(119515-38 CCC(C)OC(C12H23NO3	229.32 229.1678 Y 11	1 67 1.82E-11	3.81105 5.17405 251.8
11 DTXSID0020440 Dichlorprop	MZHCENG 120-36-5 CC(OC1=C C9H8Cl2O3	235.06 233.985 Y 16	4 89 1.16E-11	3.54397 3.53597 298.4
12 DTXSID9034816 Monocrotophos	KRTSDMXI 6923-22-4 CNC(=O)\(C7H14NO5P	223.165 223.061 Y 15	2 274 2.77E-11	0.922318 4.13837 301.7
13 DTXSID8021301 Tamoxifen citrate	FQZYTYWI54965-24- OC(=O)CC C32H37NO8	563.647 563.2519 Y 9	0 17257 2.9E-11	1209.93 3.36316 419.3
14 DTXSID7032553 Flumetralin	PWNAWO 62924-70- CCN(CC1= C16H12ClF4N3O4	421.73 421.0452 Y 11	7 1.38E-11	35265.1 3.54617 347.7
15 DTXSID6024048 Difenzoquat metilsulfate	XQEMNBN 43222-48- COS([O-])(C18H20N2O4S	360.43 360.1144 Y 7	9 20 Y 1.93E-11	565.107 13.7793 335
16 DTXSID3024104 Fluoranthene	GVEPBJHC 206-44-0 C1=CC2=C C16H10	202.256 202.0783 Y 21	1 398 Y 4.98E-11	3528.4 147.199 393.9
17 DTXSID8023890 Asulam	VGPYEHKC 3337-71-1 COC(=O)N C8H10N2O4S	230.24 230.0361 Y 13	3 19 Y 1.21E-11	2.50573 4.63676 254.8
18 DTXSID4032532 Carfentrazone-ethyl	MLKCGVH 128639-02 CCOC(=O) C15H14Cl2F3N3O	3 412.19 411.0364 Y 13	3 9 2.16E-11	192.141 4.88739 352.4
19 DTXSID5032498 Triclosan	XEFQLINVI 3380-34-5 OC1=C(OC C12H7Cl3O2	289.54 287.9512 Y 24	6 2221 1.74E-11	52.8927 4.50619 342.3
20 DTXSID1021160 Picloram	NQQVFXU 1918-02-1 NC1=C(CI) C6H3Cl3N2O2	241.45 239.926 Y 18	6 133 Y 8.15E-12	2.72427 4.09513 296.1
21 DTXSID9020160 Bifenthrin	OMFRMAI82657-04- CC1=C(C=(C23H22ClF3O2	422.87 422.126 Y 17	2 246 Y 3.32E-11	4990.65 3.54377 370.5
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Cheminformatics "PoC Modules"





- Hazard Comparison Profiling profile chemicals based on hazard
- Alerts structure, substructure, SMARTS based alerts and flags
- Predict batch prediction using WebTEST (100s of structures)
- Search structure/substructure/similarity searches
- Standardize convert structures into QSAR/MS-Ready forms
- ToxPrints generate ToxPrint substructural fragments and profile

Module 1: Hazard Module



r d C												🛠 haz	ARD	PF	EDICT	SQ S Hazar	EARCH d assess	lly : nent prof	STANDARI
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				Toxicity:	VH - Ver	y High <mark>H</mark>	- High <mark>N</mark> Human	<mark>1</mark> - Mediu Health	um <mark>L</mark> - Lo Effects	w I - Inc	onclusive N	I/A - Not App	licable	Authority.	Authorita	Custo Emerg	m jency Re pecific S	sponse creening	Ū
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 Unlikely (0) Filters (0) Sorting (0) Structure CAS Name 	Oral	Inhalation	Dermal	Carcinogenicity	Genotoxicity Mutag	Endocrine Disruptior Reproductive	Reproductive Developmental	Repeat Exposure	Single Exposure	Repeat Exposure	Single Exposure	Skin Sensitization	Skin Irritation	Eye Irritation	Acute Aquatic Toxic	Acute Aquatic Toxic Chronic Aquatic To	Persistence	Bioaccumulation	
60-35-5 Acetamide	L	T	L	νн	VH	L	М	М	1	Т	L	Т	1	T	1	L	L	L	L
107-13-1 Acrylonitrile	н	н	н	VH	VH	L	Н	Н	н	н	Н	м	н	н	VH	н	н	н	Ľ
1912-24-9 Atrazine	М	н	L	VH	L	н	н	н	Н	м	м		н	L	М	VH	VH	Н	L



Most useful form for your needs..Excel



The Hazard Compa	arison Dash	board is a prototype tool and	l a compila	tion of inf	ormation se	ourced fro	m many sit	es, databa	ses and sou	irces includ	ling U.S. Fe	deral and	state sourc	es and inter	national	bodies that	t saves the	e user time l	oy providir	ng informati	ion in
The data are not re	eviewed by	USEPA – the user must apply	judgment i	in use of tł	ne informat	tion. The re	esults do no	ot indicate	EPA's posit	ion on the	use or regu	ulation of t	these chem	icals.							
			VH - Ve	erv High	Н-	High	M - N	1edium	L-	Low	I - Incor	nclusive	No	Data		Authorita	tive	Screening		QSAR Mor	del
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DTXSID	CAS	Name	Oral	Inhalation	Dermal	Carcinogenicity	Genotoxicity Mutagenici	Endocrine Disruption	Reproductive	Developmental	Repeat Exposure	Single Exposure	Repeat Exposure	Single Exposure	Skin Sensitization	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicit	Persistence	Biochellissen
DTXSID6020438	107-06-2	1,2-Dichloroethane	м	н	L	VH	VH	L	Н	L	Н	н	м	м	М	н	н	L	L	Н	l
DTXSID7024031	156-60-5	(E)-1,2-Dichloroethylene	М	L	L	L.	L	I	1	L	I.		М	Н	1	н	н	L		н	l
DTXSID5021380	79-00-5	1,1,2-Trichloroethane	М	м	м	VH	L	L	1	L	Н		н	Н	1	Н	м	м	м	н	1
DTXSID0020448	78-87-5	1,2-Dichloropropane	м	н	L	VH	VH	L	М	М			L	Н	Н	Н	н	м	м	Н	1
DTXSID1020437	75-34-3	1,1-Dichloroethane	м	М	1	VH	VH	L	1 I -	L	- I	Н	L	м	1	н	н	L	м	Н	1
DTXSID3020203	106-99-0	1,3-Butadiene	L	L	1 - C	VH	VH	L	Н	н			H	М	1.1	1	Н	м	L	L	1
DTXSID6020430	95-50-1	1,2-Dichlorobenzene	M	Н	L	- I	VH	н	1 I -	L	Н		Н	М	1.1	н	н	VH	VH	н	N
DTXSID0021383	79-01-6	Trichloroethylene	L	М	L	VH	VH	1	н	н	н	Н	Н	м	Н	н	н	н	VH	н	1
DTXSID8020250	56-23-5	Carbon tetrachloride	Н	н	Н	VH	VH	Н	М	L		Н	Н	Н	Н	Н	Н	м	М	Н	1
DTXSID4020533	123-91-1	1,4-Dioxane	М	M	L	VH	VH	L	1	L	н	Н	Н	м	1	н	н	н	L	Н	1
DTXSID6020856	872-50-4	N-Methyl-2-pyrrolidone	L	L	L	1 I I	L	L	Н	н	М		М	м	1.1	н	н	н		L	1

Module 2: Alerts



Hazard Cor version: UAT, bu	mparison Dashboard iild: 2021-10-26 21:27:37 UTC		HAZARD 🔇 ALERTS	🖬 predict 🕄 search 🕼 stand	DARDIZE @ TOXPRINTS
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6	50594-66-6			\diamond	bond:CX_halide_alkenyl- X_dihalo_(1_2-), bond:CX_halide_alkyl- Cl_dichloro_(1_1-), bond:CX_halide_alkyl- X_dihalo_(1_3),
10	309-00-2				bond:CX_halide_generic- X_dihalo_(1_2-)
14	82-28-0			\diamond	♦
15	3775-55-1			\$ ²	1

Module 3: WebTEST Batch Prediction





Module 4: Structure/Substructure/Similarity







- These modules, and their future updates, are presently being deployed to the public
- Intended URL is : <u>https://cheminformatics.epa.gov</u>

Summary and Conclusion



- United States Environmental Protection Agency
- CompTox Chemicals Dashboard a central hub for environmental data
 - ~900k chemical substances
 - Integrating property data, hazard data, exposure data, *in vitro* bioactivity data
 - Interrogation of bioactivity data -
 - Multiple types of searches



- Batch search for thousands of chemicals
- Real-time property and toxicity predictions
- Downloadable files CSV, TSV and Excel

Some Related Publications of Interest





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 ^a, Antony J. Williams ^a, Inthirany Thillanadarajah ^b, Ann M. Richard ^a 🙁 🖾

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Enabling High-Throughput Searches for Multiple Chemical Data Using the U.S.-EPA CompTox Chemicals Dashboard

Charles N. Lowe* and Antony J. Williams*

 ♥ Cite this: J. Chem. Inf. Model. 2021, 61, 2, 565–570

 Publication Date: January 22, 2021 ~

 https://doi.org/10.1021/acs.jcim.0c01273

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Journal of Cheminformatics

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Database Open Access Published: 28 November 2017

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

Antony J. Williams ^{CI}, <u>Christopher M. Grulke</u>, Jeff Edwards, <u>Andrew D. McEachran</u>, <u>Kamel Mansouri</u>, <u>Nancy C. Baker</u>, <u>Grace Patlewicz</u>, <u>Imran Shah</u>, John F. Wambaugh, <u>Richard S. Judson</u> & <u>Ann M. Richard</u>

Journal of Cheminformatics 9, Article number: 61 (2017) Cite this article



Environment International Volume 154, September 2021, 106566



Review article

Sourcing data on chemical properties and hazard data from the US-EPA CompTox Chemicals Dashboard: A practical guide for human risk assessment

Antony J. Williams ^a A 🖾, Jason C. Lambert ^a, Kris Thayer ^b, Jean-Lou C.M. Dorne ^c

You want to know more...



- Lots of resources available
 - Presentations: <u>https://tinyurl.com/w5hqs55</u>

🔼 YouTube

Communities of Practice Videos: <u>https://rb.gy/qsbno1</u>

Search

- Manual: <u>https://rb.gy/4fgydc</u>
- Latest News: https://comptox.epa.gov/dashboard/news_info

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Where are we now? Celebrating the 10th Incremental Release of the CompTox Chemicals Dashboard

CompTox Chemicals Dashboard primer videos

The CompTox Chemicals Dashboard is a one-stop-shop for chemistry, toxicity and exposure information for over 875,000 chemicals. Data and models within the Dashboard also help with efforts to identify chemicals of most need of further testing and reducing the use of animals in chemical testing.

Explore the wealth of data and features available in the CompTox Chemicals Dashboard with these insructional videos narrated by EPA scientists.

General Chemistry and Search Capabilities

CompTox Chemicals Dashb	oard Primer. Watch In Landau and Annual Annua
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Acknowledgments



- Contact: <u>Williams.Antony@epa.gov</u>
- Feedback and follow-up is welcomed! Your questions help
- The dashboard is based on the efforts of many more team members than us. Many collaborators provide data also.



EPA's Center for Computational Toxicology and Exposure