

### Accessing Environmental Chemistry Data via Data Dashboards

### **Antony Williams**

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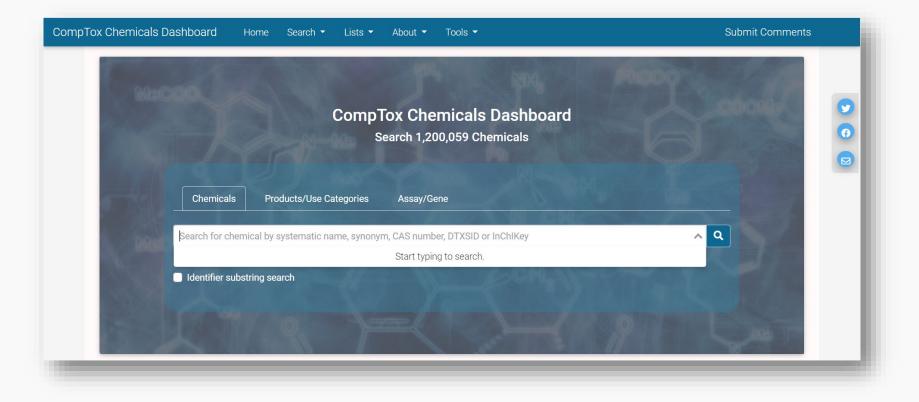
The views expressed in this presentation are those of the author and do not necessarily reflect the views or policies of the U.S. EPA



- 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 >1.2 million chemicals





### Over two decades of curation work



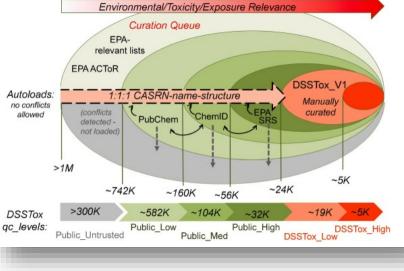


Computational Toxicology Volume 12, November 2019, 100096



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 <sup>b</sup>, Ann M. Richard ª 🙁 🖾



### **BASIC** Search



Chemic	als Product/Use Categories Assay/Gene
<b>Q</b> Benz	o(a)pyrene
<i>4</i> \$>	Benzo(a)pyrene DTXSID2020139
-93 <del>4</del> -	Benzo(a)pyrene diolepoxide 1 DTXSID9036779
с <mark>у</mark>	Benzo(a)pyrene- 7,8,9-triol,7,8,9,10-tetrahydro-, (7-alpha,8-beta,9-beta)- DTXSID00210066
3	Benzo(a)pyrene-1-methanol DTXSID40235374
ŝ	Benzo(a)pyrene-1,6-dione, 7-methyl- <i>DTXSID70229645</i>
-\$	Benzo(a)pyrene-10-methanol DTXSID20235817
ж,	Benzo(a)pyrene-10-sulfonic acid, 7,8,9,10-tetrahydro-7,8,9-trihydroxy-, (7alpha,8beta,9beta DTXSID80154378
<del>}</del>	Benzo(a)pyrene-11,12-diol DTXSID70215609
<b>2</b> 23	Benzo(a)pyrene-11,12-diol, 11,12-dihydro-, cis- DTXSID20214501

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

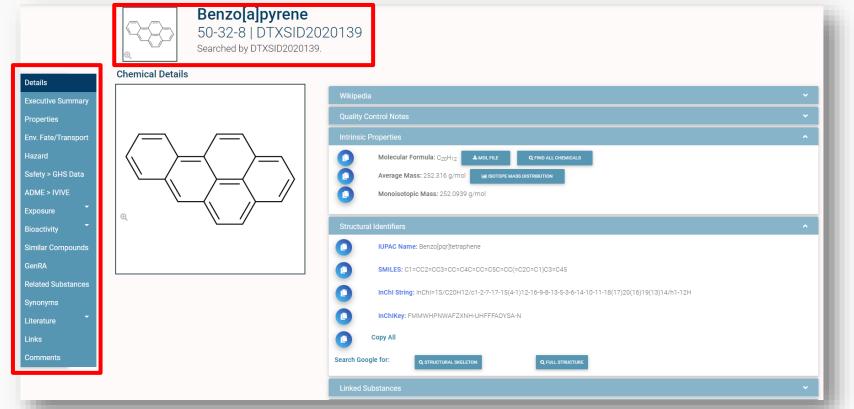
#### Search Results

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

183 chemicals

### **Detailed Chemical Pages**





Intrinsic properties, structural identifiers, linked substances

### "Executive Summary"



Executive	Summary		
Quantitative Risk Assessment Values			
IRIS values available 🗹			
No PPRTV values     EPA RSL values available C	REGION	AL SCREENING	
Minimum RID: 0.00030 mg/kg-day (chronic, IRIS, oral, 8)	Class	THQ	Value
Minimum RfC: 0.0000020 mg/m3 (chronic, IRIS, inhalation, 8) 🗹	GIABS (-)	THQ = 0.1	1
VIVE POD not calculated	ABS (-)	THQ = 0.1	0.13
Quantitative Hazard Values	MCL (ug/L)	THQ = 0.1	0.2
Minimum oral POD: 0.070 mg/kg-day (chronic, EFSA, oral, 5) 2 Minimum inhalation POD: 0.0046 mg/m3 (chronic, IRIS, Inhalation, 8) 2	MCLbased.SSL (mg/kg)	THQ = 0.1	0.24
Lowest Observed Bloactivity Equivalent Level: AR			
Cancer Information	cancer slope factor ((mg/kg-day)-1)	THQ = 0.1	1
Cancer slope factor: 23.5 (mg/kg-day)-1 (ACToR, dermal, 4)	cancer unit risk ((ug/m3)-1)	THQ = 0.1	0.0006
Inhalation unit risk: 2.4 (mg/m3)-1 (IRIS, inhalation, 8)      Carcinogenicity data available: IARC; undefinedEPA OPP cancer class: undefinedNTP Report on Carcinogens	RFDo (mg/kg-day)	THQ = 0.1	0.0003
Calcinogenicity data available. URC: Undermeder A OPP cancer class: undermeder P Report on Calcinogenis (ROC 12): undefined NLM ToxNet HSDB carcinognicity warningUniversity of Maryland carcinogenicity warning;	RIFCi (mg/m3)	THQ = 0.1	0.000002
No genotoxicity findings reported	Resident.soil (mg/kg)	THQ = 0.1	0.11
Reproductive Toxicology	Industrial.soil (mg/kg)	THC = 0.1	2.1
Reproductive toxicity PODs available C	Residen air (ug/m3)	THQ = 0.1	0.00021
Chronic Toxicology	Industrial air ug/m3)	THQ = 0.1	0.00088
Chronic toxicity PODs available C	Tapwater (ug/L)	THQ = 0.1	0.025
Subchronic Toxicology			
Subchronic toxicity PODs available C	Riskbased.SSL (mg/k)	THQ = 0.1	0.029
Developmental Toxicology	GIABS (-)	THQ = 1	1
8 No developmental toxicity data available.	ABS (-)	THQ = 1	0.13
Acute Toxicology	MCL (ug/L)	THQ = 1	0.2
Acute toxicity PODs available 🗷	MCLbased.SSL (mg/kg)	THQ = 1	0.24
Subacute Toxicology	cancer slope factor ((mg/kg-day)-1)	THQ = 1	1
No subacute toxicity data available.	cancer unit risk ((ug/m3)-1)	THQ = 1	0.0006
Neurotoxicology	RFDo (mg/kg-day)	THQ = 1	0.0003
8 No neurotoxicology data available.		THQ = 1	0.00002
Endocrine System	RFCI (mg/m3)		
Endocrine Disruption Potential. Significant Estrogen Receptor activity seen. Chemical was positive in 7 ER assays	Resident soil (mg/kg)	THQ = 1	0.11
(out of 12) and was positive in 3 AR assays (tested in 6).	Industrial.soil (mg/kg)	THQ = 1	2.1
ADME	Resident.air (ug/m3)	THQ = 1	0.0017
😵 No HTTK data	Industrial.air (ug/m3)	THQ =	0.0088
Fate and Transport	Tapwater (ug/L)	THQ = 1	0.025
No bloaccumulation concern.	Riskbased.SSL (mg/kg)	THQ = 1	0.029
<ul> <li>No volatility concern.</li> <li>Biodegradation predictions are available C<sup>*</sup></li> </ul>	· · · · · · · · · · · · · · · · · · ·		
BCF predictions are available 🖾			$\mathbf{X}$
🔇 Vapor Pressure predictions are available 🗹	• PUVOQU		$\mathbf{X}$
Exposure	GPHYSCH	EM PARAMETERS	$\sim$
Exposure Estimates have been predicted using the SEEM modeling methodology 2 <sup>*</sup>	640	3.04 .826	
AOP Information	6.13	-8.26	
AOP Links: 36, 61, 66, 107, 150, 163, 187, 200	-5 0 5 10 15 -5 0	5 10 15	4 -2 0 2
Other Notes	logP	log(BCF)	log(VP)
No water quality values available.			
18 Air quality values available.     Consumitional expension available.			
Occupational exposure values available.			

#### Overview of toxicity-related info

- Quantitative values
- Info re. toxicology subsets
- Physchem. and Fate & Transport
- Adverse Outcome Pathway links
- In vitro bioactivity summary plot

# Quantitative Risk Assessment Values IRIS values available I No PPRTV values EPA RSL values available I Minimum RfD: 0.00030 mg/kg-day (chronic, IRIS, oral, 8) I Minimum RfC: 0.0000020 mg/m3 (chronic, IRIS, inhalation, 8) I IVIVE POD not calculated Quantitative Hazard Values Minimum oral POD: 0.070 mg/kg-day (chronic, EFSA, oral, 5) I Minimum inhalation POD: 0.0046 mg/m3 (chronic, IRIS, inhalation, 8) I

S Lowest Observed Bioactivity Equivalent Level: AR

### **Experimental and Predicted Data**



50-32	ZO(a)pyrene 2-8   DTXSID202 by DSSTox Substance Id.	20139
Download      Columns     Property	<ul> <li>Experimental average</li> </ul>	✓ Predicted average
Water Solubility	8.40e-9 (4)	1.75
LogKow: Octanol-Water	6.13 (2)	6.24
Vapor Pressure	5.49e-9 (1)	3.61e-9
Boiling Point	495 (3)	480
Henry's Law	4.57e-7 (1)	4.59e-7
Melting Point	177 (8)	189
Surface Tension	-	53.9
Flash Point	-	234

- Physchem and Fate & Transport experimental and predicted data
- Data can be downloaded as Excel, TSV and CSV files
- Predictions: multiple algorithms
  - EPI Suite: Estimation Program Interface
  - ACD/Labs (commercial)
  - TEST: Toxicity Estimation Software
     Tool
  - OPERA: OPEn structure—activity/ property Relationship App

### **Chemical Hazard Data**



### ToxVal Database

- ~30k chemicals
- >1M tox. values
- 46 sources of data
- 220 journals cited
- ~50k citations



#### Bisphenol A 80-05-7 | DTXSID7020182 Searched by Expert Validated Synonym.

#### Hazard: Point of Departure

	int of Depa	rture		~ Q	Search Hazard								iuman (	) ec
<b>4</b> , E	XPORT -													
e	Priority 1	Source =	Туре	$\equiv$ Subtype $\equiv$	Risk Assessment	$\equiv$ Qualifier	Value	≡ Units	Study Type 🛛 🚍	Exposure Route =	Critical effect	≡ Species	≡ Year	
	1	IRIS	LOAEL	-	chronic	=	50.0	mg/kg-day	-	oral	reduced mean body weight	-	2020	
ì	з	ECHA eChemPor	NOAEL		developmental	=	0.200	mg/kg-day	developmental	oral	-	rat	2001	
1	з	ECHA eChemPor	NOAEL	-	developmental	-	0.200	mg/kg-day	developmental	oral	-	rat	2001	
L	з	ECHA eChemPor	NOAEL	-	reproduction	=	0.200	mg/kg-day	reproduction	oral	ft	rat	2001	
	3	ECHA eChemPor	NOAEL		reproduction	=	0.200	mg/kg-day	reproduction	oral	-	rat	2001	
Ľ	з	ECHA eChemPor	NOAEL	-	reproduction	-	0.200	mg/kg-day	reproduction	oral	-	rat	2001	
Ľ	з	ECHA eChemPor	LOAEL	-	short-term	-	600	mg/kg-day	short-term	oral	-	rat	2002	
Ľ	з	ECHA eChemPor	NOEL	-	repeat dose	-	30.0	ppm	repeat dose	oral	systemic	mouse	2007	
Ľ	з	ECHA eChemPor	NOAEL	-	repeat dose	-	300	ppm	repeat dose	oral	systemic	mouse	2007	
Ē	з	ECHA eChemPor	NOEL	-	repeat dose	-	75.0	ppm	repeat dose	oral	systemic	rat	2000	
Ľ	3	ECHA eChemPor	NOAEL	-	repeat dose	=	750	ppm	repeat dose	oral	systemic	rat	2000	
								Total Rows: 224			centrilobular			

### Hazard Data for Copper

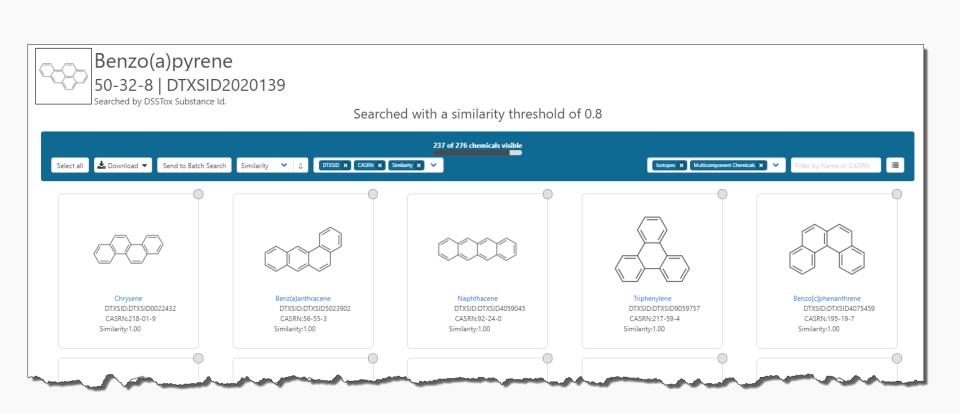


### 2246 rows of human/eco hazard data

1	SOURCE	SUB_SOU	FTOXVAL_T	TOXVAL_TYPE_ORIGINAL	TOXVAL_TYPE_SUF	TOXVAL_	TQUALIFIEF	TOXVAL_N		TOXVAL_U	TOXVAL_U	RISK_ASSE
2	ATSDR MRLs 2020	CDC	MRL	ATSDR MRL	Toxicity Value	MRL	=	0.01		mg/kg-da	mg/kg/da	acute
3	ATSDR MRLs 2020	CDC	NOAEL	NOAEL	Point of Departure	NOAEL	=	0.03	0.03	mg/kg-da	mg/kg/da	acute
4	California DPH	California	MCL	MCL California	Exposure Limit	MCL	=	1.3	1.3	mg/L	mg/L	chronic
5	California DPH	California	MCL	MCL Federal	Exposure Limit	MCL	=	1.3		mg/L	mg/L	chronic
6	California DPH	California	OEHHA PH	OEHHA PHG	Exposure Limit	Public Hea	a =	0.3	0.3	mg/L	mg/L	chronic
7	Cal OEHHA	California	MCL	MCL	Exposure Limit	MCL	=	1.3	1.3	mg/L	mg/L	chronic
8	Cal OEHHA	California	REL	REL	<b>Toxicity Value</b>	REL	=	100 1	100	ug/m3	ug/m3	acute
9	Copper Manufacturers	Copper D	eadequate	AI (adequate intake)			=	0.4	.4 .4	mg/day	mg/day	chronic
10	Copper Manufacturers	Copper D	eadequate	AI (adequate intake)			=	0.7		mg/day	mg/day	chronic
11	Copper Manufacturers	Copper D	eadequate	AI (adequate intake)			=	1 1	1	mg/day	mg/day	chronic
12	Copper Manufacturers	Copper D	eadequate	AI (adequate intake)			=	1.1	1.1	mg/day	mg/day	chronic
13	Copper Manufacturers	Copper D	eadequate	AI (adequate intake)			=	1.3	1.3	mg/day	mg/day	chronic
14	Copper Manufacturers	Copper D	eadequate	AI (adequate intake)			=	1.5	1.5	mg/day	mg/day	chronic
15	Copper Manufacturers	Copper D	eadequate	AI (adequate intake)			=	1.6	1.6	mg/day	mg/day	chronic
16	Copper Manufacturers	Copper D	edrinking w	GDWQ (guideline for drink	king water quality)		=	2 2		mg/L	mg/L	chronic
17	Copper Manufacturers	Copper D	<b>ELOAEL</b>	LOAEL	Point of Departure	LOAEL	=	7	7	mg/day	mg/day	subchroni
18	Copper Manufacturers	Copper D	eoptimal in	Optimal intake value	<b>Misc Information</b>	Optimal in	n =	2.6	2.6	mg/day	mg/day	chronic
19	Copper Manufacturers	Copper D	e RDA	RDA (recommended dieta	ry allowance)		=	0.2	).2	mg/day	mg/day	chronic
20	Copper Manufacturers	Copper D	e RDA	RDA (recommended dieta	ry allowance)		=	0.34	0.34	mg/day	mg/day	chronic
21	Copper Manufacturers	Copper D	e RDA	RDA (recommended dieta	ry allowance)		=	0.7		mg/day	mg/day	chronic
	Cover Sheet   Main	Data To	xval Detail	s (+)				: •		<b>,</b>	,.	

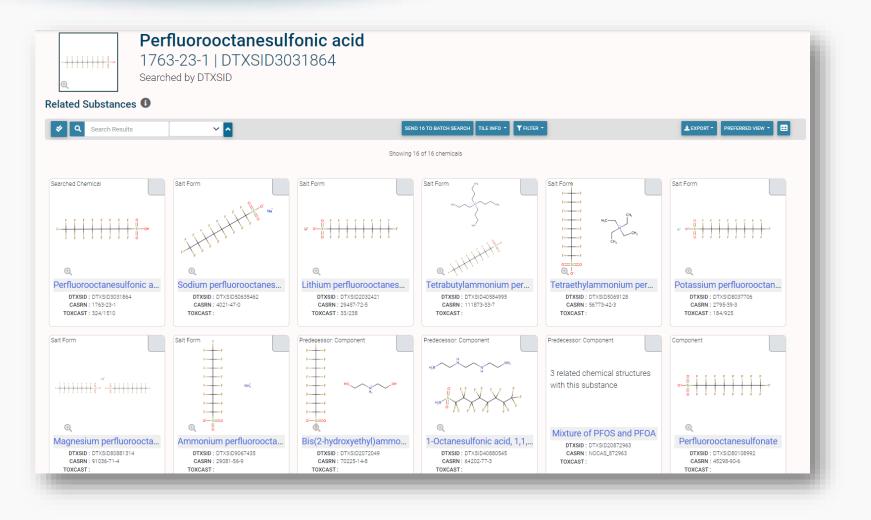
### Similarity Searching





### **Related Substances**







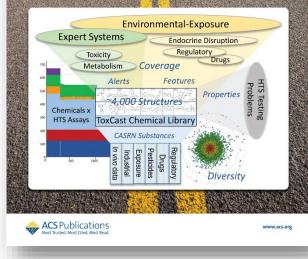
## **Bioactivity Data**

### ToxCast





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



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

Ann M. Richard<sup>\*†</sup>, Richard S. Judson<sup>†</sup>, Keith A. Houck<sup>†</sup>, Christopher M. Grulke<sup>†</sup>, Patra Volarath<sup>‡</sup>, Inthirany Thillainadarajah<sup>§</sup>, Chihae Yang<sup>II, J</sup>, James Rathman<sup>1,#</sup>, Matthew T. Martin<sup>†</sup>, John F. Wambaugh<sup>†</sup>, Thomas B. Knudsen<sup>†</sup>, Jayaram Kancherla<sup>v</sup>, Kamel Mansouri<sup>v</sup>, Grace Patlewicz<sup>†</sup>, Antony J. Williams<sup>†</sup>, Stephen B. Little<sup>†</sup>, Kevin M. Crofton<sup>†</sup>, and Russell S. Thomas<sup>†</sup>

#### View Author Information $\sim$

 ♥ Cite this: Chem. Res. Toxicol. 2016, 29, 8, 1225– 1251
 Publication Date: July 1, 2016 ∨ https://doi.org/10.1021/acs.chemrestox.6b00135



LEARN ABOUT THESE METRICS

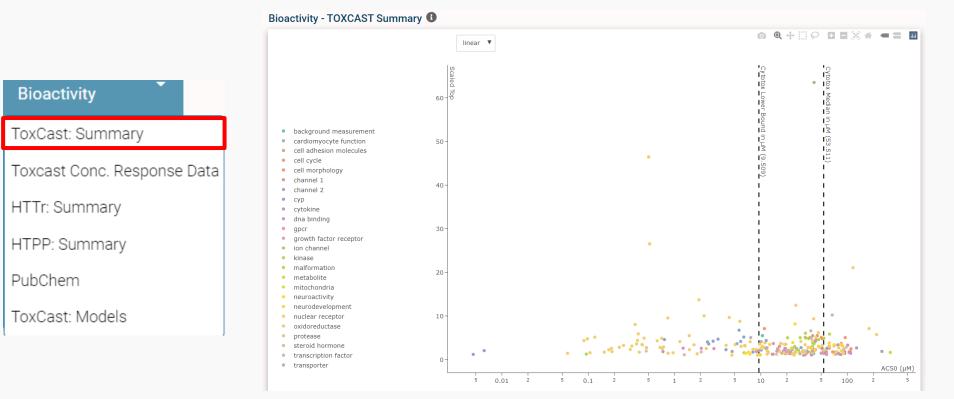
Share

Add to Export

### Bioactivity Data

Summary views of >2000 Assay Endpoints





### Bioactivity Data Full transparency of data...



#### Concentration Response Data 🖲

Analytical Data on Tox21 Browser 🗹

🛃 EXPORT 👻

#### **Bioactivity**

#### ToxCast: Summary

Toxcast Conc. Response Data

HTTr: Summary

HTPP: Summary

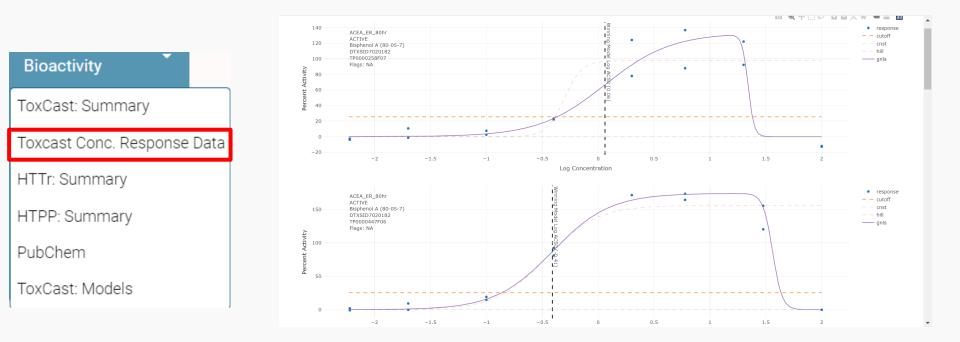
PubChem

ToxCast: Models

Name	ve ↑	=	Description	≡	Endpoint Name		Active	=	Details	Rep. Plot	All Plots	Gene	=	Intended Target	$\equiv$ Cell Line	≡ Cell Fo	mat 🗄
		$\nabla$		$\nabla$		₽		$\nabla$					V		♥	7	
ASS	SAY SOURCE: ACEA		ACEA Biosciences		ACEA_AR_agonist_80hr		Inactive		6	₩.	⊞	AR		steroidal	prostate	cell li	ne
ASS	SAY SOURCE: ACEA		ACEA Biosciences		ACEA_AR_agonist_AUC_viability		Active		6	₩.	<b>=</b>	-		cytotoxicity	prostate	cell li	ne
ASS	SAY SOURCE: ACEA		ACEA Biosciences		ACEA_AR_antagonist_80hr		Active		E .	₩.	⊞	AR		steroidal	prostate	cell li	ne
ASS	SAY SOURCE: ACEA		ACEA Biosciences		ACEA_AR_antagonist_AUC_viability		Active		Ē.	₩.	<b>=</b>	-		cytotoxicity	prostate	cell li	he
ASS	SAY SOURCE: ACEA		ACEA Biosciences		ACEA_ER_80hr		Active		6	<b>₩</b>	Ħ	ESR1		steroidal	breast	cell li	ne
ASS	SAY SOURCE: ACEA		ACEA Biosciences		ACEA_ER_AUC_viability		Inactive			M	Ħ			cytotoxicity	breast	cell li	ne
ASS	SAY SOURCE: APR		Apredica		APR_HepG2_CellCycleArrest_1h_dn		Inactive		1	2	<b>=</b>	-		proliferation	liver	cell li	ne
ASS	SAY SOURCE: APR		Apredica		APR_HepG2_CellCycleArrest_1h_up		Inactive		Ē.	M	Ħ	-		arrest	liver	cell li	he
ASS	SAY SOURCE: APR		Apredica		APR_HepG2_CellCycleArrest_24h_dn		Inactive			2	<b>=</b>	÷		proliferation	liver	cell li	he
ASS	SAY SOURCE: APR		Apredica		APR_HepG2_CellCycleArrest_24h_up		Inactive		6	₩.	<b>=</b>	-		arrest	liver	cell li	ne
ASS	SAY SOURCE: APR		Apredica		APR_HepG2_CellCycleArrest_72h_dn		Inactive		Ē.	M	æ	-		proliferation	liver	cell li	he
ASS	SAY SOURCE: APR		Apredica		APR_HepG2_CellCycleArrest_72h_up		Inactive		-	₩.	<b>=</b>	-		arrest	liver	cell li	ne
ASS	SAY SOURCE: APR		Apredica		APR_HepG2_CellLoss_1h_dn		Inactive		Ē.	₩.	<b>=</b>	-		cytotoxicity	liver	cell li	he
ASS	SAY SOURCE: APR		Apredica		APR_HepG2_CellLoss_1h_up		Inactive			E.	<b>=</b>	-		proliferation	liver	cell li	ne
ASS	SAY SOURCE: APR		Apredica		APR_HepG2_CellLoss_24h_dn		Active		6	E.	<b>=</b>			cytotoxicity	liver	cell li	ne -

## Bioactivity Data ... including concentration-response





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



#### 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
- FCHA Infocard
- ChemAgora
- Consumer Product Information Database
- ChEBI
- NIST Chemistry Webbook
- **WEBWISER**
- PubChem Safety Sheet
- Consumer Product Information Database
- PubChem: Chemical Vendors

#### Toxicology

- ACToR OH DrugPortal
- CCRIS
- ChemView
- CTD eChemPortal
- Gene-Tox
- ACToR PDF Report
- CREST
- National Air Toxics Assessment
- FCOTOX
- ChemView
- Chemical Checker
- BindingDB
- INIOSH IDLH Values
- actMed
- € FCOTOX

Publications

#### Toyline

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

#### Analytical

- RSC Analytical Abstracts
- A Tox21 Analytical Data
- MONA: MassBank North America
- area mzCloud
- NIST IR Spectrum
- NIST MS Spectrum

#### Prediction

- 2D NMR HSQC/HMBC Prediction
- Carbon-13 NMR Prediction
- Proton NMR Prediction
- ChemRTP Predictor
- € LSERD
- MassBank
- NIST Antoine Constants
- IR Spectra on PubChem
- NIST Kovats Index values
- Protein DataBank
- National Environmental Methods Index

### **External Links**



Print 🖨 👘 English 🗸



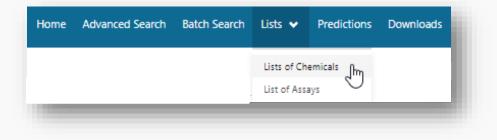
Links to ~90 websites providing access to additional data on the chemical of • interest 

BETTER POLIC	IES FOR BETTER LIVES								
	e	Cheml	Portal				Infor	al Portal t mation o Substance	n
Home	Substance Search	Property Search		Schedules of Assessments	Data sources	About 🝷	Help 🕶	Contact Us	
	hemical S	ubstance	Search						
Substa	nce (50-32-8)								*
Source	s and type of info	ormation							^
Select all	Deselect all								
Types (	D		Data sources						
Prope	erty information		ACTOR <sup>0</sup>	AGRITO	X 0	<b>~</b> A	ICIS assessm	ents O	
🔽 Expo	sure and use information		APVMA-CR 🔍	CCR 🔍		C	ESAR <sup>0</sup>		
GHS of	classifications		Chemicals Dashbo	oard <sup>0</sup> ChemIn	fo <sup>0</sup>	C	ombined Exp	osures <sup>0</sup>	



## Chemical Lists and Categories

### **Example: PFAS Structure Lists**



United States Environmental Protection

### **Example: PFAS Structure Lists**

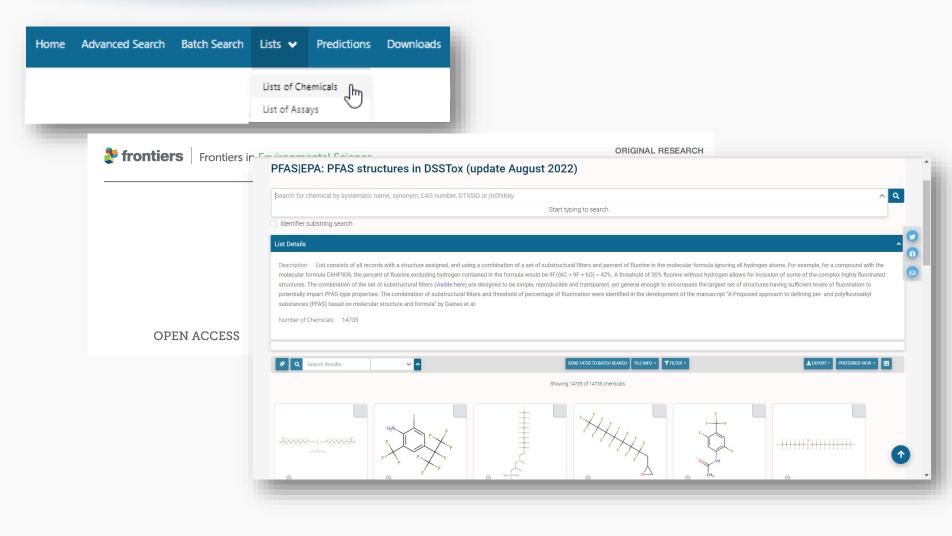
**OPEN ACCESS** 

Home	Advanced Search	Batch Search	Lists 🗸	Predictions	Downloads					
			Lists of Ch	4'')						
	frontie	<b>rs</b> Frontiers in	n Environmo	ental Science				doi: 1	<b>L RESE</b> 1: 05 April 1s.2022.85	20
				-	and C Polyflu					-

#### Per- and Polyfluoroalkyl Substance (PFAS) to Support Environmental Science Research

Antony J. Williams<sup>1</sup>\*, Linda G. T. Gaines<sup>2</sup>, Christopher M. Grulke<sup>1†</sup>, Charles N. Lowe<sup>1</sup>, Gabriel F. B. Sinclair<sup>3</sup>, Vicente Samano<sup>4</sup>, Inthirany Thillainadarajah<sup>4</sup>, Bryan Meyer<sup>4</sup>, Grace Patlewicz<sup>1</sup> and Ann M. Richard<sup>1</sup> invironmental Protection

### **Example: PFAS Structure Lists**



Environmental Protection

### **PFAS** lists of Chemicals



			Select I	ist
Download       Columns         List Acronym       List Name       Last Updated       Number of Chemicals       List Description         FPAPFAS7551       PFAS[EPA: List of 75 Test       2018-06-29       74       PFAS list corresponds to 75 samples (Set 1) submitted for initial testing screens conducted by EPA researchers in collaboration with researchers at the National Toxicology Program.         EPAPFAS7552       PFAS[EPA: List of 75 Test       2019-02-21       75       PFAS list corresponds to a second set of 75 samples (Set 2) submitted for testing screens conducted by EPA researchers in collaboration with researchers at the National Toxicology Program.         EPAPFASCAT       PFAS[EPA: List of 75 Test]       2018-06-29       64       List of registered DSSTox "category substances" representing PFAS categories created using ChemAxon's Markush structure-based query representations.         EPAPFASINSOL       PFAS[EPA: ToxCast]       2018-06-29       43       PFAS chemicals included in EPA's expanded ToxCast chemical inventory found to be insoluble in DMSO above 5mM.         EPAPFASINV       PFAS[EPA: ToxCast]       2018-06-29       430       PFAS chemicals included in EPA's expanded ToxCast chemical inventory and available for testing.         EPAPFASINV       PFAS[EPA: ToxCast]       2017-11-16       199       PFAS (Per- & Poly-fluorinated alkyl substances) compiled from various internal, literature and public sources by EPA researchers and program office representatives.         EPAPFASENI       PFAS: List				
List Acronym \$	List Name 🗘	Last Updated 🗢	Number of Chemicals 🕈	List Description \$
EPAPFAS75S1		2018-06-29	74	conducted by EPA researchers in collaboration with researchers at the National
EPAPFAS75S2		2019-02-21	75	screens conducted by EPA researchers in collaboration with researchers at the
EPAPFASCAT		2018-06-29	64	
EPAPFASINSOL	Inventory Insoluble in	2018-06-29	43	
EPAPFASINV		2018-06-29	430	
EPAPFASRL		2017-11-16	199	PFAS (Per- & Poly-fluorinated alkyl substances) compiled from various internal, literature and public sources by EPA researchers and program office
PFASKEMI	PFAS: List from the Swedish Chemicals Agency (KEMI) Report	2017-02-09	2416	Perfluorinated substances from a Swedish Chemicals Agency (KEMI) Report on the occurrence and use of highly fluorinated substances.
PFASMASTER	PFAS Master List of PFAS Substances	2018-07-26	5061	PFASMASTER is a consolidated list of PFAS substances spanning and bounded by the below lists of current interest to researchers and regulators worldwide.
PFASOECD	PFAS: Listed in OECD Global Database	2018-05-16	4729	OECD released a New Comprehensive Global Database of Per- and Polyfluoroalkyl Substances, (PFASs) listing more than 4700 new PFAS
PFASTRIER	PFAS Community- Compiled List (Trier et al., 2015)	2017-07-16	597	PFASTRIER community-compiled public listing of PFAS (Trier et al, 2015)

10 ......

### MTOX biomarkers



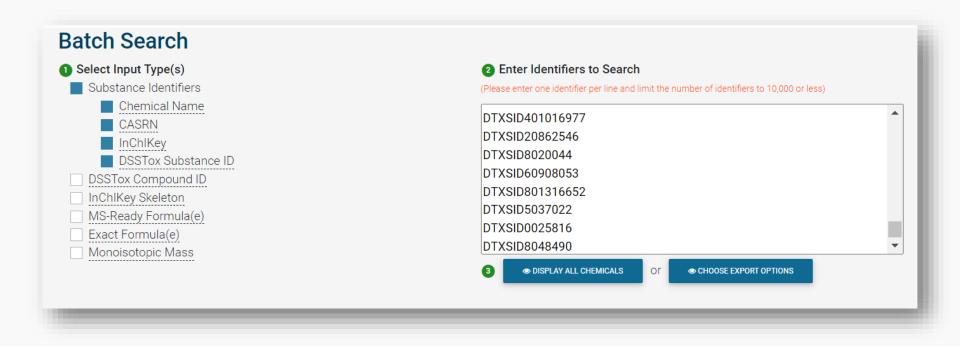
1Tox700+ metabo	lic biomarkers				
Search for chemical by systema	tic name, synonym, CAS number, DTX	SID or InChIKey			<u>୍</u> ବ
Identifier substring search					
.ist Details					
Description: List of metabolic binner of Chemicals: 627	omarkers associated with the publication	"Knowledge-Driven Approaches to Crea	te the MTox700+ Metabolite Panel for F	redicting Toxicity" authored by Viant et	: al.
Search Results	~ ^		SEND 1000 TO BATCH SEARCH TILE INFO - T	ALTER -	LEXPORT - PREFERRED VIEW - E
	CH Q				
Cholic acid	(8Z,11Z,14Z)-8,11,14-Eico DTXSID : DTXSID00912351	Uroporphyrin III DTXSID : DTXSID70896977	Cyclic AMP DTXSID : DTXSID8040436	L-Valine DTXSID : DTXSID40883233	5-Methylcytosine DTxsib:DTXSID50203948



## **Batch Searching**

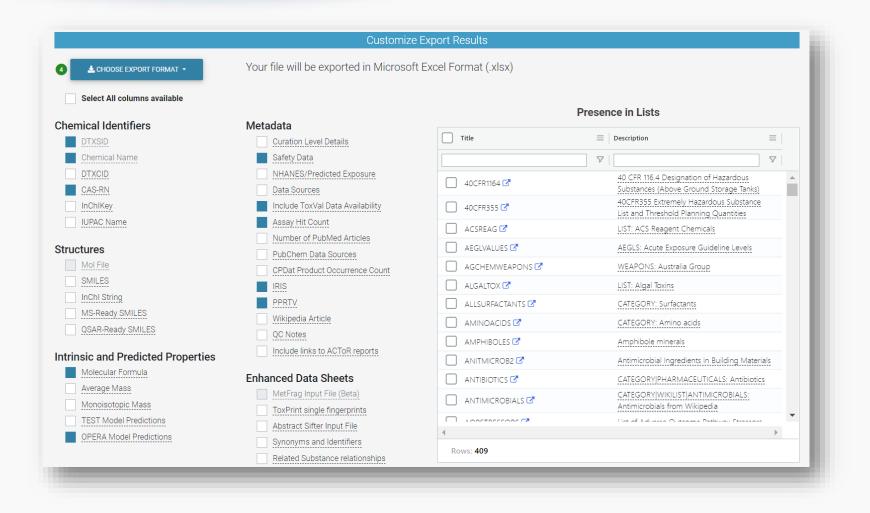
### Batch Search CASRNs Mtox 700 Biomarkers





### **Download Batches of Data**





### Chemistry Data in one sheet



A1		≺ √ ƒx DTX	SID														
	А	В	С	D	E	F	G	н	I	J	К	L	М	N	0	Р	Q
1	DTXSID	PREFERRED_NAME	CASRN	MOLECUL	TOXVAL	_C SAFETY_C	IRIS_LINK	PPRTV_LII	ATMOSPH	BIOCONCE	BIODEGRA	BOILING_F	HENRYS_L	OPERA_KN	OCTANOL	SOIL_ADS	OCTANOL
2	DTXSID6020143	Benzoic acid	65-85-0	C7H6O2	Υ	Υ	Υ	Υ	2.29E-12	3.72629	6.6407	249.237	2.67E-07	0.262557	5.90758	31.66	1.87054
3	DTXSID5024057	Dimethylamine	124-40-3	C2H7N	Υ	Υ	Υ		6.49E-11	1.41638	7.56049	6.89746	1.77E-05	0.118492	2.0199	2.5819	-0.37918
4	DTXSID4021426	Urea	57-13-6	CH4N2O	Υ	Υ	Υ		1.2E-12	2.04926	7.5801	257.615	5.44E-09	0.111874	7.35722	1.41784	-1.88328
5	DTXSID5039224	Acetaldehyde	75-07-0	C2H4O	Υ	Υ	Υ		1.58E-11	2.45935	7.56818	20.1228	6.61E-05	0.169684	1.79446	2.57283	-0.33813
6	DTXSID6023991	Cyanide	57-12-5	CN	Υ	Υ	Υ		3E-14	1.9792	8.20889	25.6428	0.000134	0.171334	0.437106	2.76794	-0.24944
7	DTXSID2024115	Formic acid	64-18-6	CH2O2	Y	Υ	Υ	Υ	4.5E-13	4.43184	6.10776	101.081	1.68E-07	0.097207	2.61624	5.39642	-0.54024
8	DTXSID8020044	Allyl alcohol	107-18-6	C3H6O	Y	Υ	Υ	Υ	2.59E-11	4.03901	4.44729	97.0571	5.01E-06	0.095317	3.75884	5.00251	0.169344
9	DTXSID6040660	Cholic acid	81-25-4	C24H40O	Υ	Υ			2.03E-11	12.2751	158.787	377.012	6.84E-12	0.729327	9.42532	41583.4	2.02413
10	DTXSID00912351	(8Z,11Z,14Z)-8,11,14-	1783-84-2	C20H34O2	2	Υ			1.35E-10	65.0338	4.4549	347.357	3.34E-08	0.829383	11.3756	4877.36	8.03065
11	DTXSID70896977	Uroporphyrin III	18273-06-	C40H38N4	1	Υ			1.85E-10	3.23875	199.454	356.404	1.51E-11	0.230449	9.6107	21193.3	1.77471
12	DTXSID8040436	Cyclic AMP	60-92-4	C10H12N5	5	Υ			1.76E-11	4.46912	5.66829	315.51	1.4E-10	0.915775	9.32545	47.8154	-2.95715
13	DTXSID40883233	L-Valine	72-18-4	C5H11NO	Y	Υ			8.36E-12	4.25743	4.07071	199.843	5.28E-07	0.090285	7.18036	18.2108	-2.25735
14	DTXSID50203948	5-Methylcytosine	554-01-8	C5H7N3O		Υ			9.02E-12	3.51614	3.54576	245.899	4.17E-08	0.207629	5.96017	47.0387	-0.84538
15	DTXSID7022679	Biotin	58-85-5	C10H16N2	Y	Υ			1.45E-11	2.86486	4.11633	255.156	1.01E-09	0.314873	9.22248	88.9387	1.44715
16	DTXSID00883219	L-Ornithine	70-26-8	C5H12N20		Υ			8.65E-12	2.79981	3.55454	272.761	4.35E-10	0.08733	7.25812	10.0694	-4.21283
17	DTXSID2020260	Chenodeoxycholic ac	474-25-9	C24H40O4	Y	Υ			2.02E-11	65.1383	161.947	383.963	1.12E-09	0.769439	9.32373	98509.3	3.00931
18	DTXSID70187059	N-Formylanthranilic	3342-77-6	C8H7NO3		Y			2.43E-11	3.48632	3.54972	285.649	8.73E-10	0.123782	8.09494	34.795	0.797736
19	DTXSID6022559	Adenosine triphosph	56-65-5	C10H16N5	5	Υ			2.48E-11	2.60734	3.67994	347.902	2.36E-11	0.142466	9.56326	53.8001	-1.3349
20	DTXSID101031182		2922-05-0	CIUNIZNZ													
4	Cover Shee	et Main Data As	sociated To	oxCast Assa	ys To	xval Details	(+)										

### **Bioactivity Data in another sheet**

	А	В	С	D	Е	F	G	н	1	J	К	L	М	N	0	Р	
1	INPUT	DTXSID70	DTXSID80	DTXSID50	DTXSID80	DTXSID20	DTXSID90	DTXSID30	DTXSID704	DTXSID20	DTXSID90	DTXSID20	DTXSID80	DTXSID90	DTXSID80	DTXSID40	DT
2	ACEA_AR_agonist_80hr	-	0	-	0	-	-	-	-	-	-	-	-	0	-	1	-
3	ACEA_AR_agonist_AUC_viability	-	Ó	-	0	-	-	-	-	-	-	-	-	0	-	0	-
4	ACEA_AR_antagonist_80hr	-	Ó	-	1	-	-	-	-	-	-	-	-	0	-	0	-
5	ACEA_AR_antagonist_AUC_viability	-	Ó	-	1	-	-	-	-	-	-	-	-	0	-	1	-
6	ACEA_ER_80hr	-	Ó	-	1	-	-	-	-	-	-	-	-	0	-	1	-
7	ACEA_ER_AUC_viability	-	Ó	-	0	-	-	-	-	-	-	-	-	1	-	0	-
8	APR_HepG2_CellCycleArrest_1h_dn	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
9	APR_HepG2_CellCycleArrest_1h_up	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
10	APR_HepG2_CellCycleArrest_24h_dn	-	-	-	0	-	-	-	-	-	-	-	-	-	-	0	-
11	APR_HepG2_CellCycleArrest_24h_up	-	-	-	0	-	-	-	-	-	-	-	-	-	-	0	-
12	APR_HepG2_CellCycleArrest_72h_dn	-	-	-	0	-	-	-	-	-	-	-	-	-	-	0	-
13	APR_HepG2_CellCycleArrest_72h_up	-	-	-	0	-	-	-	-	-	-	-	-	-	-	0	-
14	APR_HepG2_CellLoss_1h_dn	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
15	APR_HepG2_CellLoss_1h_up	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
16	APR_HepG2_CellLoss_24h_dn	-	-	-	0	-	-	-	-	-	-	-	-	-	-	0	-
17	APR_HepG2_CellLoss_24h_up	-	-	-	0	-	-	-	-	-	-	-	-	-	-	0	-
18	APR_HepG2_CellLoss_72h_dn	-	-	-	1	-	-	-	-	-	-	-	-	-	-	0	-
19	APR_HepG2_CellLoss_72h_up	-	-	-	0	-	-	-	-	-	-	-	-	-	-	0	-
20	APR HepG2 MicrotubuleCSK 1h dn	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
4	Cover Sheet Main Data As	sociated T	oxCast As	says Tox	val Details	+			E 💽								►

€FP

United States Environmental Protection

## Toxicity Value Data in another sheet >5000 rows of quantitative data



	A	В	С	D	E	F	G	Н	1	J	K	L	Μ	Ν	0	Р	Q	R	S	
	L SEARC	IECDTXSID	CASRN	NAME	SOURCE	SUB_SOUF	TOXVAL_1	TOXVAL_T	TOXVAL	_S TOXVAL_	T TOXVAL	T QUALIFI	IEFTOXVAL_N	TOXVAL_	TOXVAL_U	TOXVAL_U	RISK_ASSE	STUDY_T	STUDY_T	Y ST
1	2 Cholic	acic DTXSID60	481-25-4	Cholic aci	CECHA IUC	LEU REACH	concentra	dose level	-	Exposure	-	=	500	500	mg/kg-da	mg/kg-da	repeat do	repeat do	repeat do	<b>)</b> !-
3	3 Cholic	acic DTXSID60	481-25-4	Cholic aci	CECHA IUC	LEU REACH	LD50	LD50	-	Lethality	E LD	=	2300	2300	mg/kg-da	ymg/kg	acute	acute	acute	-
4	4 Cholic	acic DTXSID60	481-25-4	Cholic aci	CECHA IUC	LEU REACH	LD50	LD50	-	Lethality	ELD	=	4600	4600	mg/kg-da	ymg/kg	acute	acute	acute	-
1	5 Cholic	acic DTXSID60	481-25-4	Cholic aci	CECHA IUC	LEU REACH	LD50	LD50	-	Lethality	ELD	=	4950	4950	mg/kg-da	ymg/kg	acute	acute	acute	-
(	6 Cholic	acic DTXSID60	481-25-4	Cholic aci	CECHA IUC	LEU REACH	NOEC	NOEC	-	Point of I	NOEC	=	30.64	30.64	mg/L	mg/L	chronic	chronic	chronic	-
	7 Cholic	cic DTXSID60	481-25-4	Cholic aci	CECHA IUC	LEU REACH	NOEC	NOEC	-	Point of I	NOEC	=	70.29	70.29	mg/L	mg/L	acute	acute	acute	-
8	3 Cholic	acic DTXSID60	481-25-4	Cholic aci	CECHA IUC	LEU REACH	NOEC	NOEC	-	Point of I	NOEC	=	75.52	75.52	mg/L	mg/L	acute	acute	acute	-
9	Cholic	acic DTXSID60	481-25-4	Cholic aci	COTOX	EPA ORD	LOEC	LOEC	-	Point of I	Di-	-	1	1	%	%	acute repr	Reproduc	Reproduc	tac
1	0 L-Valin	e DTXSID40	872-18-4	L-Valine	COSMOS	US FDA CF	HNEL	HNEL	-	Point of I	HNEL	=	1	1	mM	mМ	genotoxic	genotoxic	i Genetic to	<b>o</b> -
1	1 L-Valin	e DTXSID40	872-18-4	L-Valine	COSMOS	US FDA CF	HNEL	HNEL	-	Point of I	HNEL	=	2	_	mg/ml	mg/ml	genotoxic	genotoxic	i Genetic t	<b>o</b> -
1	2 L-Valin	e DTXSID40	872-18-4	L-Valine	COSMOS	US FDA CF	HNEL	HNEL	-	Point of I	HNEL	=	5	5	mg/plate	mg/plate	genotoxic	genotoxic	i Genetic t	o -
1	3 L-Valin	e DTXSID40	872-18-4	L-Valine	COSMOS	US FDA CF	HNEL	HNEL	-	Point of I	HNEL	=	1853	1853	mg/kg-da	ymg/kg bw	subchroni	subchron	i Subchron	d -
1	4 L-Valin	e DTXSID40	872-18-4	L-Valine	COSMOS	US FDA CF	LEL	LEL	-	Point of I	DELL	=	1	1	mM	mМ	genotoxic	genotoxic	i Genetic t	o -
1	5 L-Valin	e DTXSID40	872-18-4	L-Valine	COSMOS	US FDA CF	LEL	LEL	-	Point of I	DELL	=	3721	3721	mg/kg-da	ymg/kg bw	subchroni	subchron	i Subchron	d -
1	6 L-Valin	e DTXSID40	872-18-4	L-Valine	ECHA	eChemPor	NOAEL	NOAEL	repeat	do: Point of I	NOAEL	=	628	628	mg/kg-da	mg/kg bw	subchroni	subchron	i subchron	d -
1	7 L-Valin	DTXSID40	872-18-4	L-Valine	ECHA	eChemPor	NOAEL	NOAEL	repeat	do: Point of I	NOAEL	=	666	666	mg/kg-da	ymg/kg bw	subchroni	subchron	i subchron	d -
1	8 L-Valin	e DTXSID40	872-18-4	L-Valine	ECHA	eChemPor	NOEC	NOEC	eco aqu	iat Point of I	NOEC	=	3.2	3.2	g/L	g/L	chronic	static	static	-
1	9 L-Valin	e DTXSID40	872-18-4	L-Valine	ECHA eCh	ECHA REA	LD50	LD50	-	Lethality	E LD	>	2000	-	mg/kg	mg/kg bw	acute	acute	acute tox	icac
2	0 L-Valin			L-Valine		ECHA REA		NOAEL	-	Point of I	NOAEL	=	610	610	mg/kg-da	mg/kg bw	developm	developm	developm	ו de ד
	$\rightarrow $	Cover She	et Main	Data As	ssociated To	oxCast Assay	/s Tox	al Details	+			:	•							



### Cheminformatics Proof-of-Concept Modules

### (PUBLICLY AVAILABLE)

### **Disclaimer and Info**



- Software is available at
- <u>https://www.epa.gov/chemical-research/cheminformatics</u>
- Please understand it is proof-of-concept so reach out to me for help if necessary

## LIVE DEMO

How to Use HCD

- Always start with INPUTs
- - Search based on CAS RNs, Names, DTXSIDs from the Dashboard







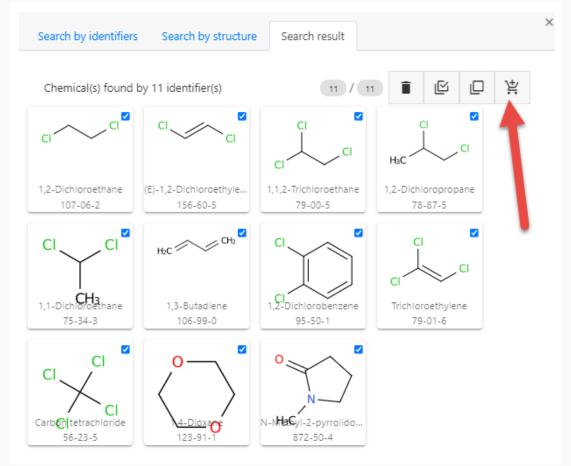
Paste them into the search box. Click Search

Search by identifiers	Search by structure	Search result	×
107-06-2 156-60-5 79-00-5 78-87-5 1,1-Dichloroethane 1,3-Butadiene 1,2-Dichlorobenzene DTXSID0021383 DTXSID8020250 DTXSID4020533			
			SEARCH

### Add to "Cart"

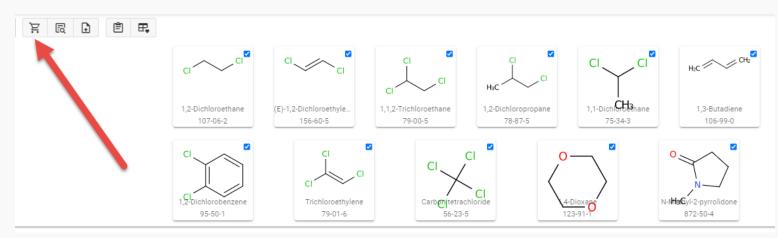


### Review the chemicals and "Add to Cart"





 "Process the Cart" searches the chemicals against the database and serves them up



• The blue check marks (top RHS of structure) select or deselect chemicals Default is ALL.

# Navigating the Matrix



Chemicals: 11				Toxici	ty: VH -	Very Higi	n <mark>H</mark> - Hig	h <mark>M</mark> -N	/ledium L	- Low I	- Inconclus	ive N/A - N	lot Applic	able Au	thority: A	uthoritati	i <b>ve</b> 🛈 Scr	eening (	D QSAR	Model 🤅
						ł	Human I	Health	Effects							Ecoto	oxicity		Fate	
Skipped (0) Unlikely (0) Filters (0) Sorting (0) Structure CAS Name	Oral	lammaliar Inhalation	Toxicity Jeman	Carcinogenicity	Genotoxicity Mutagenicit	Endocrine Disruption	Reproductive	Developmental	Repeat Exposure	Single Exposure	Systemic Kebeat Exposure	Single Exposure	Skin Sensitization	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation	Exposure
107-06-2 AIGBT 1,2-Dichloroethane	м	н	L	νн	н	L	н	L	н	н	м	м	м	н	н	L	L	н	L	
156-60-5 IGBTP (E)-1,2-Dichloroet	м	L	L	I.	L	N/A	N/A	L	N/A		м	н	N/A	н	н	L		н	L	
79-00-5 AIGBT 1,1,2-Trichloroeth	м	м	м	νн	L	L	N/A	L	н		н	н	N/A	н	м	м	м	н	L	
78-87-5 AIGBT 1,2-Dichloropropa	м	н	L	νн	L	L	М	м			L	н	н	н	н	м	м	н	L	
75-34-3 AIGBT 1,1-Dichloroethane	м	м	N/A	νн	VH	L	N/A	L	N/A	н	L	м	N/A	н	н	L	м	н	L	
106-99-0 AIGBT 1,3-Butadiene	L	L	N/A	νн	νн	L	н	н			н	м	N/A	N/A	н	М	L	L	L	
95-50-1 IGBT 1,2-Dichlorobenze	м	н	L	I.	н	н	N/A	L	н		н	м	N/A	н	н	νн	νн	н	L	
79-01-6 AIGBT Trichloroethylene	L	м	L	νн	νн	N/A	н	н	н	н	н	м	н	н	н	н	VH	н	L	
56-23-5 AIGBT Carbon tetrachlori	н	н	н	νн	L	н	м	L		н	н	н	н	н	н	м	м	н	L	
123-91-1 AIGBT 1,4-Dioxane	м	м	L	νн	VH	L	N/A	L	н	н	н	м	N/A	н	н	н	L	н	L	
872-50-4 GBT N-Methyl-2-pyrroli	L	L	L	N/A	L	L	н	н	м		м	м	N/A	н	н	н		L	L	

## What are the Sources



 Hover over the informational icon to understand sources for Authoritative, Screening and QSAR Model

														(	*	HAZARD	•	ALER
_		Authorita	tive sour	ces														
		<ul> <li>Europea</li> <li>EPA mid</li> <li>Germany Area;</li> </ul>	-Atlantic R	egion Hur	man Hea	lth Risk-B	Based Co	oncentrat	ions;			al Compou	inds in th	e Work		Authorit	ative <sup>()</sup> S	creenin
			ealth Orga	nization li	nternatio	nal Ager	ncy for R	esearch o	on Cance	r (IARC) I	Monograph	ns on the Ev	aluation	of		Eco	toxicity	
	Acute	Carcinog Integrate US Natio Californi EU Europ Candida	enic Risks ed Risk Info onal Institut a Office of bean Chem te List of Si rtment of I	to Humar prmation ! te for Occ Environm icals Age ubstances Health an	ns; System ( pental He ncy (ECF of Very d Huma	IRIS); al Safety ealth Haz IA) Regis High Cor n Service	and Hea ard Asse tration, I ncern fo s Nation	lith (NIOS essment F Evaluation r Authoria al Toxico	iH) list of Proposition, Author zation; logy Proj	f potentia on 65 List rization a gram Rep	al occupatio ; nd Restrict port on Car	onal carcino	ogens;			Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence
IGBT	м	н	L	νн	н	L	н	L	н	н	м	м	М	н	н	L	L	н

## Hover over Cell – Summary Call

 Hover on the cell gives the summary call for the chemical. CLICK to expand...

AIGBT	м	н	L VH L L M M L H H	Н	н	м	м	н
AIGBT			Trichloroethylene   Skin Irritation					
ane	м	М	Source ECHA CLP	н	н	L	м	н
AIGBT	L	L	Authority Authoritative Score H	N/A	н	М	L	L
IGBT	м	н	Route	н	н	VH	νн	н
AIGBT	L	м	Category Skin Irrit. 2 Hazard Code H315	н	н	н	VH	н
ne	-	141	Hazard Statement Causes skin irritation				viii	
AIGBT	н	н	Rationale Score of H was assigned based on a hazard code of H315	Н	н	м	м	н
AIGBT	М	м	Note	н	н	н	L	н
GBT	1	1		ц	ц	н		I

opmental Protection

## **Detail Table**

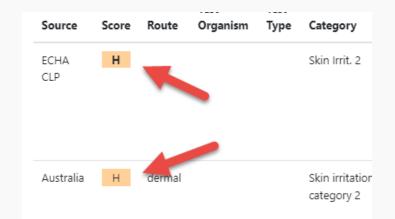


Skin Irritation for Trichloroethylene (79-01-6 Q)

		Toxicity: VH	- Very High H	- High <mark>M</mark>	- Medium L - Low I - Inc	onclusive N/A	- Not Applicable	Authority: Autho	ritative <sup>(1)</sup> Screening <sup>(1)</sup> QSAR Model
Source	Score	Route	Test Organism	Test Type	Category	Hazard Code	Hazard Statement	Rationale	Note
ECHA CLP	Н				Skin Irrit. 2	H315	Causes skin irritation	Score of H was assigned based on a hazard code of H315	
Australia	Н	dermal			Skin irritation - category 2	H315	Causes skin irritation	Score of H was assigned based on a hazard code of H315	N (The classification information for this entry was provided by the National Industrial Chemical Notification and Assessment Scheme)
Canada	Η				Skin corrosion/irritation - Category 2	H315	Causes skin irritation	Score of H was assigned based on a hazard code of H315	
Japan	Н				Category 2	H315	Causes skin irritation	Score of H was assigned	From a report that in the case of humans, dermatitis and erythema were caused by



- : Authority: Authoritative <sup>(i)</sup> Screening <sup>(i)</sup> QSAR Model <sup>(i)</sup>
- BOLD: Authoritative Sources
- Normal: Screening Sources
- Italic: QSAR Models (TEST and SEEM3)



# Multi-sorting of columns



# Click on a column-heading...carcinogenicity selected below...

Chemicals: 11				Toxici	ity: VH -	Very High	n <mark>H</mark> - Hig	gh <mark>M</mark> - N	ledium L	- Low I	- Inconclus	ive N/A -N	lot Applic	able Au	thority: A	uthoritati	ve 🛈 Scr	reening (	D QSAR	Model 🛈
						ł	Human	Health	Effects							Ecoto	xicity		Fate	
Skipped (0)	Acute M	lammaliar	n Toxicity		nicit				Neuro	toxicity	Systemic	c Toxicity				≥	city			
<ul> <li>Unlikely (0)</li> <li>Filters (0)</li> <li>Sorting (1)</li> <li>Structure</li> <li>CAS</li> <li>Name</li> </ul>	Oral	Inhalation	Dermal	Carcinogenicity	Genotoxicity Mutagenicit	Endocrine Disruption	Reproductive	Developmental	Repeat Exposure	Single Exposure	Repeat Exposure	Single Exposure	Skin Sensitization	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation	Exposure
Sorting	Carcino	ogenicity	Ŕ					×												Reset
107-06-2 AIGBT 1,2-Dichloroethane	м	н	L	νн	н	L	н	L	н	н	м	м	м	н	н	L	L	н	L	
79-00-5 AIGBT 1,1,2-Trichloroeth	м	м	м	νн	L	L	N/A	L	н		н	н	N/A	н	м	м	м	н	L	
78-87-5 AIGBT 1,2-Dichloropropa	м	н	L	νн	L	L	м	м			L	н	н	н	н	м	м	н	L	
75-34-3 AIGBT 1,1-Dichloroethane	м	м	N/A	νн	VH	L	N/A	L	N/A	н	L	м	N/A	н	н	L	м	н	L	
106-99-0 AIGBT 1,3-Butadiene	L	L	N/A	νн	νн	L	н	н			н	м	N/A	N/A	н	М	L	L	L	
79-01-6 AIGBT Trichloroethylene	L	м	L	νн	νн	N/A	н	н	н	н	н	м	н	н	н	н	νн	н	L	

# Multi-sort, multi-columns

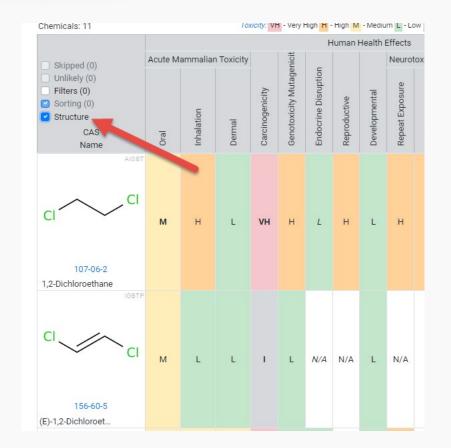


- Multiple columns can be sorted in order
- Click the check mark to remove that sort
- Click Reset to remove ALL sorts

						ŀ	luman	Health	Effects							Ecoto	oxicity		Fate	
Skipped (0)	Acute M	lammaliar	n Toxicity		nicit	-			Neurot	toxicity	Systemic	c Toxicity				ty	city			
<ul> <li>Unlikely (0)</li> <li>Filters (0)</li> <li>✓ Sorting (2)</li> <li>Structure</li> <li>CAS</li> <li>Name</li> </ul>	Oral	Inhalation	Dermal	Carcinogenicity	Genotoxicity Mutagenicit	Endocrine Disruption	Reproductive	Developmental	Repeat Exposure	Single Exposure	Repeat Exposure	Single Exposure	Skin Sensitization	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation	Exposure
Sorting		ogenicity ` xicity Mut	لا tagenicity	Ŕ				××												Rese
106-99-0 AIGBT 1,3-Butadiene	L	L	N/A	νн	νн	L	н	н			н	м	N/A	N/A	н	М	L	L	L	
79-01-6 AIGBT Trichloroethylene	L	м	L	νн	VH	N/A	н	н	н	н	н	м	н	н	н	н	VH	н	L	

## **Click Structure to Show**

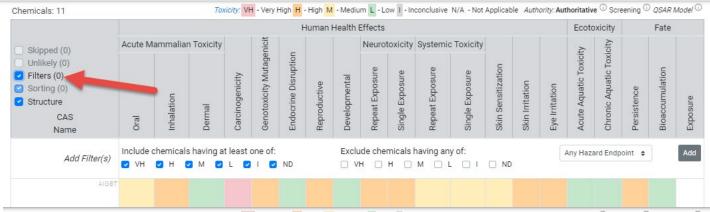




## Filters



# Filter hazard ratings IN or OUT...select Endpoint – should be self explanatory



Chemicals: 11

Toxicity: VH - Very High H - High M - Medium L - Low I - Inconclusive N/A - Not Applicable Authority: Authority: Authoritative 🛈 Screening 🛈 QSAR Model 🛈

nemicais. II																				
						ŀ	Human I	Health	Effects							Ecoto	xicity		Fate	
Skipped (0) Unlikely (0)	Acute M	ammalia	n Toxicity		agenicit	tion			Neurot	oxicity	Systemi	c Toxicity	_			Toxicity	Toxicity			
<ul> <li>Filters (2)</li> <li>Sorting (0)</li> <li>Structure</li> </ul>		ition	le	Carcinogenicity	Genotoxicity Mutagenicit	srine Disruption	Reproductive	Developmental	Repeat Exposure	Single Exposure	Repeat Exposure	Exposure	Sensitization	Skin Irritation	Eye Irritation	Aquatic	Chronic Aquatic 1	Persistence	Bioaccumulation	
CAS Name	Oral	Inhalation	Dermal	Carcir	Genot	Endocrine	Repro	Develo	Repea	Single	Repea	Single	Skin S	Skin Ir	Eye Irr	Acute	Chron	Persis	Bioaco	
Filters			I: [ "VH", "I Itagenicity			-												××	l	Res
Add Filter(s)	Include o	chemical И	s having a • M •	t least o L 🔽		ND				nicals H 🗌	having an M 🗌 I	·	□ ND			Genotoxi	city Mut	agen 🗢		A
AIGBT																				

## Filter out individual/multiple sources



									Full	;	
Toxicity: VH - Very High H - High M - Medium L - Low 1	- Inconclusive N/A - N	lot Applicable	Authority: A			reening <sup>(</sup>	DQSAR	Model			
Hazard Report Filters				Ecoto	-	-	Fate				
✓ Hide No-Data chemicals				Acute Aquatic Toxicity	Chronic Aquatic Toxicity		ion				
Data sources filter		UOITE	ation	quatic	Aqua	nce	Bioaccumulation	ω			
Authoritative		and the second se	Eye Irritation	ute A	ronic	Persistence	oaccu	Exposure			
Screening		X	Ē	Ac	-S	Pe	Bio	Ē			
🕨 🔽 QSAR Model		H	н	L	L	Н	L	VH			
Test types filter				-				10			
🕨 🗹 Cancer			Н	L		н	L	Н			
EC Values		÷.	м	м	м	н	L	н			
🕨 🗹 LC Values			-					-			
🕨 🔽 LD Values			н	М	М	н	L	Н			
🕨 🔽 LOEC Values		÷	н	L	м	Н	L	Н			
NOEC Values				м							
NOEL Values			н	IVI	L	L	L	Н			
> V Other		H.	н	VH	VH	н	м	L			
<ul> <li>Unknown</li> </ul>				100	101	2240	-	18			
Categories and Endpoints for Custom profile		-	н	н	VH	H	L	Н			
🕨 😑 Human Health Effects		÷.	н	М	м	н	L	М			
Ecotoxicity							L	н			
Fate		7	н	н	L	Н	L	9			
			н	н		L	L	Н			
	RESET	CLOSE									

## **Export SDF or Excel File**



## Most useful form for your needs..Excel



The Hazard Comparison Dashboard is a prototype tool and a compilation of information sourced from many sites, databases and sources including U.S. Federal and state sources and international bodies that saves the user time by providing information in The data are not reviewed by USEPA – the user must apply judgment in use of the information. The results do not indicate EPA's position on the use or regulation of these chemicals.

		VH - Ve	ery High	Н-	High	M - M	edium	L-I	Low	I - Incor	nclusive	Nol	Data		Authorita	tive	Screening		QSAR Mo
					0			Huma	an Health E	ffects								oxicity	1
		Acute N	1ammalian	Toxicity		enicity	-			Neurot	toxicity	Systemic	Toxicity				₽	≿	
DTXSID	CAS Name	Oral	Inhalation	Dermal	Carcinogenicity	Genotoxicity Mutageni	Endocrine Disruption	Reproductive	Developmental	Repeat Exposure	Single Exposure	Repeat Exposure	Single Exposure	Skin Sensitization	Skin Irritation	Eye Irritation	Acute Aquatic Toxicit	Chronic Aquatic Toxicity	Persistence
XSID6020438	107-06-2 1,2-Dichloroethane	М	Н	L	VH	VH	L	н	L	Н	Н	М	М	М	н	н	L	L	Н
XSID7024031	156-60-5 (E)-1,2-Dichloroethylene	М	L	L	1	L	1	1	L	1		М	Н	1	н	н	L		Н
XSID5021380	79-00-5 1,1,2-Trichloroethane	м	м	м	VH	L	L	1	L	Н		н	н	1	н	м	M	м	Н
XSID0020448	78-87-5 1,2-Dichloropropane	м	н	L	VH	VH	L	М	М			L	Н	н	н	н	м	м	Н
XSID1020437	75-34-3 1,1-Dichloroethane	м	М	1	VH	VH	L	1	L	1	н	L	м	1	н	н	L	м	н
XSID3020203	106-99-0 1,3-Butadiene	L	L	1	VH	VH	L	н	н			Н	М	1.1	1	н	М	L	L
XSID6020430	95-50-1 1,2-Dichlorobenzene	м	H	L	1	VH	Н	- 1	L	Н		Н	м	1	н	н	VH	VH	Н
KSID0021383	79-01-6 Trichloroethylene	L	М	L	VH	VH	1	н	н	Н	н	н	м	н	н	н	н	VH	н
XSID8020250	56-23-5 Carbon tetrachloride	н	н	н	VH	VH	Н	М	L		Н	н	н	Н	н	н	м	м	Н
(SID4020533	123-91-1 1,4-Dioxane	М	М	L	VH	VH	L	1	L	Н	н	Н	М	1	Н	н	н	L	н
KSID6020856	872-50-4 N-Methyl-2-pyrrolidone	L	L	L	1	L	L	н	н	м		M	м	1	н	н	н		L

## Check SECOND Worksheet



A	В	С	D	
Hazard Name	CAS	Name	Source	Original Source
Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	ECHA CLP	
Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	UMD	
Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	Canada	
Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	ChemIDplus	
Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	ChemIDplus	
Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	ChemIDplus	
Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	Japan	
Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	Malaysia	
Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	New Zealand	
. Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	T.E.S.T. (experimental value)	
Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	ToxVal	<u>ECHA</u>
Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	ToxVal	<u>ECHA</u>
Acute Mammalian Toxicity Oral	107-06-2	1,2-1/ichloroethane	ToxVal	<u>ECHA</u>
Acute Mammalian Toxicity Oral	107-06-2	1Dichloroethane	ToxVal	<u>ECHA</u>
Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	ToxVal	<u>ECHA</u>
Acute Mammalian Toxicity Oral	107-06-1	1,2-Dichloroethane	ToxVal	ECHA IUCLID
Acute Mammalian Toxicity Oral	107-0 -2	1,2-Dichloroethane	ToxVal	ECHA IUCLID
Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	ToxVal	ECHA IUCLID
Acute Mammalian Toxicity Oral	1 J7-06-2	1,2-Dichloroethane	ToxVal	ECHA IUCLID
. Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	ToxVal	ECHA IUCLID
Acute Mammalian Toxicity Oral 💦 🖌	107-06-2	1,2-Dichloroethane	T.E.S.T. (predicted value)	



# (Work in Progress)



 Building the database of reactions under the Chemical Transformation Simulator



<b>Environmental Topics</b>	Laws & Regulations	About EPA	Search EPA.gov	٩
CTS: Chemical	Transforma	tion Simulator 1.2.3	Contact Us	

### About

CTS Home

CTS Basic Information

Execute CTS Workflows

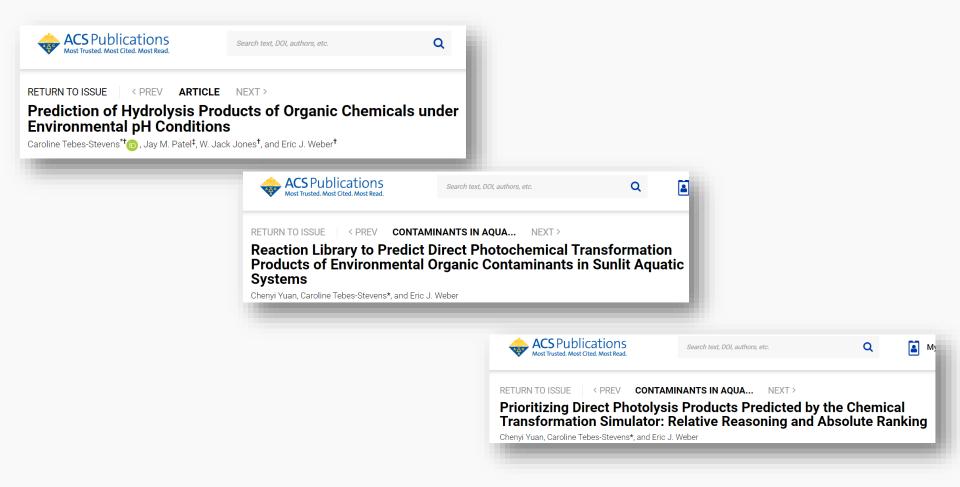
> Calculate Chemical Speciation

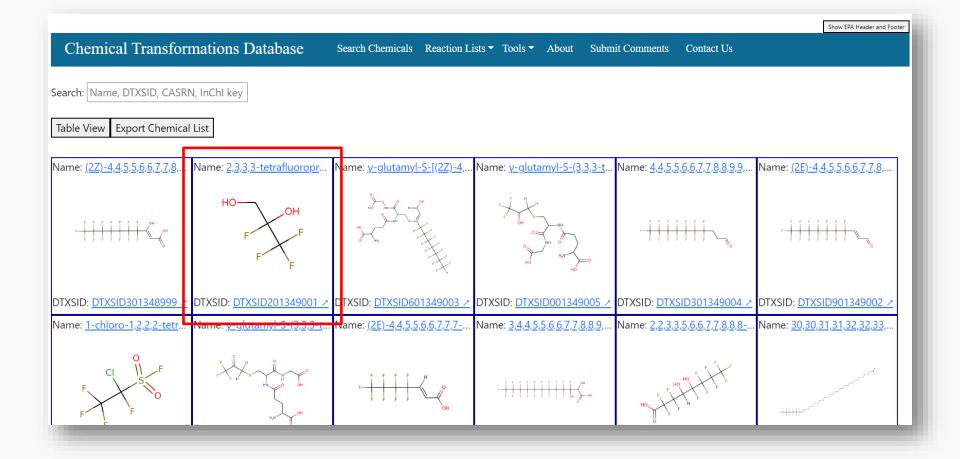


Calculate Dhysicochemical



# Building the database of reactions under the Chemical Transformation Simulator





Invironmental Protection

Agency

## Reaction, Original References etc

Chemical Transformations Database

Search Chemicals Reaction Lists 

Tools 

About Contact Us Submit Comments

### <u>2-Fluoro-2-(trifluoromethyl)oxirane</u> $\rightarrow$ <u>2,3,3,3-tetrafluoropropane-1,2-diol</u>

$F \xrightarrow{F} F \xrightarrow{HO} F$	OH F F	
Reaction Process:		
Reaction Type: <u>Hydrolysis</u>		
Reaction Scheme: <u>Epoxide to diol PTP</u>		
Reaction Details		
T Half Life (days) Reaction System	Metabolic Environmental Notes	Reference
rat	1	Schuster et al., 2008

**Export Reaction Details** 

Delete Delete

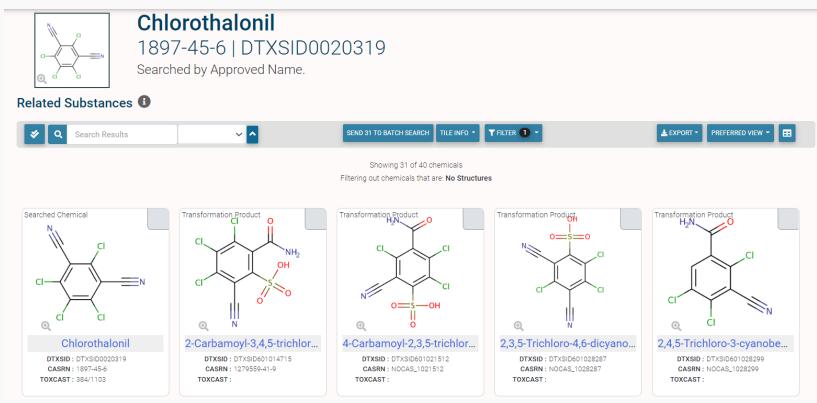
Invironmental Protection

Agency





 Adding Thousands of Parent-Product mappings from the Dashboard





# Cheminformatically Enabling Analytical Methods

# (Work in Progress)

# **Building a Methods Database**



- Simple Vision: I want to find the best method(s) associated with a chemical (class)
- The Approach:
  - Aggregate MS method documents
  - Extract chemistry (mostly CASRN and Names)
  - Map CASRN and Names to structures
  - Search a database by names and synonyms, CASRNs, InChIKeys and ultimately structure
  - "I cannot find my chemical in any method" CHEMINFORMATICS can help....

## Where are there methods?



# 900 method documents

Related Topics: Pesticide Analytical Methods

CONTACT US

## Environmental Chemistry Methods (ECM) Index - 0-9

 $\textbf{0-9} \hspace{0.1cm} \mid \hspace{0.1cm} \underline{A} \hspace{0.1cm} \mid \hspace{0.1cm} \underline{B} \hspace{0.1cm} \mid \hspace{0.1cm} \underline{C} \hspace{0.1cm} \mid \hspace{0.1cm} \underline{D} \hspace{0.1cm} \mid \hspace{0.1cm} \underline{E} \hspace{0.1cm} \mid \hspace{0.1cm} \underline{G} \hspace{0.1cm} \mid \hspace{0.1cm} \underline{H} \hspace{0.1cm} \mid \hspace{0.1cm} \underline{I} \hspace{0.1cm} \mid \hspace{0.1cm} \underline{M} \hspace{0.1cm} \mid \hspace{0.1cm} \underline{N} \hspace{0.1cm} \mid \hspace{0.1cm} \underline{O} \hspace{0.1cm} \mid \hspace{0.1cm} \underline{P} \hspace{0.1cm} \mid \hspace{0.1cm} \underline{Q} \hspace{0.1cm} \mid \hspace{0.1cm} \underline{S} \hspace{0.1cm} \mid \hspace{0.1cm} \underline{I} \hspace{0.1cm} \mid \hspace{0.1cm} \underline{V} \hspace{0.1cm} \mid \hspace{0.1cm} \underline{Z} \hspace{0.1cm}$ 

Analyte(s) by Pesticide	ECM MRID	Matrix	Method Date
<u>1,2,4-triazole</u>	49762553	Water	2/19/13
<u>1,3-dichloropropene &amp; 1,2-dichloropropane</u>	44536511	Soil	3/27/98
<u>1,3-dichloropropene &amp; 1,2-dichloropropane</u>	44536511	Water	3/27/98
<u>1,3-dichloropropene Degradate 3-chloroallyl Alcohol</u>	44536505	Water	12/12/97

## ECM – New and Old



### ECM for 1,3-dichloropropene & 1,2dichloropropane in Soil - MRID 44536511

- MRID: 44536511
- Date: 3/27/98
- Matrix: Soil
- Registrant: Dow Elanco
- Analysis: GC/MS
- Limit of Quantitation (LOQ):  $0.2\,\mu g/kg$

### DISCLAIMER

EPA makes no claim of validity by posting these methods, but recognizes that the methods may be of some utility to state, tribal, and local authorities. In addition, not all methods listed are independently validated.

- ECM 1,3-dichloropropene & 1,2-dichloropropane in Soil MRID 44536511 (pdf) (945.98 KB)
- 🖹 ILV 1,3-dichloropropene & 1,2-dichloropropane in Soil MRID 44536508 (pdf) (108.78 KB)
- DER 1,3-dichloropropene & 1,2-dichloropropane in Water & Soil MRID 44536511 (pdf) (180.26 KB)

## Many Scanned Documents!!!

United States Environmental Protection Agency

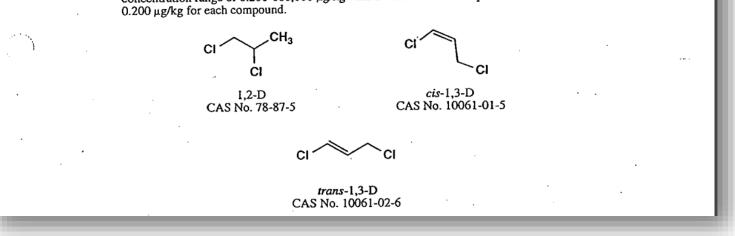
GRM.: 94.13 EFFECTIVE: July 26, 1995 SUPERSEDES: New

Determination of Residues of 1,2-Dichloropropane and *cis*- and *trans*-1,3-Dichloropropene in Soil by Purge and Trap Extraction, Capillary Gas Chromatography and Mass Selective Detection

S. C. Dolder, C. E. Kubitschek and H. E. Dixon-White North American Environmental Chemistry Laboratory DowElanco Indianapolis, Indiana 46268 - 1053

A. <u>Scope</u>

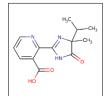
This method is applicable for the quantitative determination of residues of 1,2dichloropropane (1,2-D) and *cis*- and *trans*-1,3-dichloropropene (1,3-D) in soil over the concentration range of 0.200-160,000  $\mu$ g/kg with a validated limit of quantitation of 0.200  $\mu$ g/kg for each compound.



## Embedding old Method PDFs



### Search Results for "Imazapyr"



(Preferred) Name: Imazapyr DTXSID: <u>DTXSID8034665</u> CASRN: 81334-34-1 InChIKey: CLQMBPJKHLGMQK-UHFFFAOYNA-N Molecular Formula: C13H15N3O3 Mass: 261.281

#### Imazapyr

MRID: 41891501 Date: 10/1/89 Matrix: Water Registrant: American Cyanamide Co Analysis: HPLC/UV Limit of Quantitation: 5.0 µg/L

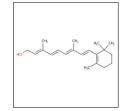
Spectrum Type ↑	Source	Record Type	View	😑 US EPA - ECM for Imazapyr 1 / 8   - 90% +   🗄 🚸 🛃 🖶
	Environmental Chemistry Methods	Method	PDF	
	Environmental Chemistry Methods	Method	PDF	418915-\$1
.C-MS+	MoNA	Spectrum	Spectrum	
.C-MS+	MassBank EU	Spectrum	<u>Spectrum</u>	C3197 CONFIDENTIAL
.C-MS+	MassBank EU	Spectrum	Spectrum	C3197 CONFIDENTIAL Page 5 of 22
.C-MS+	MassBank EU	Spectrum	Spectrum	SOP M1900
.C-MS+	MassBank EU	Spectrum	Spectrum	A. Khunachak/hm
.C-MS+	MassBank EU	Spectrum	Spectrum	09/05/89 Approved by:
				AMERICAN CYANAMID COMPANY AGRICULTURAL RESEARCH DIVISION CHEMICAL DEVELOPMENT P. O. Bax 400 Princeton, New Jersey 08540 USA RECOMMENDED METHOD OF ANALYSIS
				Imazzpyr (CL 243,997): HPLC Method for the Determination of CL 243,997 Residues in Water
				A. <u>Principle</u>
				Residues of CL 243,997 are extracted from water by using a C18 solid phase extraction (SPE) cartridge. Additional cleanup and specificity are achieved by

## **Embedding New Method PDFs**





### Search Results for "Retinol"



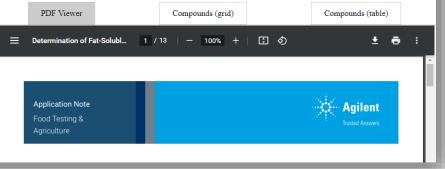
(Preferred) Name: Retinol DTXSID: <u>DTXSID3023556</u> CASRN: 68-26-8 InChIKey: FPIPGXGPPPQFEQ-OVSJKPMPSA-N Molecular Formula: C20H30O Mass: 286.459

#### Determination of Fat-Soluble Vitamins in Foods Using Agilent Chem Elut S Extraction with LC/DAD and LC/MS/MS Triple-Quadrupole

#### Author: Hui Zhao

Focus/Analyte: Reliable sample preparation and identification/quantitation in various food matrices Synopsis: This application note describes a method for the determination of fat-soluble vitamins, including vitamin A (retinol), vitamin D3 (cholecalciferol), vitamin D2 (ergocalciferol), and vitamin E (a-tocopherol) in complex food matrices, including infant formula, egg, canned tuna, and mushroom. Samples were saponified as sample pretreatment, extracted using Agilent Chem Elut S (Supported Liquid Extraction (SLE)) 12 mL cartridges, and fat-soluble vitamins were then simultaneously identified and quantified by an Agilent 1290 Infinity II LC coupled to an Agilent diode array detector (DAD) and Agilent 6470 triple quadrupole LC/MS in series. Data were analyzed using Agilent MassHunter workstation software.

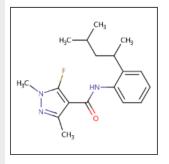
GC-MS			
OC-IVIS	Spectrabase	Spectrum	External Link
GC-MS	<u>Spectrabase</u>	Spectrum	External Link
GC-MS	Spectrabase	Spectrum	External Link
GC-MS	<u>Spectrabase</u>	Spectrum	External Link
GC-MS	<u>Spectrabase</u>	Spectrum	External Link
GC-MS	Spectrabase	Spectrum	External Link
GC-MS	Spectrabase	Spectrum	External Link
GC-MS	<u>Spectrabase</u>	Spectrum	External Link
LC-MS	Agilent	Method	<u>PDF</u>
LC-MS+	<u>MoNA</u>	Spectrum	<u>Spectrum</u>



## Structure Tables/Tiles view



### Search Results for "DTXSID9058107"



(Preferred) Name: Penflufen DTXSID: <u>DTXSID9058107</u> CASRN: 494793-67-8 InChIKey: GOFJDXZZHFNFLV-UHFFFAOYNA-N Molecular Formula: C18H24FN3O Mass: 317.408

### Penflufen & Degradates

MRID: 48023715 Date: 1/8/10 Matrix: Water Registrant: Bayer CropScience Analysis: LC/MS/MS Limit of Quantitation: 0.1 µg/L

Spectrum Type ↑	Source	Record Type	Info	PDF Viewer		Compou	nds (grid)	Compounds (table)	
LC/MS/MS	Environmental Chemistry Methods	Method (PDF)		Structure D	TXSID		CASRN	Compound Name	
LC/MS/MS	Environmental Chemistry Methods	Method (PDF)			17,510		CASINI	compound Name	
LC/MS/MS	Environmental Chemistry Methods	Method (PDF)			DTXSID9058107		494793-67-8	Penflufen	
LC/MS/MS	Environmental Chemistry Methods	Method ( <u>PDF</u> )			1721030	10101	494795-07-0	remulen	
					TXSID60	1024859	NOCAS_1024859	N-(2-Acetylphenyl)-5-fluoro-1,3-dime	

## How many methods do we have?



- We have 2765 method documents to extract
- 30% have been extracted ca. 25 small docs per day or 3-5 big docs per day

B1 $\rightarrow$ : $\times \checkmark f_x$								
	А	В	С	D	E	F	G	
		Refresh	button to get all file					
1	Summary		names and counts from L:					
2					r		1	
3	Text file with chemi -	Date textfile upd	Pdf file 🕞	Date pdf update	pdf size 🗖	Chen -	Folder	
4	GJ-014.txt	8/8/2022 12:45	CLG_AVR_1_03.pdf	8/4/2022 14:08	540323	7	:\Lab\NCCT_Richard\GregoryJa	
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• <u>williams.antony@epa.gov</u>