Accessing Environmental Chemistry Data via Data Dashboards

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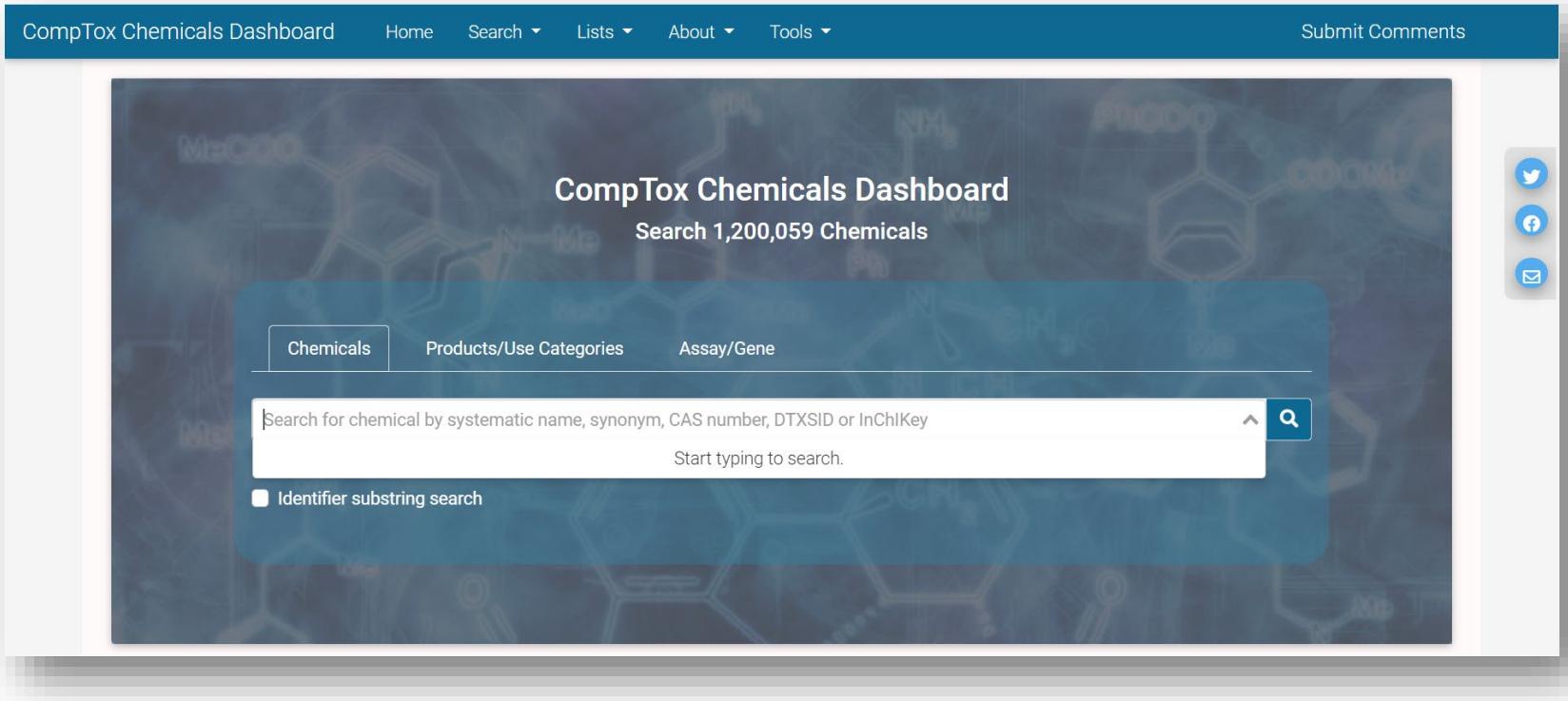
The Charge for the Dashboard

- 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

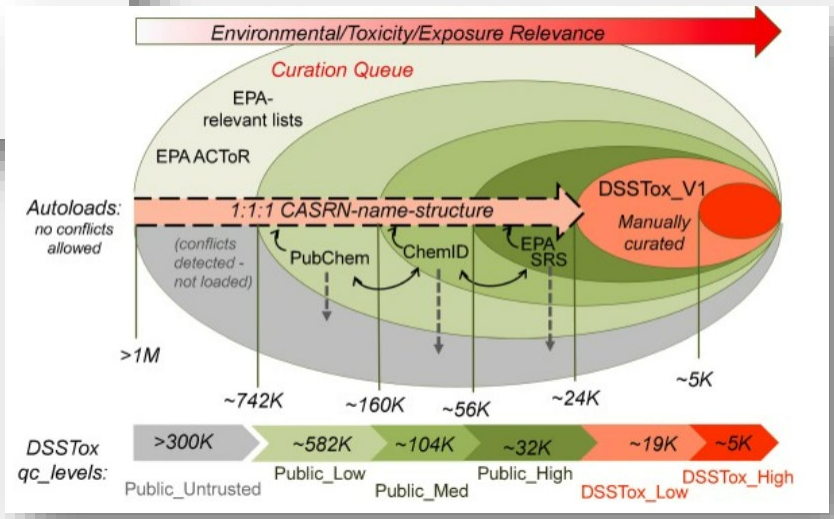
ELSEVIER

Computational Toxicology

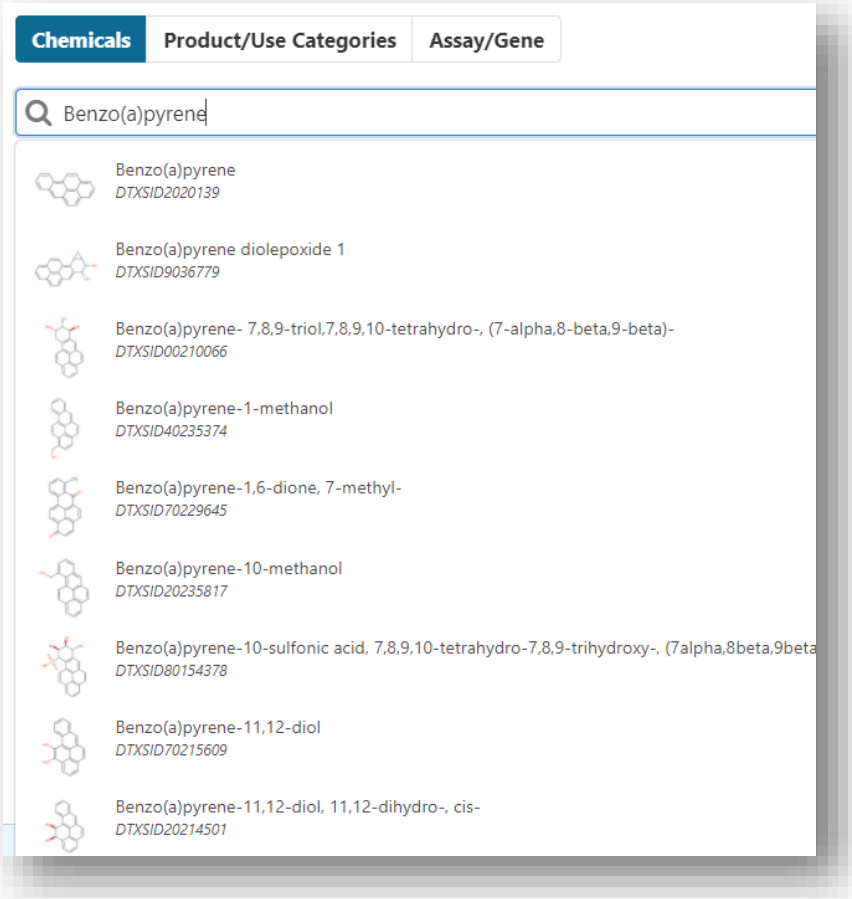
Volume 12, November 2019, 100096

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

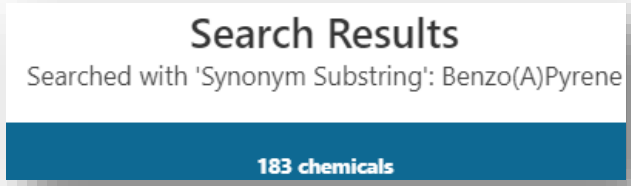
Christopher M. Grulke [a], Antony J. Williams [a], Inthirany Thillanadarajah [b], Ann M. Richard [a]



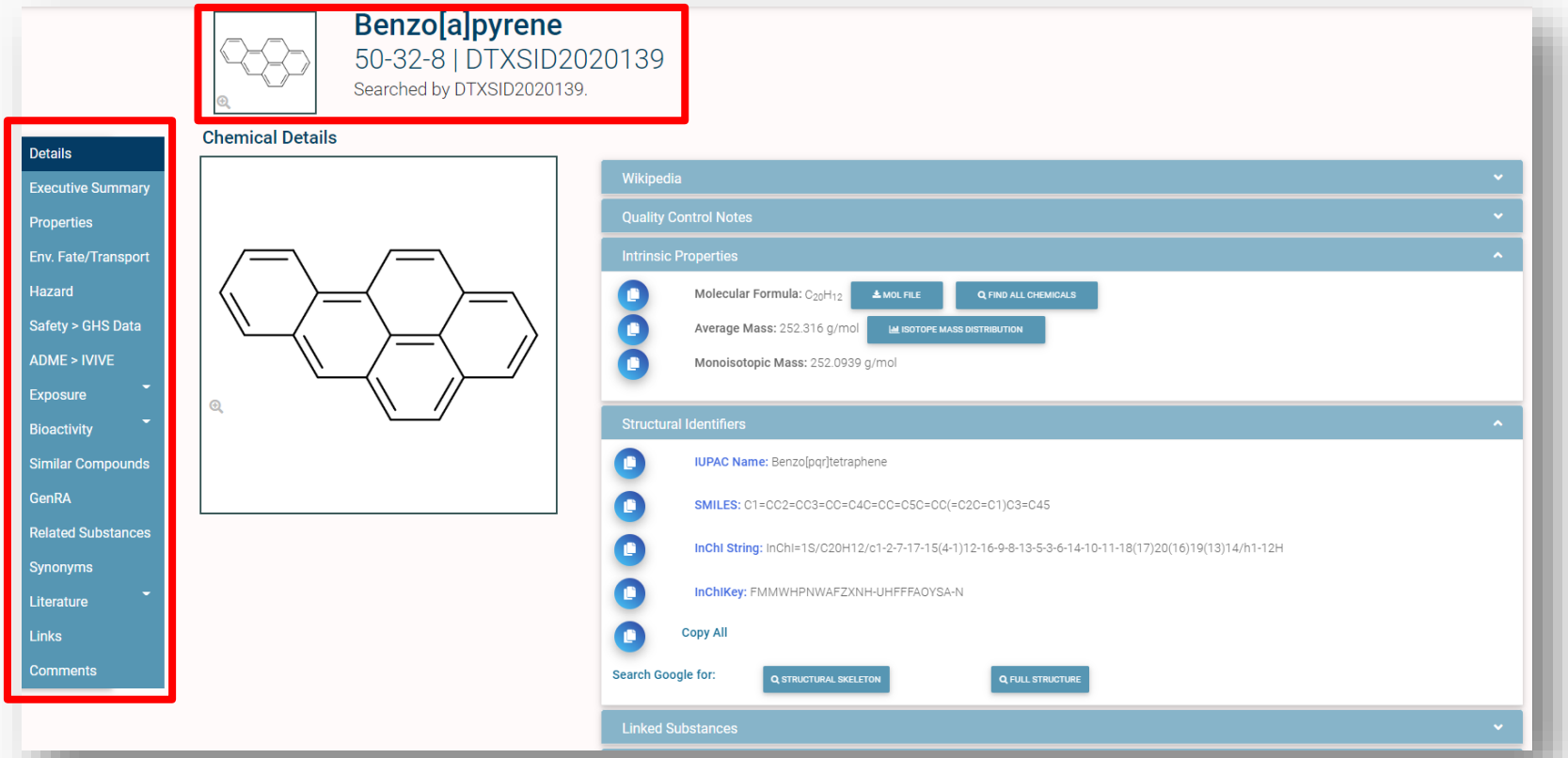
BASIC Search



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

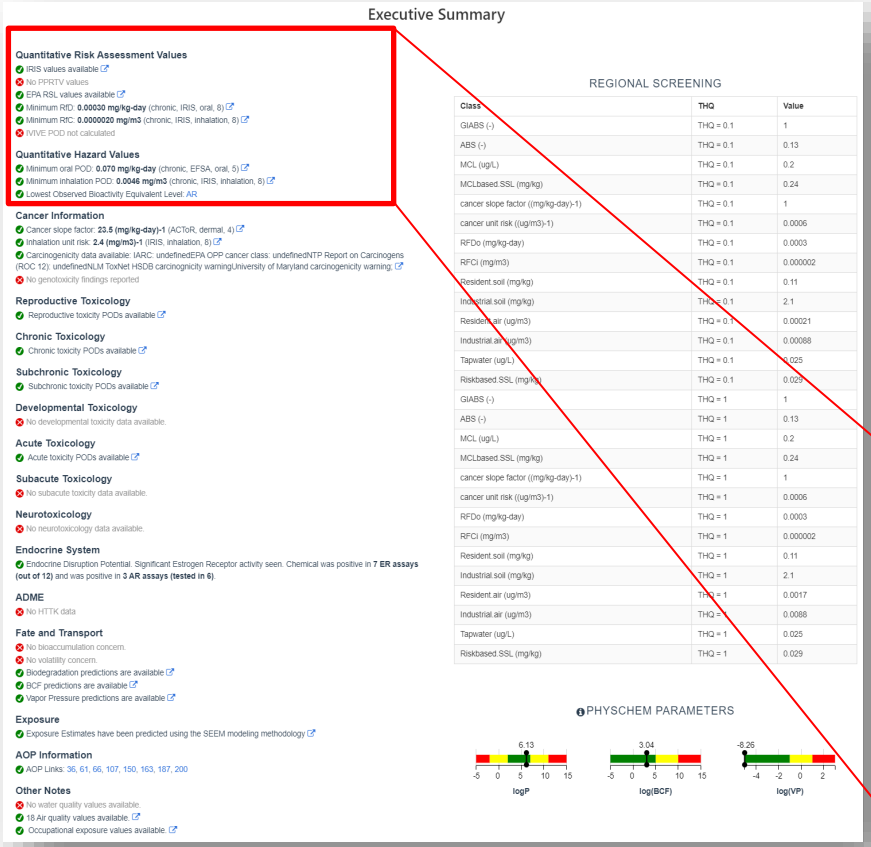


Detailed Chemical Pages



- Intrinsic properties, structural identifiers, linked substances

“Executive Summary”



- Overview of toxicity-related info
  - Quantitative values
  - Info re. toxicology subsets
  - Physchem. and Fate & Transport
  - Adverse Outcome Pathway links
  - *In vitro* bioactivity summary plot

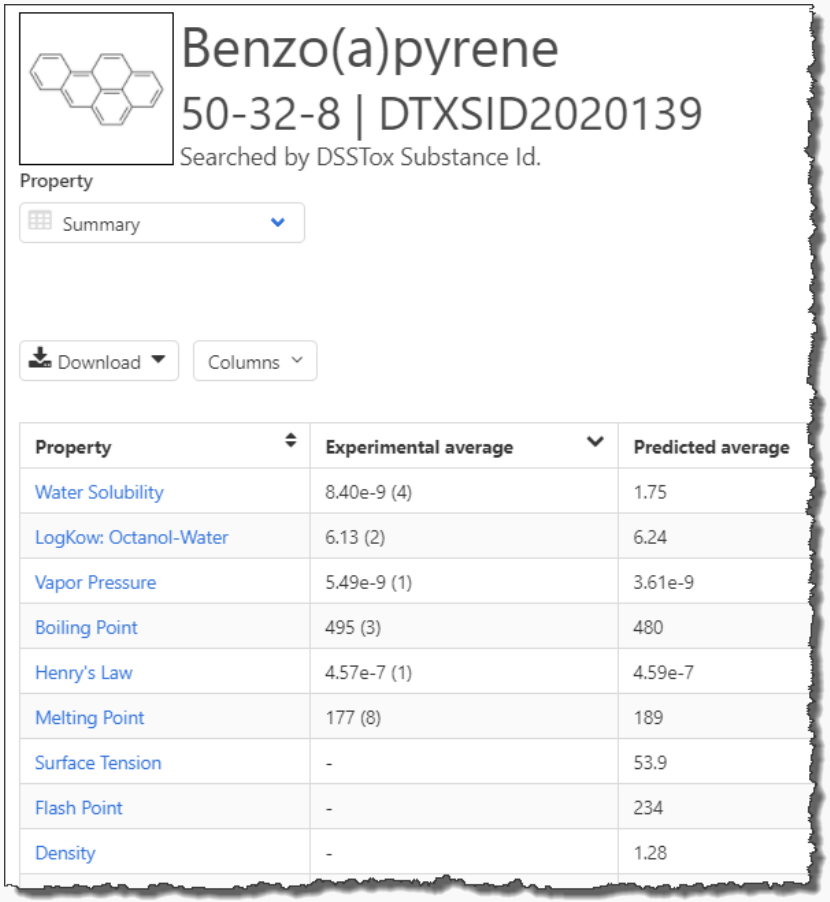
Quantitative Risk Assessment Values

- IRIS values available
- No PPRTV values
- EPA RSL values available
- Minimum RfD: **0.00030 mg/kg-day** (chronic, IRIS, oral, 8)
- Minimum RfC: **0.0000020 mg/m3** (chronic, IRIS, inhalation, 8)
- IVIVE POD not calculated

Quantitative Hazard Values

- Minimum oral POD: **0.070 mg/kg-day** (chronic, EFSA, oral, 5)
- Minimum inhalation POD: **0.0046 mg/m3** (chronic, IRIS, inhalation, 8)
- Lowest Observed Bioactivity Equivalent Level: AR

Experimental and Predicted Data



Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

Property

Summary

Download Columns

Property	Experimental average	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
Density	-	1.28

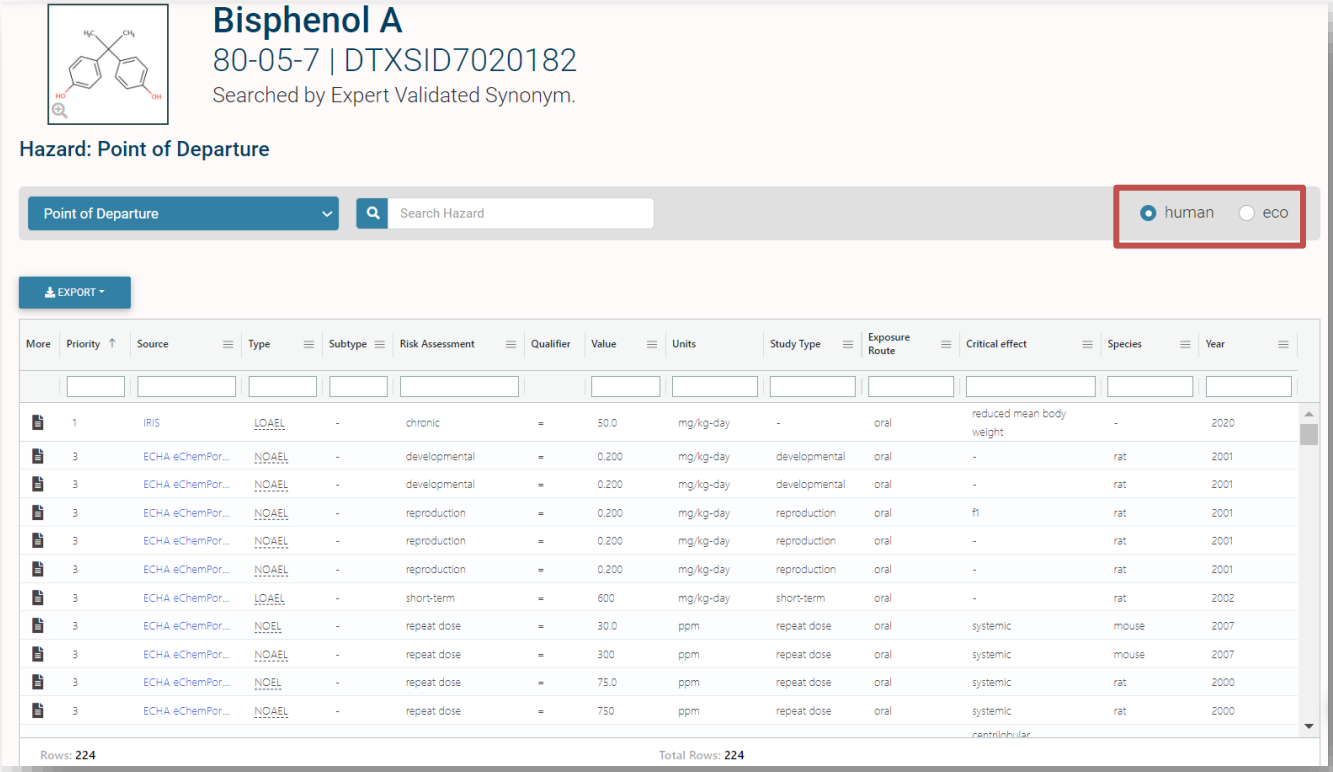
- Physchem and Fate & Transport experimental and predicted data
- Data can be downloaded as Excel, TSV and CSV files
- Predictions: multiple algorithms
  - EPI Suite: Estimation Program Interface
  - ACD/Labs (commercial)
  - TEST: Toxicity Estimation Software Tool
  - OPERA: OPEn structure–activity/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

Chemical Hazard Data

EPA United States Environmental Protection Agency

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

Point of Departure | Search Hazard | human | eco

EXPORT

More	Priority	Source	Type	Subtype	Risk Assessment	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
	3	ECHA eChemPor...	NOAEL	-	developmental	=	0.200	mg/kg-day	developmental	oral	-	rat	2001
	3	ECHA eChemPor...	NOAEL	-	developmental	=	0.200	mg/kg-day	developmental	oral	-	rat	2001
	3	ECHA eChemPor...	NOAEL	-	reproduction	=	0.200	mg/kg-day	reproduction	oral	fl	rat	2001
	3	ECHA eChemPor...	NOAEL	-	reproduction	=	0.200	mg/kg-day	reproduction	oral	-	rat	2001
	3	ECHA eChemPor...	NOAEL	-	reproduction	=	0.200	mg/kg-day	reproduction	oral	-	rat	2001
	3	ECHA eChemPor...	LOAEL	-	short-term	=	600	mg/kg-day	short-term	oral	-	rat	2002
	3	ECHA eChemPor...	NOEL	-	repeat dose	=	30.0	ppm	repeat dose	oral	systemic	mouse	2007
	3	ECHA eChemPor...	NOAEL	-	repeat dose	=	300	ppm	repeat dose	oral	systemic	mouse	2007
	3	ECHA eChemPor...	NOEL	-	repeat dose	=	75.0	ppm	repeat dose	oral	systemic	rat	2000
	3	ECHA eChemPor...	NOAEL	-	repeat dose	=	750	ppm	repeat dose	oral	systemic	rat	2000

Rows: 224 Total Rows: 224

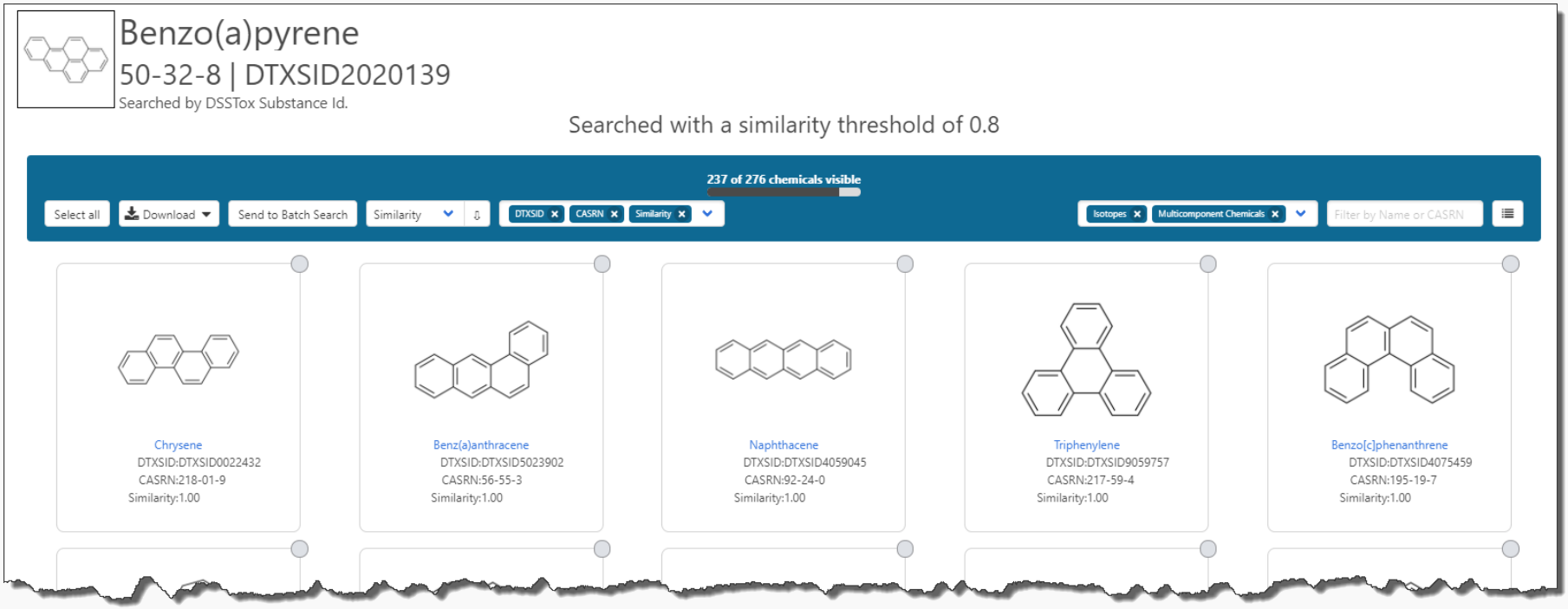
Hazard Data for Copper

- 2246 rows of human/eco hazard data

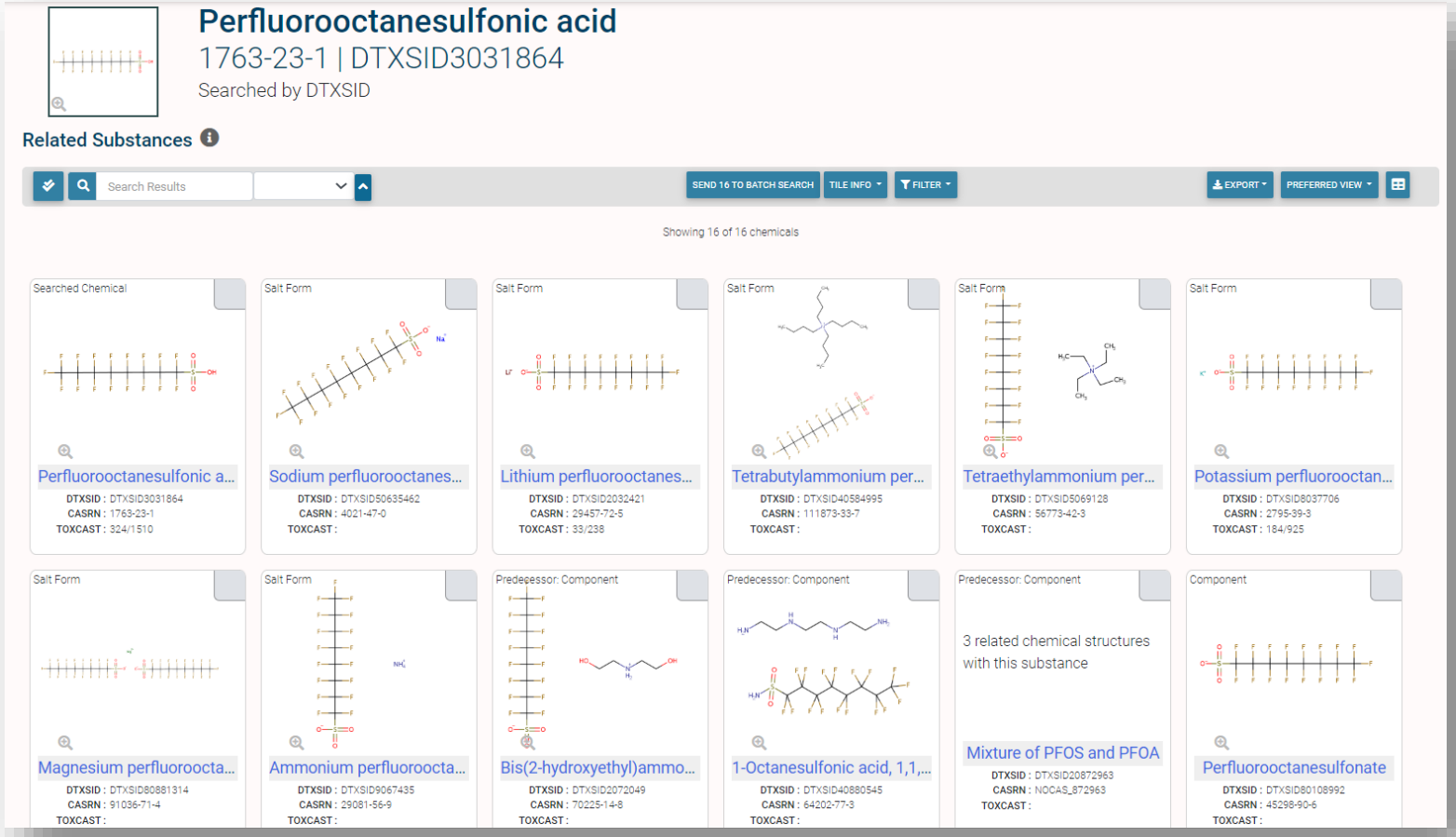
	SOURCE	SUB_SOUI	TOXVAL_T	TOXVAL_TYPE_ORIGINAL	TOXVAL_TYPE_SUP	TOXVAL_T	QUALIFIEF	TOXVAL_N	TOXVAL_N	TOXVAL_U	TOXVAL_U	RISK_ASSE
2	ATSDR MRLs 2020	CDC	MRL	ATSDR MRL	Toxicity Value	MRL	=	0.01	0.01	mg/kg-da	mg/kg/da	acute
3	ATSDR MRLs 2020	CDC	NOAEL	NOAEL	Point of Departure	NOAEL	=	0.03	0.03	mg/kg-da	mg/kg/da	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	1.3	mg/L	mg/L	chronic
6	California DPH	California	OEHHA PH	OEHHA PHG	Exposure Limit	Public Hea	=	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	Toxicity Value	REL	=	100	100	ug/m3	ug/m3	acute
9	Copper Manufacturers	Copper De	adequate	AI (adequate intake)			=	0.4	0.4	mg/day	mg/day	chronic
10	Copper Manufacturers	Copper De	adequate	AI (adequate intake)			=	0.7	0.7	mg/day	mg/day	chronic
11	Copper Manufacturers	Copper De	adequate	AI (adequate intake)			=	1	1	mg/day	mg/day	chronic
12	Copper Manufacturers	Copper De	adequate	AI (adequate intake)			=	1.1	1.1	mg/day	mg/day	chronic
13	Copper Manufacturers	Copper De	adequate	AI (adequate intake)			=	1.3	1.3	mg/day	mg/day	chronic
14	Copper Manufacturers	Copper De	adequate	AI (adequate intake)			=	1.5	1.5	mg/day	mg/day	chronic
15	Copper Manufacturers	Copper De	adequate	AI (adequate intake)			=	1.6	1.6	mg/day	mg/day	chronic
16	Copper Manufacturers	Copper De	drinking w	GDWQ (guideline for drinking water quality)			=	2	2	mg/L	mg/L	chronic
17	Copper Manufacturers	Copper De	LOAEL	LOAEL	Point of Departure	LOAEL	=	7	7	mg/day	mg/day	subchroni
18	Copper Manufacturers	Copper De	optimal in	Optimal intake value	Misc Information	Optimal in	=	2.6	2.6	mg/day	mg/day	chronic
19	Copper Manufacturers	Copper De	RDA	RDA (recommended dietary allowance)			=	0.2	0.2	mg/day	mg/day	chronic
20	Copper Manufacturers	Copper De	RDA	RDA (recommended dietary allowance)			=	0.34	0.34	mg/day	mg/day	chronic
21	Copper Manufacturers	Copper De	RDA	RDA (recommended dietary allowance)			=	0.7	0.7	mg/day	mg/day	chronic

Cover Sheet | Main Data | Toxval Details

Similarity Searching



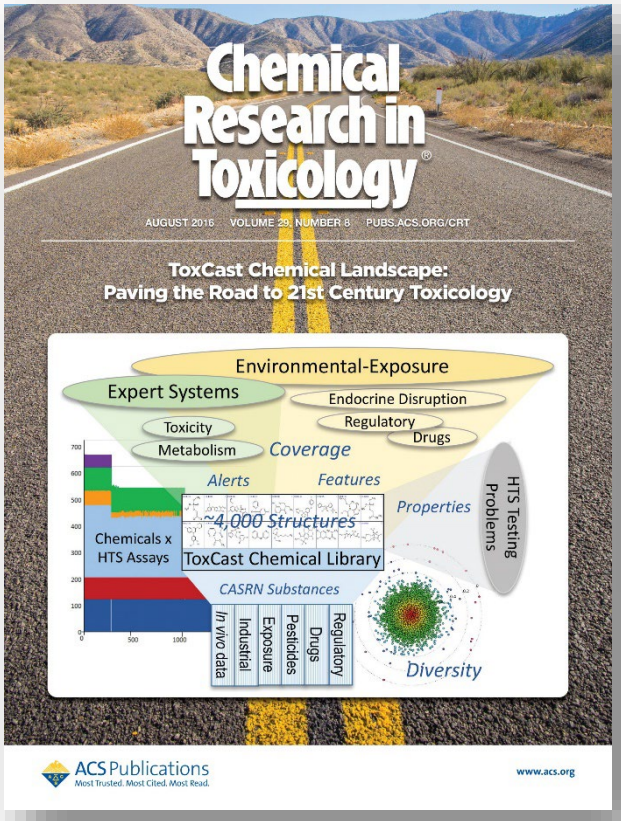
Related Substances



EPA
United States
Environmental Protection
Agency

Bioactivity Data

ToxCast



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

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

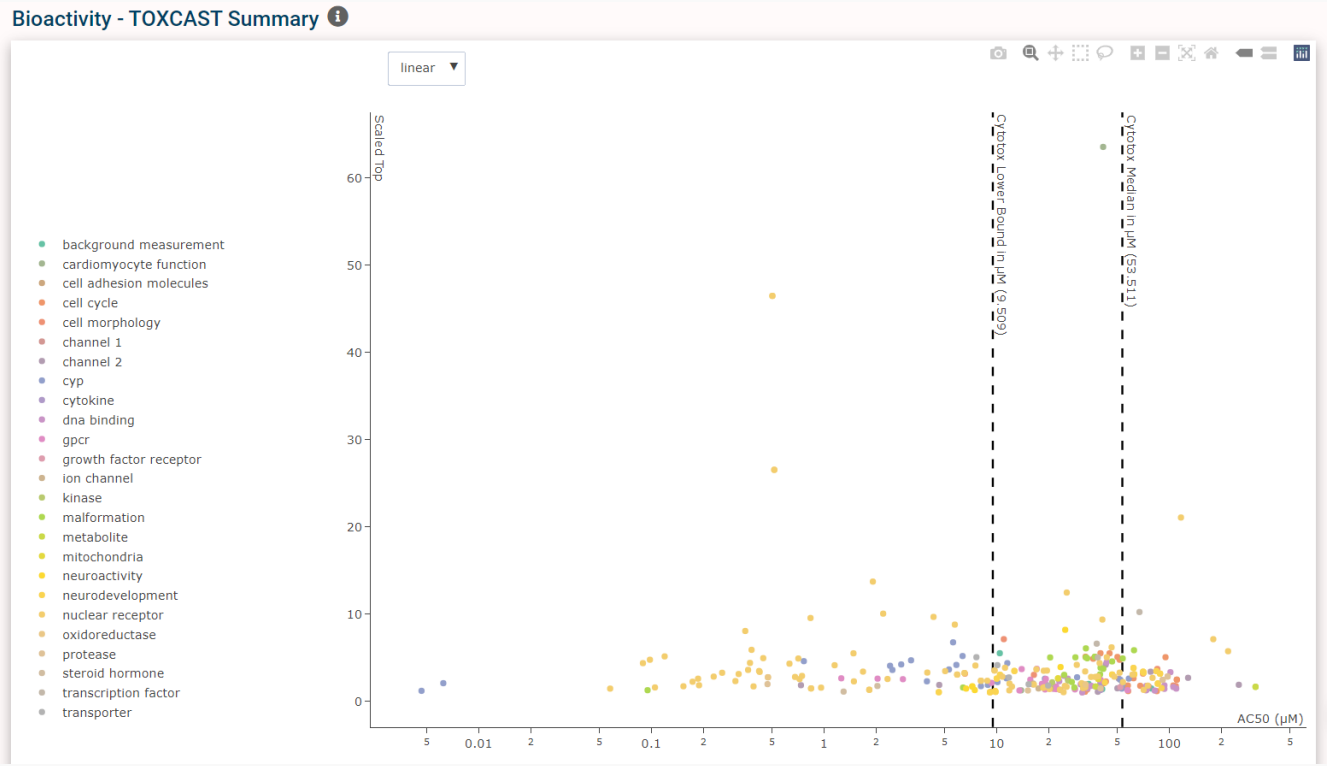
Bioactivity Data

Summary views of >2000 Assay Endpoints

EPA United States Environmental Protection Agency

Bioactivity

- ToxCast: Summary
- Toxcast Conc. Response Data
- HTTr: Summary
- HTPP: Summary
- PubChem
- ToxCast: Models



Bioactivity Data
Full transparency of data…

EPA United States Environmental Protection Agency

Bioactivity

- ToxCast: Summary
- Toxcast Conc. Response Data
- HTTr: Summary
- HTPP: Summary
- PubChem
- ToxCast: Models

Concentration Response Data

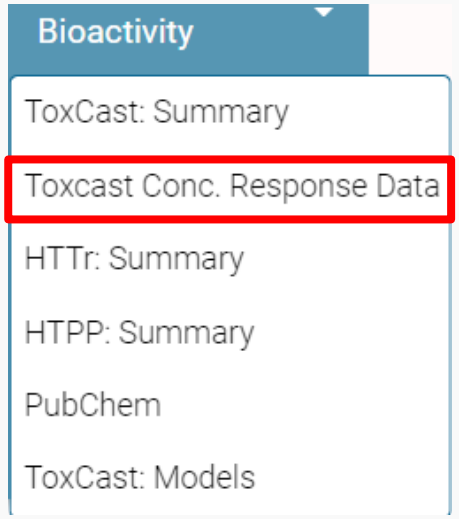
Analytical Data on Tox21 Browser

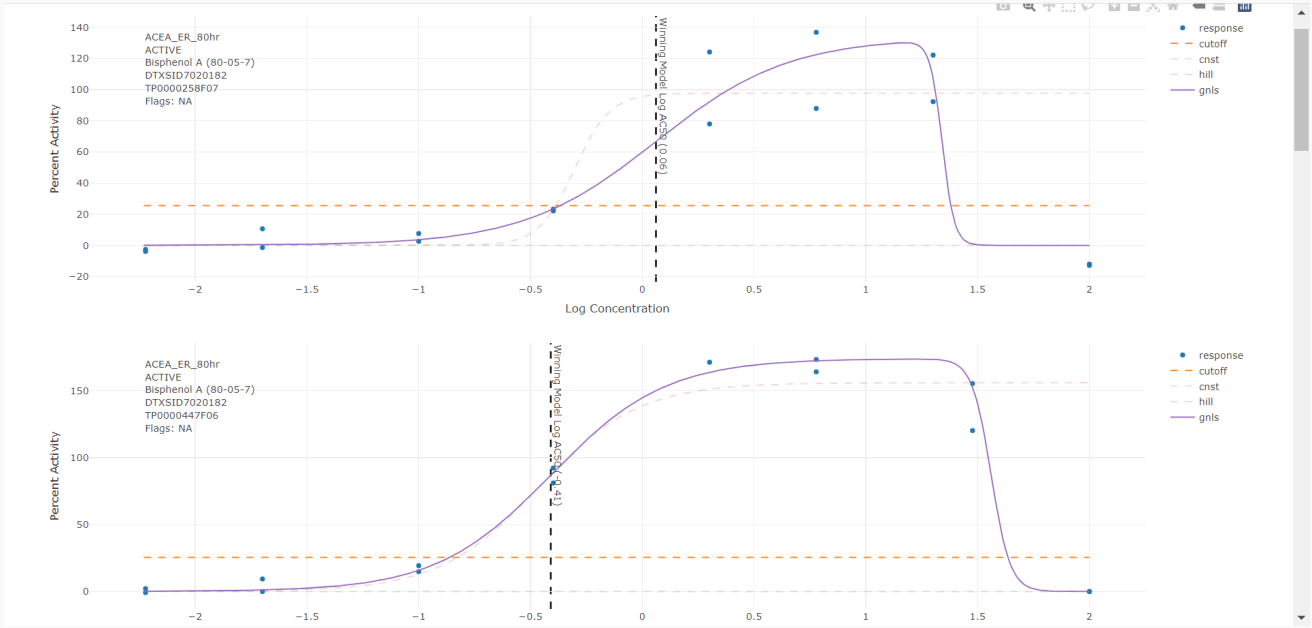
EXPORT

Name	Description	Endpoint Name	Active	Details	Rep. Plot	All Plots	Gene	Intended Target	Cell Line	Cell Format
ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_agonist_80hr	Inactive				AR	steroidal	prostate	cell line
ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_agonist_AUC_viability	Active				-	cytotoxicity	prostate	cell line
ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_antagonist_80hr	Active				AR	steroidal	prostate	cell line
ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_antagonist_AUC_viability	Active				-	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				-	cytotoxicity	breast	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_1h_dn	Inactive				-	proliferation	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_1h_up	Inactive				-	arrest	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_24h_dn	Inactive				-	proliferation	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_24h_up	Inactive				-	arrest	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_72h_dn	Inactive				-	proliferation	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_72h_up	Inactive				-	arrest	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellLoss_1h_dn	Inactive				-	cytotoxicity	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellLoss_1h_up	Inactive				-	proliferation	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellLoss_24h_dn	Active				-	cytotoxicity	liver	cell line

Rows: 1,398 Total Rows: 1,398

Bioactivity Data
…including concentration-response





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

Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

General

- EPA Substance Registry Service
- PubChem
- Chemspider
- CPCat
- DrugBank
- Wikipedia
- MSDS Lookup
- ChEMBL
- ToxPlanet
- ACS Reagent Chemicals
- Wolfram Alpha
- ECHA Infocard
- ChemAgora
- Consumer Product Information Database
- ChEBI
- NIST Chemistry Webbook
- WEBWISER
- PubChem Safety Sheet
- Consumer Product Information Database
- PubChem: Chemical Vendors

Toxicology

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

Publications

- Toxline
- PPRTVWEB
- 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
- Google Books (Text Search)
- Google Patents (Text search)
- Google Scholar (Text search)
- Google Patents (Structure search)
- Google Books (Structure Search)
- Google Scholar (Structure search)
- Federal Register

Analytical

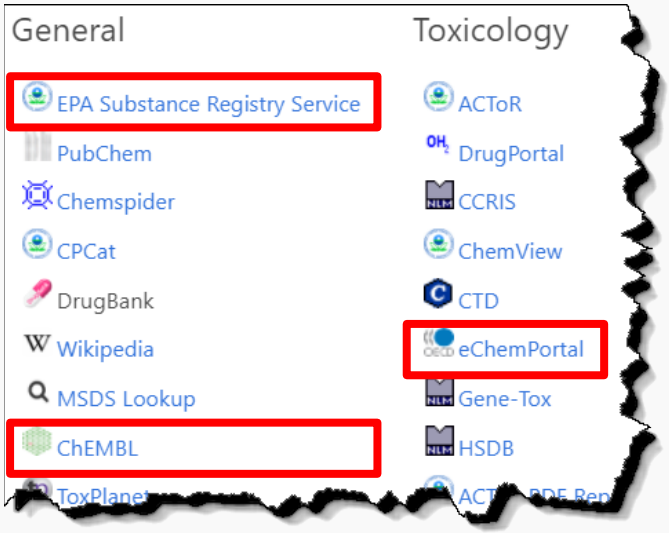
- RSC Analytical Abstracts
- Tox21 Analytical Data
- MONA: MassBank North America
- mzCloud
- NIST IR Spectrum
- NIST MS Spectrum
- MassBank
- NIST Antoine Constants
- IR Spectra on PubChem
- NIST Kovats Index values
- Protein DataBank
- National Environmental Methods Index

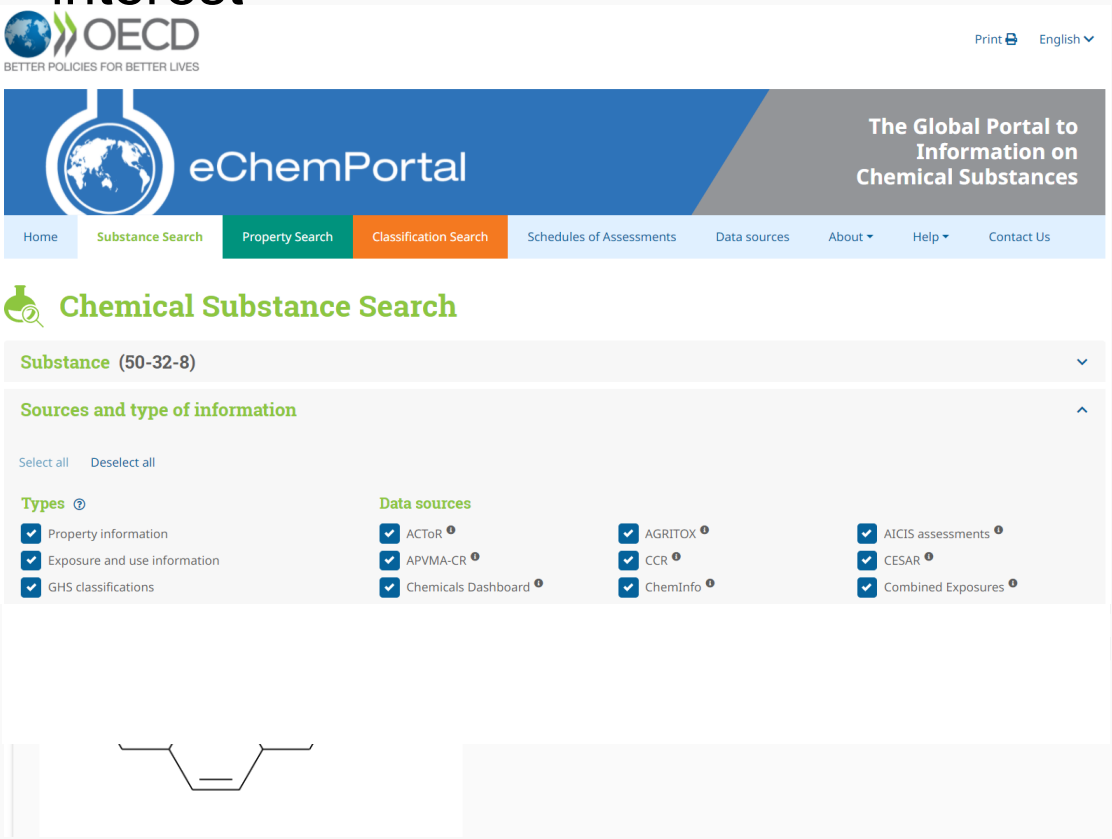
Prediction

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

External Links

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





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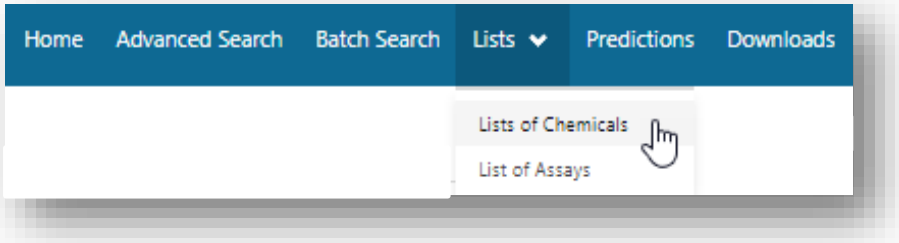
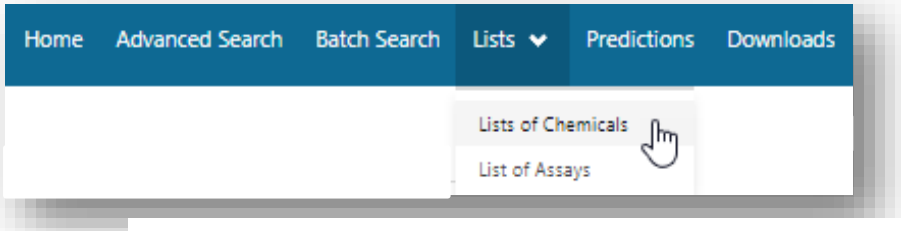
Chemical Lists and Categories

Example: PFAS Structure Lists



Example: PFAS Structure Lists



frontiers | Frontiers in Environmental Science

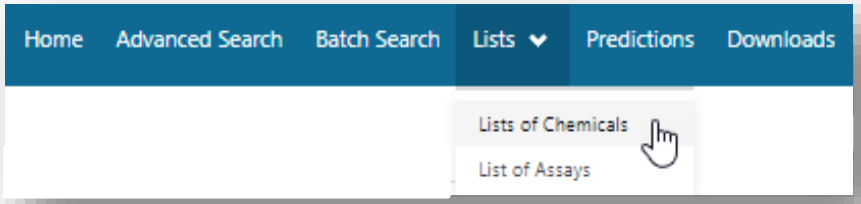
ORIGINAL RESEARCH
published: 05 April 2022
doi: 10.3389/fenvs.2022.850019

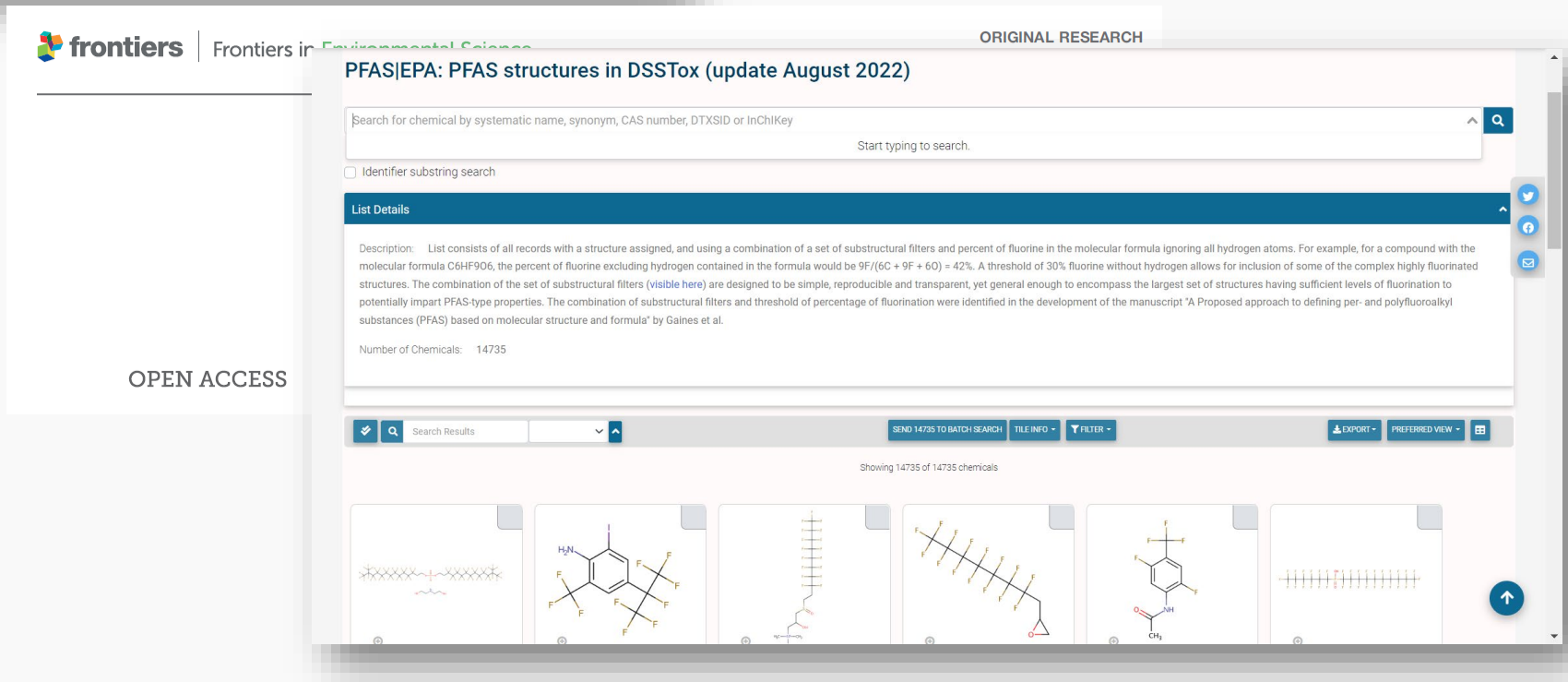
Assembly and Curation of Lists of Per- and Polyfluoroalkyl Substances (PFAS) to Support Environmental Science Research

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

OPEN ACCESS

Example: PFAS Structure Lists





PFAS lists of Chemicals

EPA United States Environmental Protection Agency

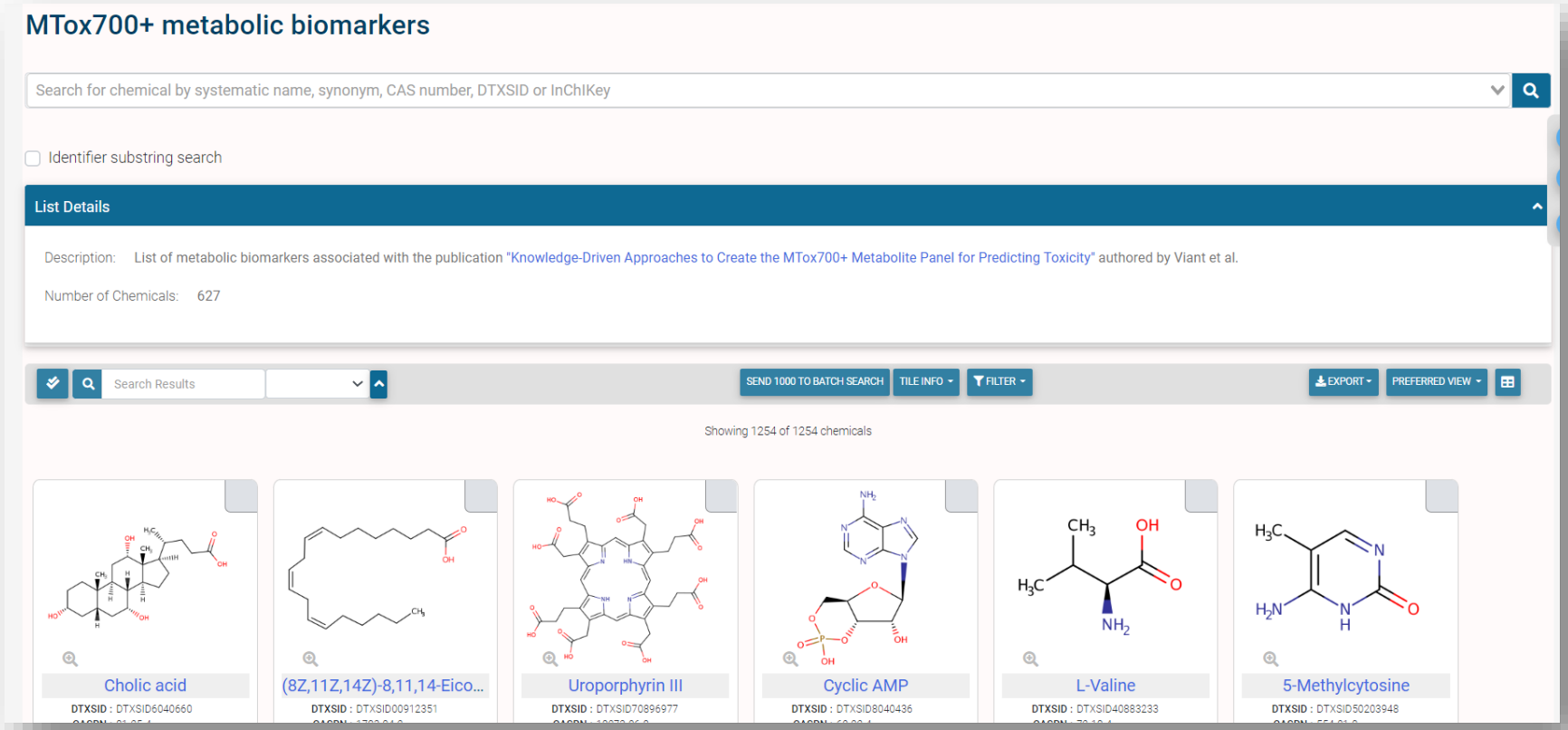
Select List

Download | Columns | PFAS | Copy Filtered Lists URL

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

10 records

MTOX biomarkers



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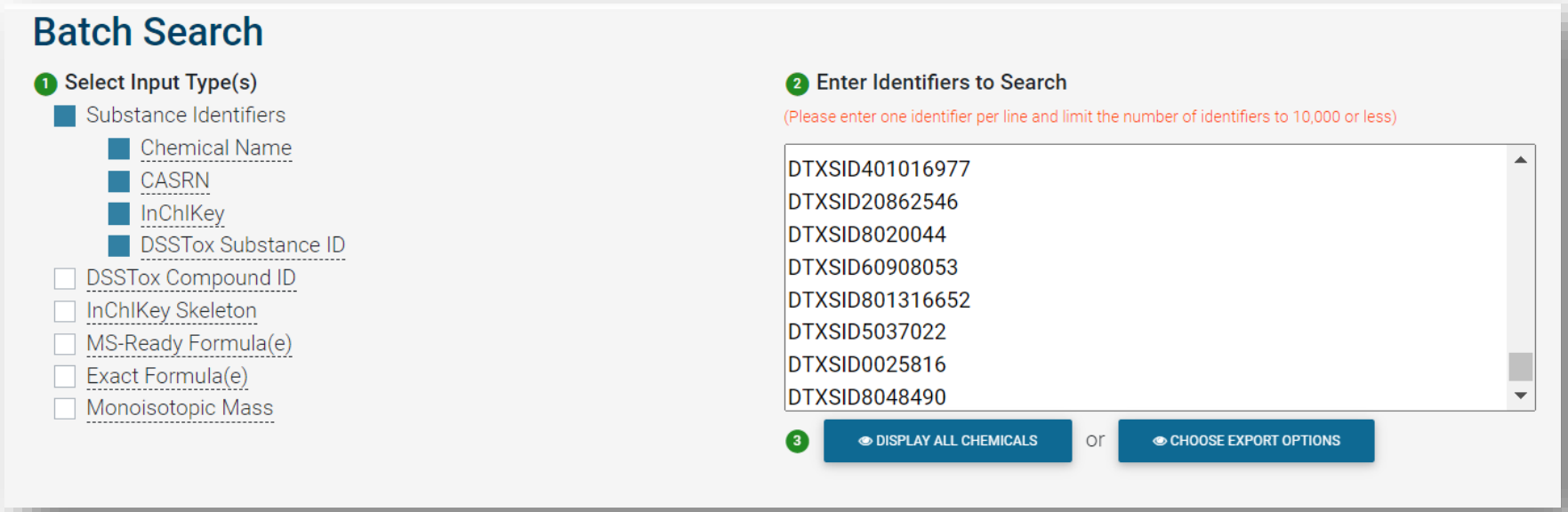
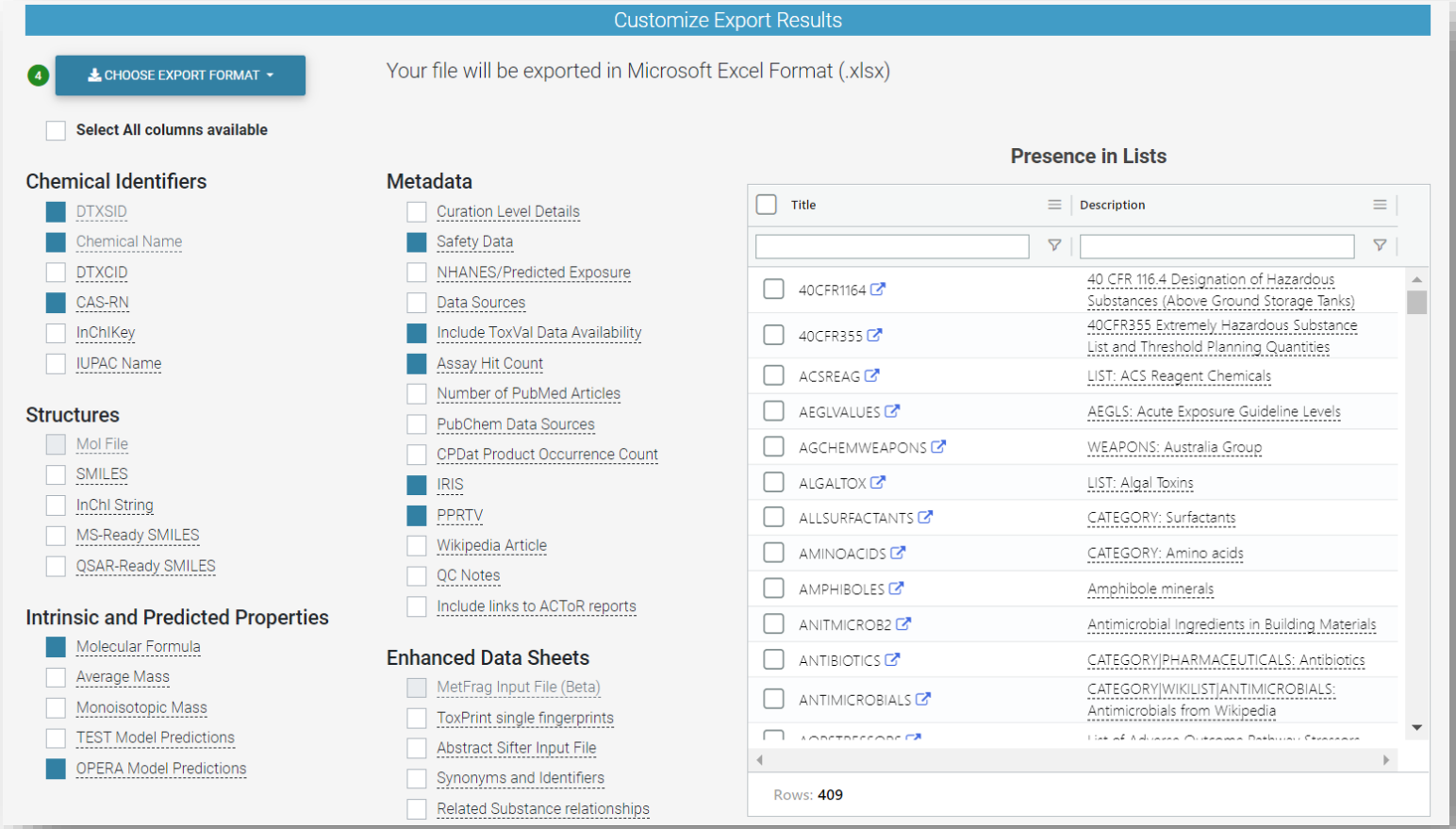
Batch Searching

Batch Search CASRNs Mtox 700 Biomarkers

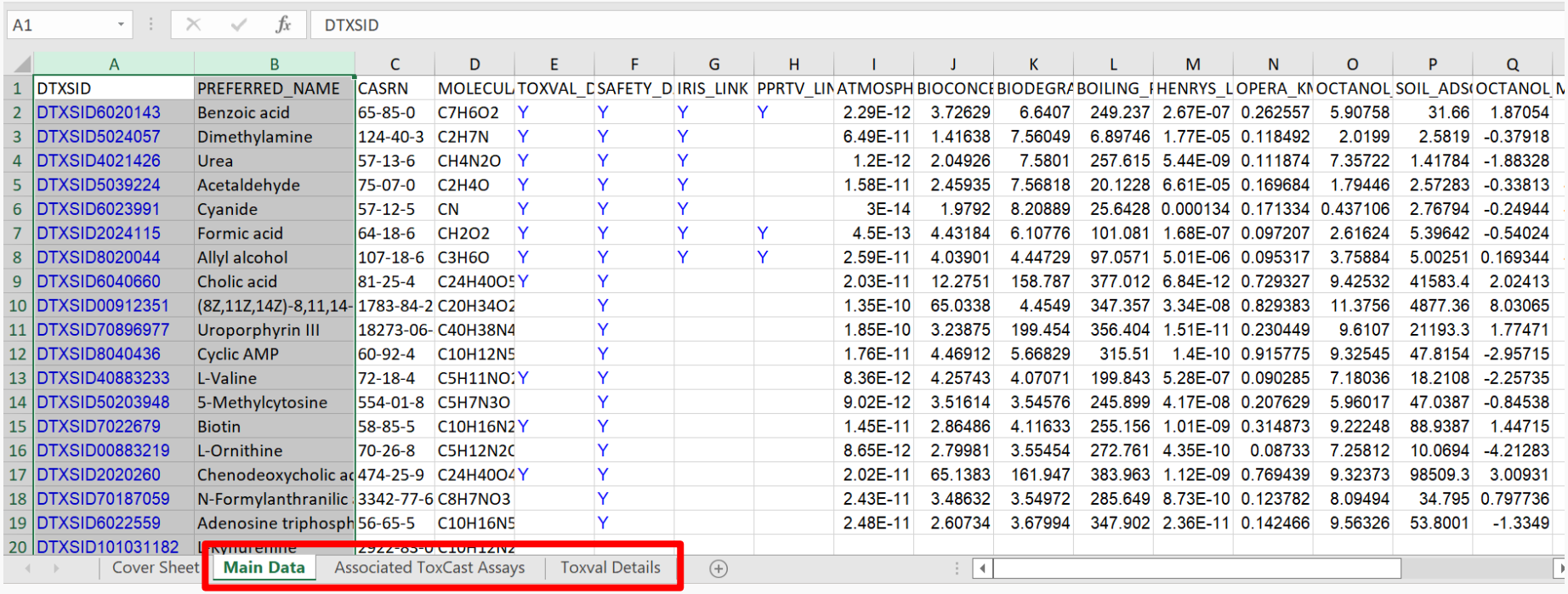


Download Batches of Data



Chemistry Data in one sheet

EPA United States Environmental Protection Agency

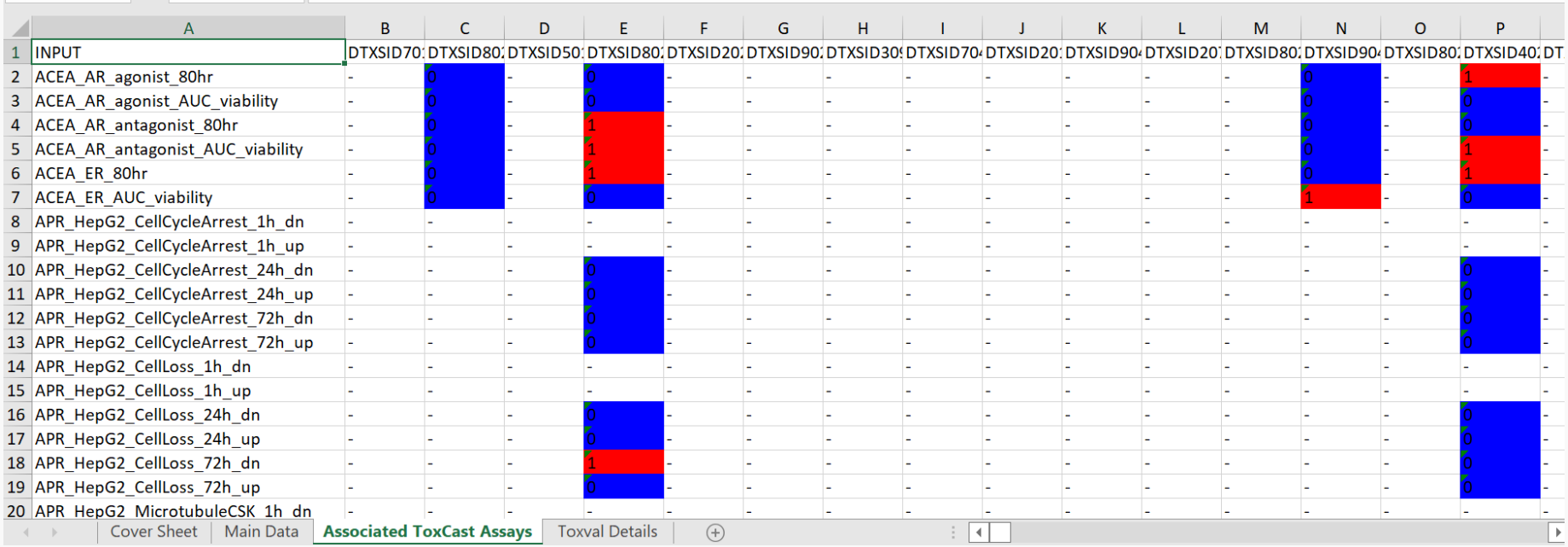


A1 | DTXSID

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	DTXSID	PREFERRED_NAME	CASRN	MOLECUL	TOXVAL_D	SAFETY_D	IRIS_LINK	PPRTV_LIN	ATMOSPH	BIOCONCE	BIODEGRA	BOILING_P	HENRYS_L	OPERA_KN	OCTANOL_	SOIL_ADS(	OCTANOL_M
2	DTXSID6020143	Benzoic acid	65-85-0	C7H6O2	Y	Y	Y	Y	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	Y	Y	Y		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	Y	Y	Y		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	Y	Y	Y		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	Y	Y	Y		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	Y	Y	Y	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	Y	Y	Y	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	C24H40O5	Y	Y			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		Y			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		Y			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		Y			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	C5H11NO2	Y	Y			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		Y			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	Y			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	C5H12N2O		Y			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	Y			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		Y			2.48E-11	2.60734	3.67994	347.902	2.36E-11	0.142466	9.56326	53.8001	-1.3349
20	DTXSID101031182	L-Kynurenine	2922-83-0	C10H12N2													

Cover Sheet | Main Data | Associated ToxCast Assays | Toxval Details

Bioactivity Data in another sheet



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	
1	INPUT	DTXSID70	DTXSID80	DTXSID50	DTXSID80	DTXSID20	DTXSID90	DTXSID30	DTXSID70	DTXSID20	DTXSID90	DTXSID20	DTXSID80	DTXSID90	DTXSID80	DTXSID40	DT
2	ACEA_AR_agonist_80hr	-	0	-	0	-	-	-	-	-	-	-	-	0	-	1	-
3	ACEA_AR_agonist_AUC_viability	-	0	-	0	-	-	-	-	-	-	-	-	0	-	0	-
4	ACEA_AR_antagonist_80hr	-	0	-	1	-	-	-	-	-	-	-	-	0	-	0	-
5	ACEA_AR_antagonist_AUC_viability	-	0	-	1	-	-	-	-	-	-	-	-	0	-	1	-
6	ACEA_ER_80hr	-	0	-	1	-	-	-	-	-	-	-	-	0	-	1	-
7	ACEA_ER_AUC_viability	-	0	-	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	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

Cover Sheet | Main Data | **Associated ToxCast Assays** | Toxval Details

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

EPA United States Environmental Protection Agency

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q	R	S	
1	SEARCHED	DTXSID	CASRN	NAME	SOURCE	SUB_SOUF	TOXVAL_T	TOXVAL_T	TOXVAL_S	TOXVAL_T	TOXVAL_T	QUALIFIEF	TOXVAL_N	TOXVAL_N	TOXVAL_U	TOXVAL_U	RISK_ASSE	STUDY_TY	STUDY_TY	ST
2	Cholic acic	DTXSID60	81-25-4	Cholic acic	ECHA IUCL	EU REACH	concentra	dose level	-	Exposure	-	=	500	500	mg/kg-da	mg/kg-da	repeat do	repeat do	repeat do	-
3	Cholic acic	DTXSID60	81-25-4	Cholic acic	ECHA IUCL	EU REACH	LD50	LD50	-	Lethality E	LD	=	2300	2300	mg/kg-da	mg/kg	acute	acute	acute	-
4	Cholic acic	DTXSID60	81-25-4	Cholic acic	ECHA IUCL	EU REACH	LD50	LD50	-	Lethality E	LD	=	4600	4600	mg/kg-da	mg/kg	acute	acute	acute	-
5	Cholic acic	DTXSID60	81-25-4	Cholic acic	ECHA IUCL	EU REACH	LD50	LD50	-	Lethality E	LD	=	4950	4950	mg/kg-da	mg/kg	acute	acute	acute	-
6	Cholic acic	DTXSID60	81-25-4	Cholic acic	ECHA IUCL	EU REACH	NOEC	NOEC	-	Point of D	NOEC	=	30.64	30.64	mg/L	mg/L	chronic	chronic	chronic	-
7	Cholic acic	DTXSID60	81-25-4	Cholic acic	ECHA IUCL	EU REACH	NOEC	NOEC	-	Point of D	NOEC	=	70.29	70.29	mg/L	mg/L	acute	acute	acute	-
8	Cholic acic	DTXSID60	81-25-4	Cholic acic	ECHA IUCL	EU REACH	NOEC	NOEC	-	Point of D	NOEC	=	75.52	75.52	mg/L	mg/L	acute	acute	acute	-
9	Cholic acic	DTXSID60	81-25-4	Cholic acic	ECOTOX	EPA ORD	LOEC	LOEC	-	Point of D	-	-	1	1	%	%	acute repr	Reproduct	Reproduct	ac
10	L-Valine	DTXSID40	72-18-4	L-Valine	COSMOS	US FDA CF	HNEL	HNEL	-	Point of D	HNEL	=	1	1	mM	mM	genotoxici	genotoxici	Genetic to	-
11	L-Valine	DTXSID40	72-18-4	L-Valine	COSMOS	US FDA CF	HNEL	HNEL	-	Point of D	HNEL	=	2	2	mg/ml	mg/ml	genotoxici	genotoxici	Genetic to	-
12	L-Valine	DTXSID40	72-18-4	L-Valine	COSMOS	US FDA CF	HNEL	HNEL	-	Point of D	HNEL	=	5	5	mg/plate	mg/plate	genotoxici	genotoxici	Genetic to	-
13	L-Valine	DTXSID40	72-18-4	L-Valine	COSMOS	US FDA CF	HNEL	HNEL	-	Point of D	HNEL	=	1853	1853	mg/kg-da	mg/kg bw	subchroni	subchroni	Subchroni	-
14	L-Valine	DTXSID40	72-18-4	L-Valine	COSMOS	US FDA CF	LEL	LEL	-	Point of D	LEL	=	1	1	mM	mM	genotoxici	genotoxici	Genetic to	-
15	L-Valine	DTXSID40	72-18-4	L-Valine	COSMOS	US FDA CF	LEL	LEL	-	Point of D	LEL	=	3721	3721	mg/kg-da	mg/kg bw	subchroni	subchroni	Subchroni	-
16	L-Valine	DTXSID40	72-18-4	L-Valine	ECHA	eChemPor	NOAEL	NOAEL	repeat do	Point of D	NOAEL	=	628	628	mg/kg-da	mg/kg bw	subchroni	subchroni	subchroni	-
17	L-Valine	DTXSID40	72-18-4	L-Valine	ECHA	eChemPor	NOAEL	NOAEL	repeat do	Point of D	NOAEL	=	666	666	mg/kg-da	mg/kg bw	subchroni	subchroni	subchroni	-
18	L-Valine	DTXSID40	72-18-4	L-Valine	ECHA	eChemPor	NOEC	NOEC	eco aquat	Point of D	NOEC	=	3.2	3.2	g/L	g/L	chronic	static	static	-
19	L-Valine	DTXSID40	72-18-4	L-Valine	ECHA eCh	ECHA REA	LD50	LD50	-	Lethality E	LD	>	2000	2000	mg/kg	mg/kg bw	acute	acute	acute toxi	ac
20	L-Valine	DTXSID40	72-18-4	L-Valine	ECHA eCh	ECHA REA	NOAEL	NOAEL	-	Point of D	NOAEL	=	610	610	mg/kg-da	mg/kg bw	developm	developm	developm	de

Cover Sheet | Main Data | Associated ToxCast Assays | **Toxval Details**

Cheminformatics Proof-of-Concept Modules

(PUBLICLY AVAILABLE)

Disclaimer and Info

- Software is available at
- https://www.epa.gov/chemical-research/cheminformatics

- Please understand it is proof-of-concept so reach out to me for help if necessary

LIVE DEMO

How to Use HCD

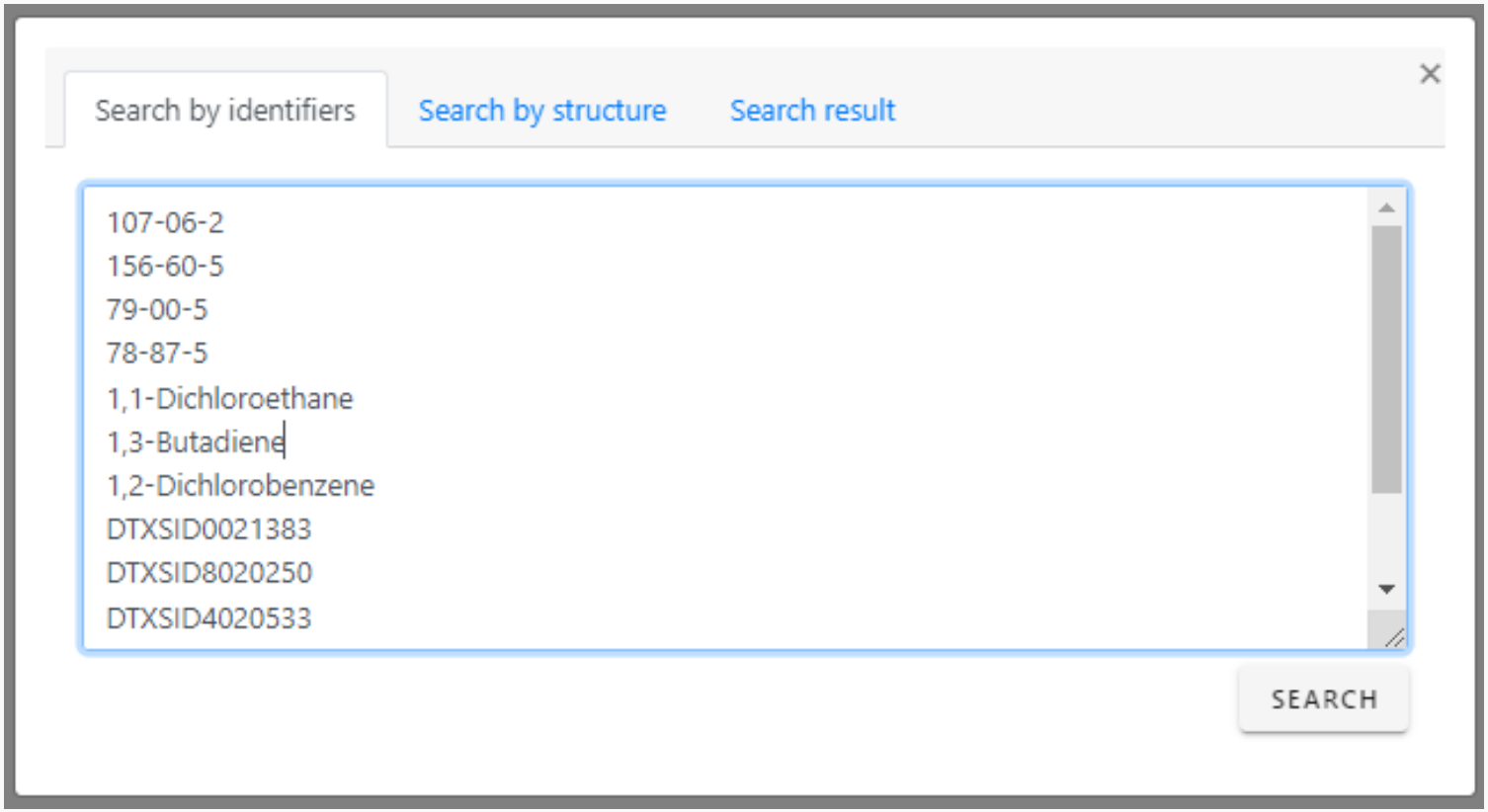
- Always start with INPUTs

- Choose the magnifying glass

- Search based on CAS RNs, Names, DTXSIDs from the Dashboard

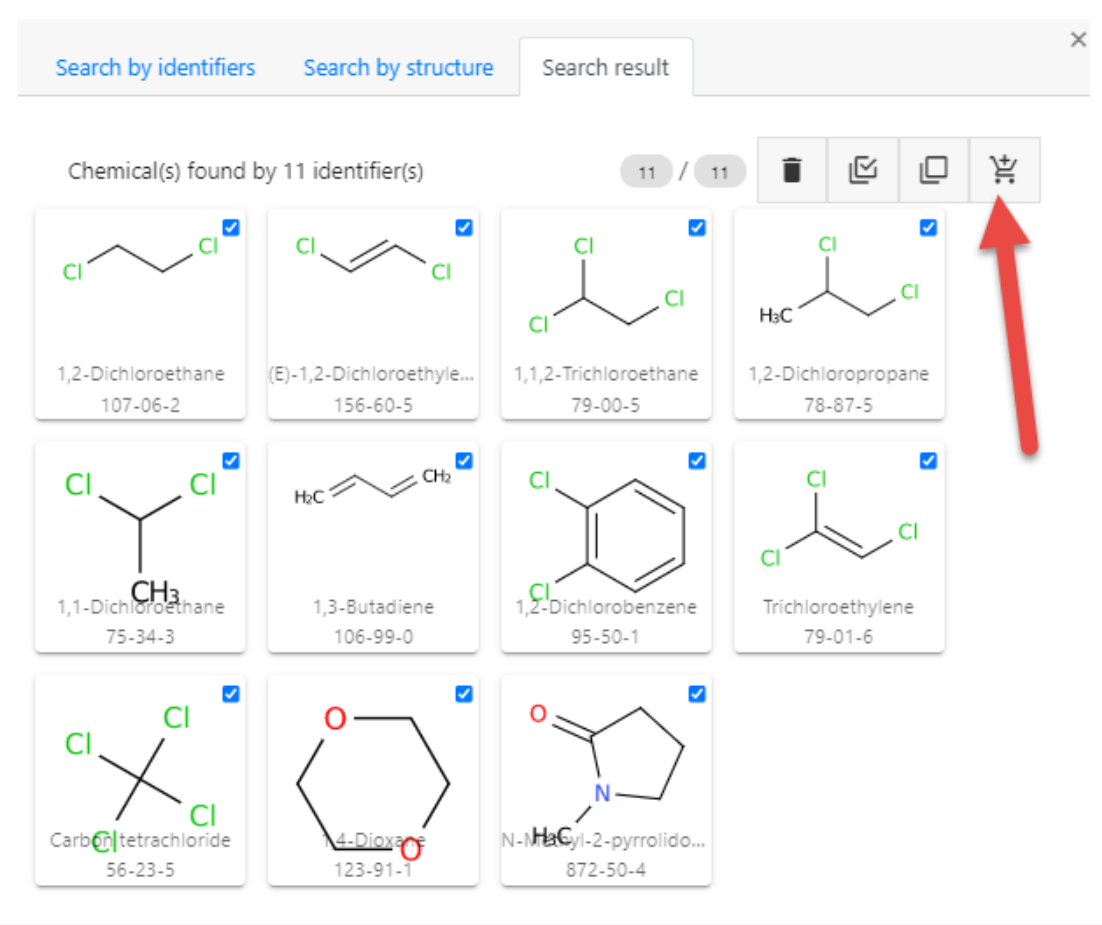
Basic Search

- Paste them into the search box. Click Search



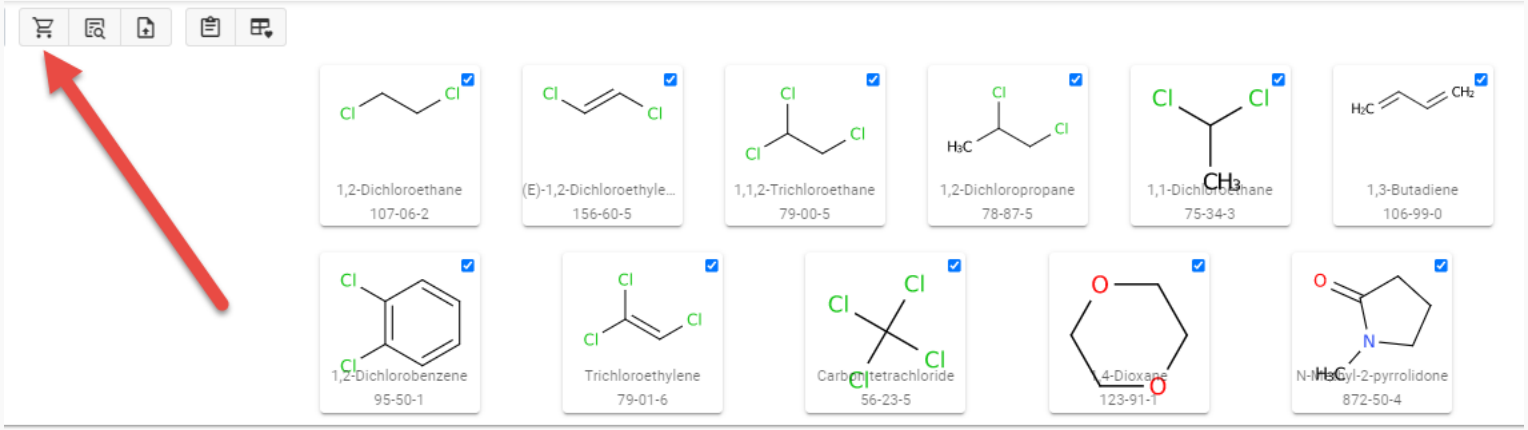
Add to “Cart”

- Review the chemicals and “Add to Cart”



“Process the Cart”

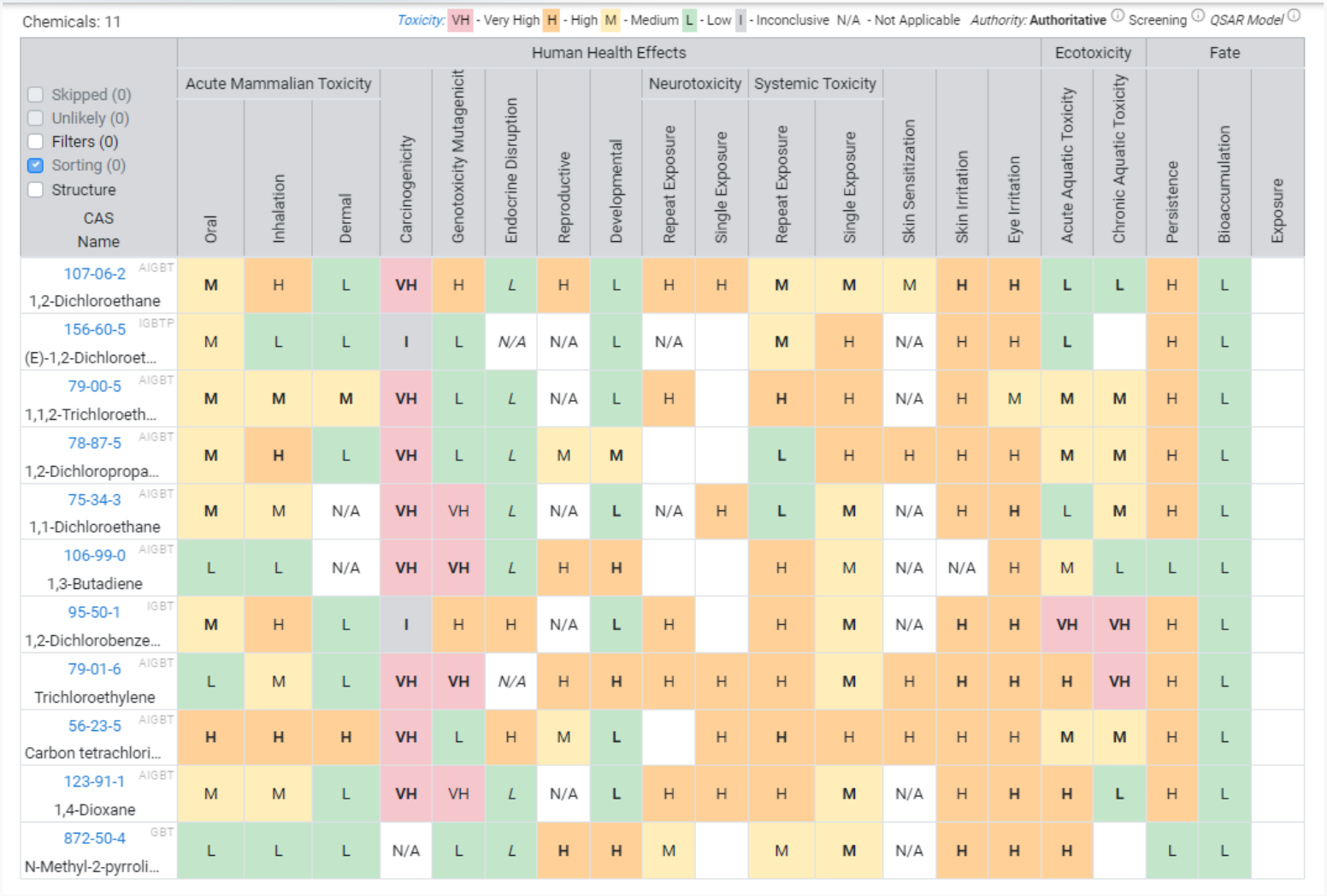
- “Process the Cart” searches the chemicals against the database and serves them up



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

Navigating the Matrix

EPA United States Environmental Protection Agency



Chemicals: 11

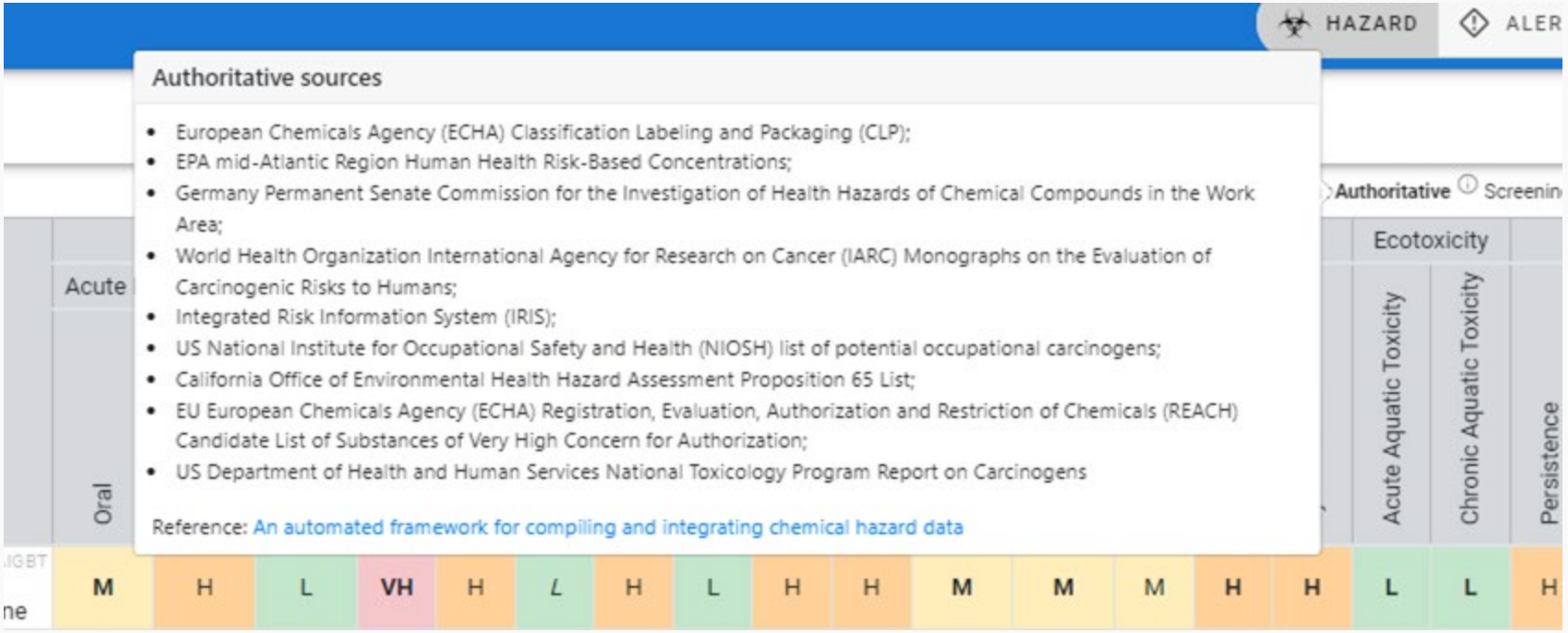
Toxicity: VH - Very High H - High M - Medium L - Low I - Inconclusive N/A - Not Applicable *Authority:* **Authoritative** Screening *QSAR Model*

Skipped (0)
Unlikely (0)
Filters (0)
Sorting (0)
Structure

CAS	Name	Human Health Effects															Ecotoxicity		Fate		
		Acute Mammalian Toxicity							Neurotoxicity		Systemic Toxicity										
		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
107-06-2 AIGBT	1,2-Dichloroethane	M	H	L	VH	H	*L*	H	L	H	H	M	M	M	H	H	L	L	H	L	
156-60-5 IGBTP	(E)-1,2-Dichloroet...	M	L	L	I	L	*N/A*	N/A	L	N/A		M	H	N/A	H	H	L		H	L	
79-00-5 AIGBT	1,1,2-Trichloroeth...	M	M	M	VH	L	*L*	N/A	L	H		H	H	N/A	H	M	M	M	H	L	
78-87-5 AIGBT	1,2-Dichloropropa...	M	H	L	VH	L	*L*	M	M			L	H	H	H	H	M	M	H	L	
75-34-3 AIGBT	1,1-Dichloroethane	M	M	N/A	VH	VH	*L*	N/A	L	N/A	H	L	M	N/A	H	H	L	M	H	L	
106-99-0 AIGBT	1,3-Butadiene	L	L	N/A	VH	VH	*L*	H	H			H	M	N/A	N/A	H	M	L	L	L	
95-50-1 IGBT	1,2-Dichlorobenze...	M	H	L	I	H	H	N/A	L	H		H	M	N/A	H	H	VH	VH	H	L	
79-01-6 AIGBT	Trichloroethylene	L	M	L	VH	VH	*N/A*	H	H	H	H	H	M	H	H	H	H	VH	H	L	
56-23-5 AIGBT	Carbon tetrachlori...	H	H	H	VH	L	H	M	L		H	H	H	H	H	H	M	M	H	L	
123-91-1 AIGBT	1,4-Dioxane	M	M	L	VH	VH	*L*	N/A	L	H	H	H	M	N/A	H	H	H	L	H	L	
872-50-4 GBT	N-Methyl-2-pyrroli...	L	L	L	N/A	L	*L*	H	H	M		M	M	N/A	H	H	H		L	L	

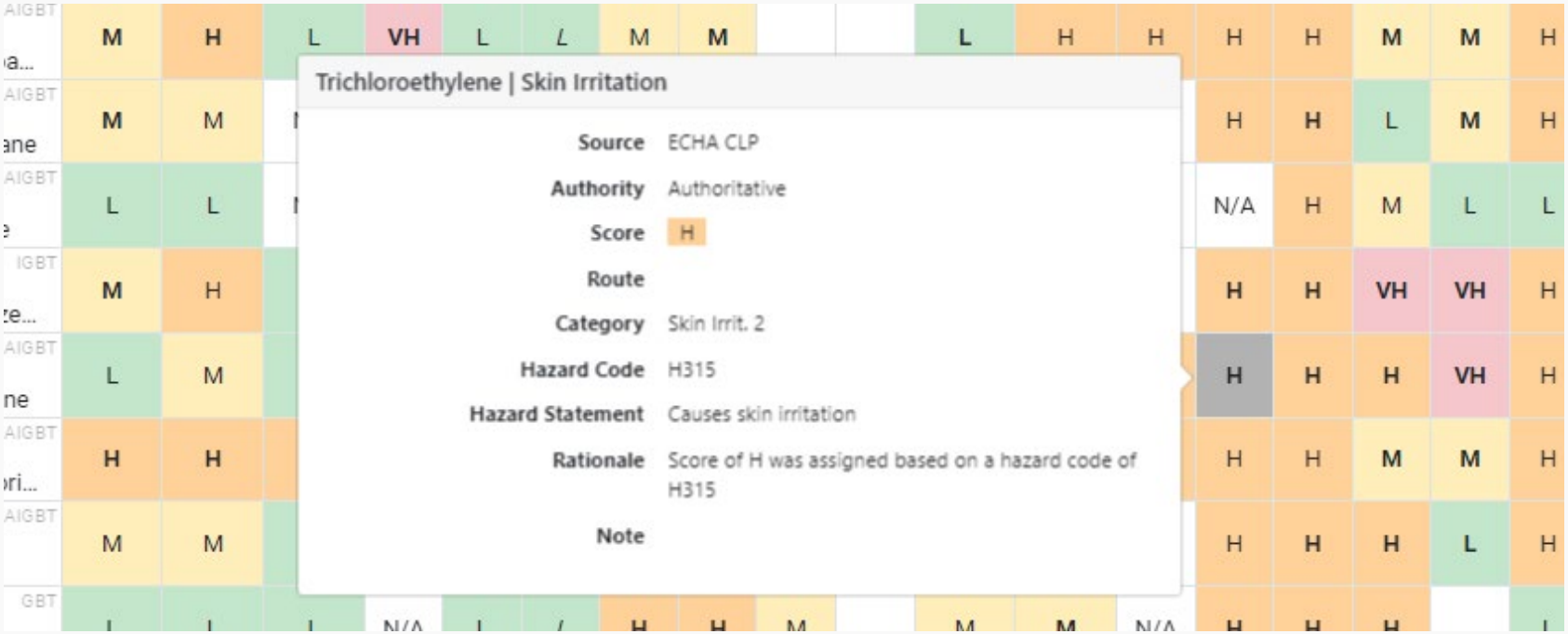
What are the Sources

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



Hover over Cell – Summary Call

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



Detail Table

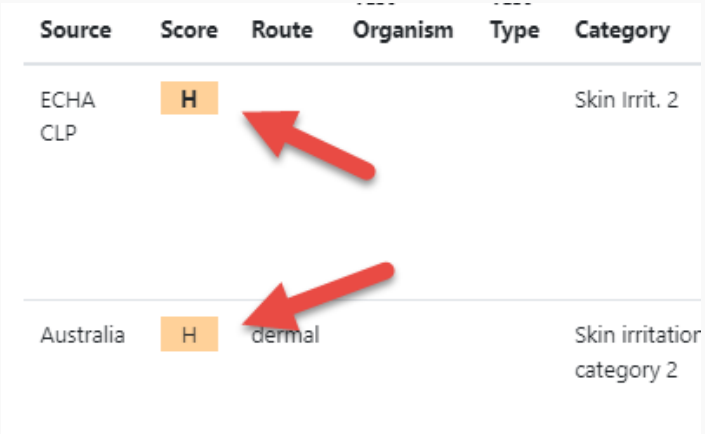
Skin Irritation for ***Trichloroethylene*** (79-01-6)

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

Source	Score	Route	Test Organism	Test Type	Category	Hazard Code	Hazard Statement	Rationale	Note
ECHA CLP	H				Skin Irrit. 2	H315	Causes skin irritation	Score of H was assigned based on a hazard code of H315	
Australia	H	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	H				Skin corrosion/irritation - Category 2	H315	Causes skin irritation	Score of H was assigned based on a hazard code of H315	
Japan	H				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

Fonts represent sources

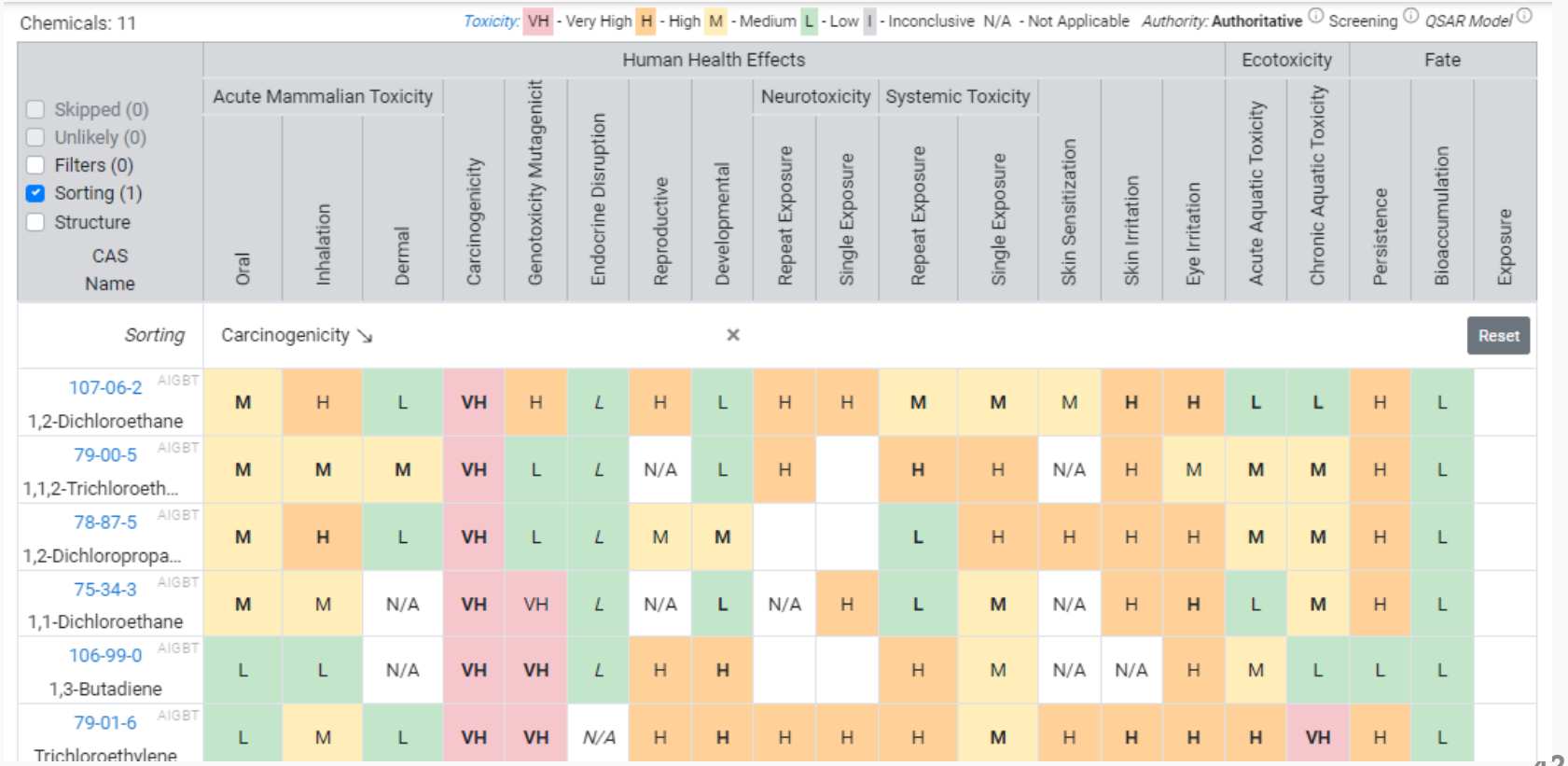
- BOLD: Authoritative Sources
- Normal: Screening Sources
- Italic: QSAR Models (TEST and SEEM3)



Source	Score	Route	Organism	Type	Category
ECHA CLP	H				Skin Irrit. 2
Australia	H	dermal			Skin irritation category 2

Multi-sorting of columns

- Click on a column-heading…carcinogenicity selected below…



Chemicals: 11

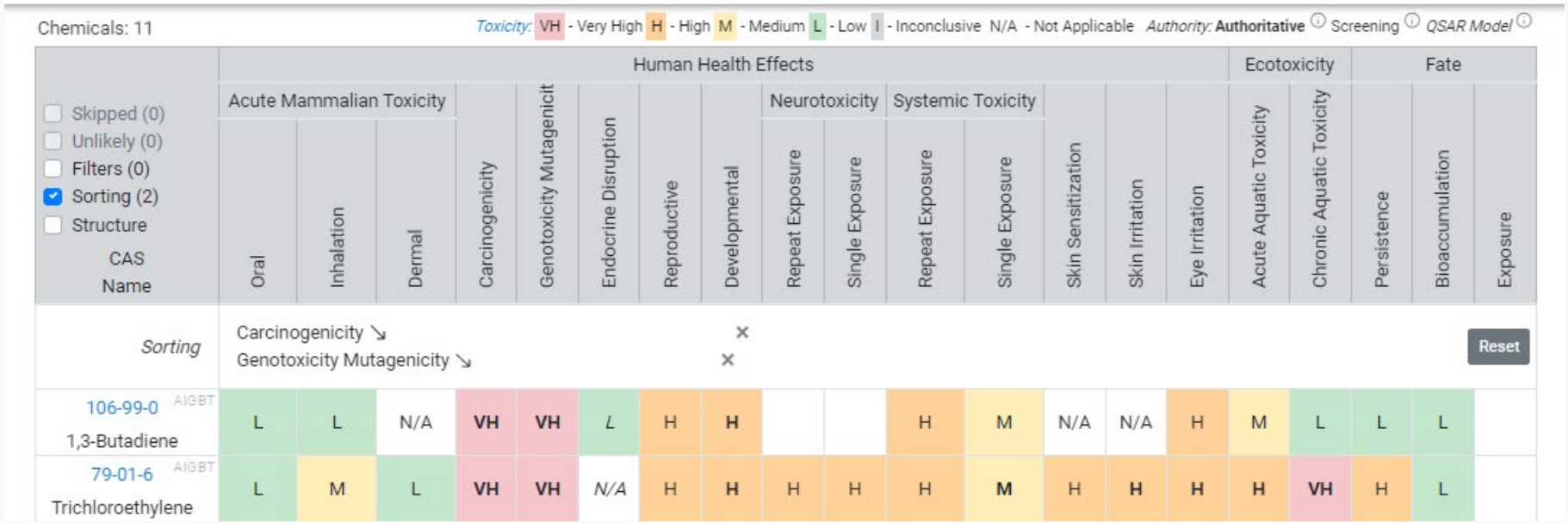
Toxicity: VH - Very High H - High M - Medium L - Low I - Inconclusive N/A - Not Applicable *Authority:* **Authoritative** Screening *QSAR Model*

Skipped (0)
Unlikely (0)
Filters (0)
Sorting (1)
Structure

CAS Name	Human Health Effects															Ecotoxicity		Fate		
	Acute Mammalian Toxicity								Neurotoxicity		Systemic Toxicity									
	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	Carcinogenicity ↘ ×																			Reset
107-06-2 AIGBT 1,2-Dichloroethane	M	H	L	VH	H	*L*	H	L	H	H	M	M	M	H	H	L	L	H	L	
79-00-5 AIGBT 1,1,2-Trichloroeth...	M	M	M	VH	L	*L*	N/A	L	H		H	H	N/A	H	M	M	M	H	L	
78-87-5 AIGBT 1,2-Dichloropropa...	M	H	L	VH	L	*L*	M	M			L	H	H	H	H	M	M	H	L	
75-34-3 AIGBT 1,1-Dichloroethane	M	M	N/A	VH	VH	*L*	N/A	L	N/A	H	L	M	N/A	H	H	L	M	H	L	
106-99-0 AIGBT 1,3-Butadiene	L	L	N/A	VH	VH	*L*	H	H			H	M	N/A	N/A	H	M	L	L	L	
79-01-6 AIGBT Trichloroethylene	L	M	L	VH	VH	*N/A*	H	H	H	H	H	M	H	H	H	H	VH	H	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



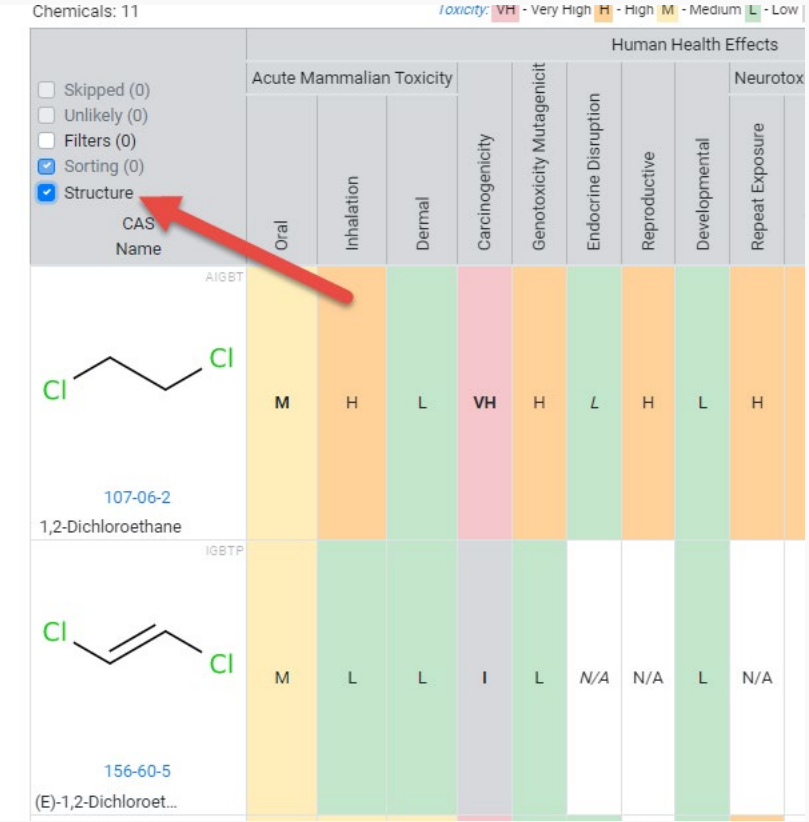
Chemicals: 11

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

- Skipped (0)
- Unlikely (0)
- Filters (0)
- Sorting (2)
- Structure

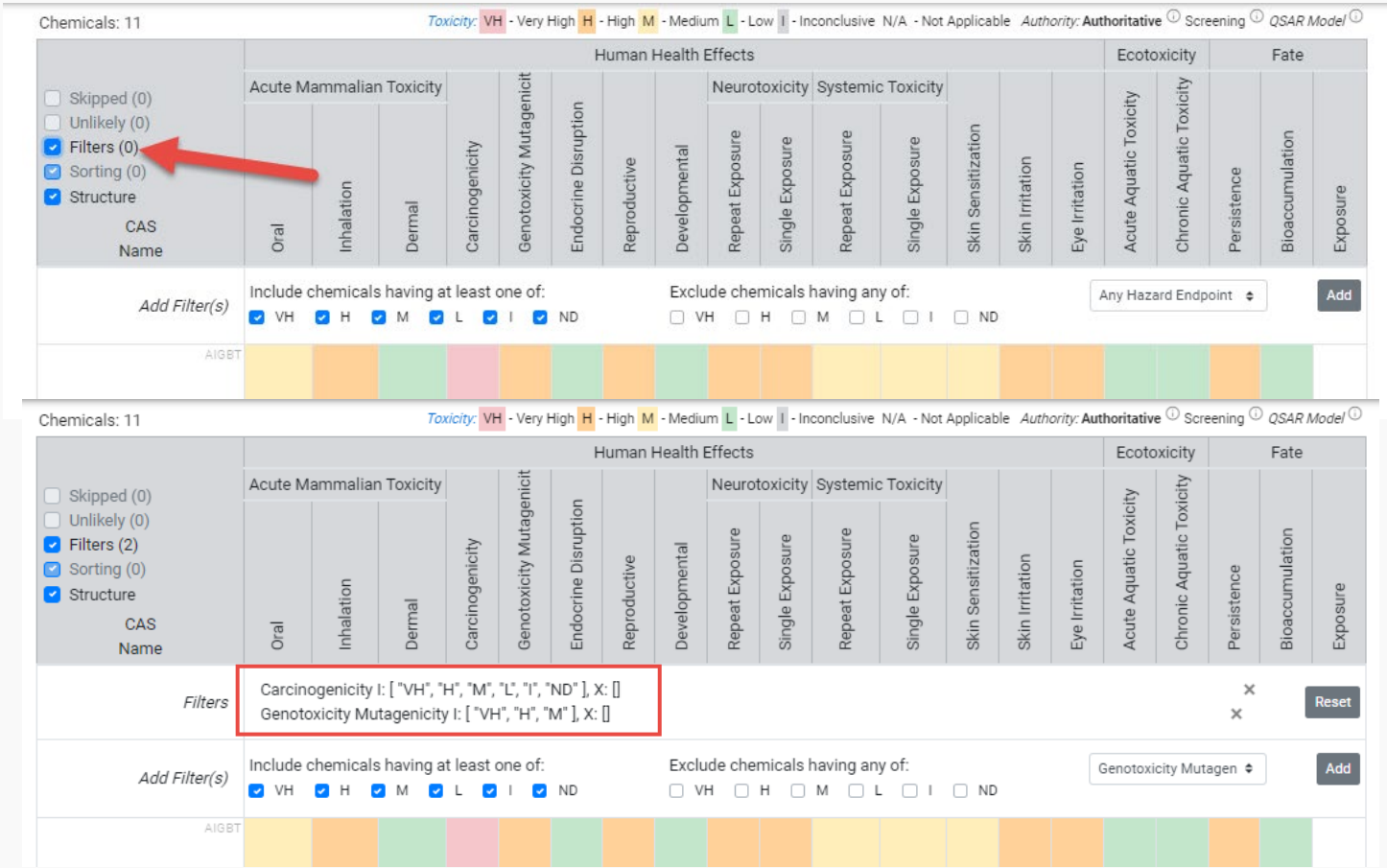
CAS / Name	Human Health Effects																Ecotoxicity		Fate		
	Acute Mammalian Toxicity								Neurotoxicity		Systemic Toxicity										
	Oral	Inhalation	Dermal	Carcinogenicity	Genotoxicity Mutagenicit	Endocrine Disruption	Reproductive	Developmental	Repeat Exposure	Single Exposure	Repeat Exposure	Single Exposure	Skin Sensitization	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation	Exposure
Sorting	Carcinogenicity ↘ × Genotoxicity Mutagenicity ↘ ×																			Reset
106-99-0 AIGBT 1,3-Butadiene	L	L	N/A	VH	VH	*L*	H	H			H	M	N/A	N/A	H	M	L	L	L	
79-01-6 AIGBT Trichloroethylene	L	M	L	VH	VH	*N/A*	H	H	H	H	H	M	H	H	H	H	VH	H	L	

Click Structure to Show

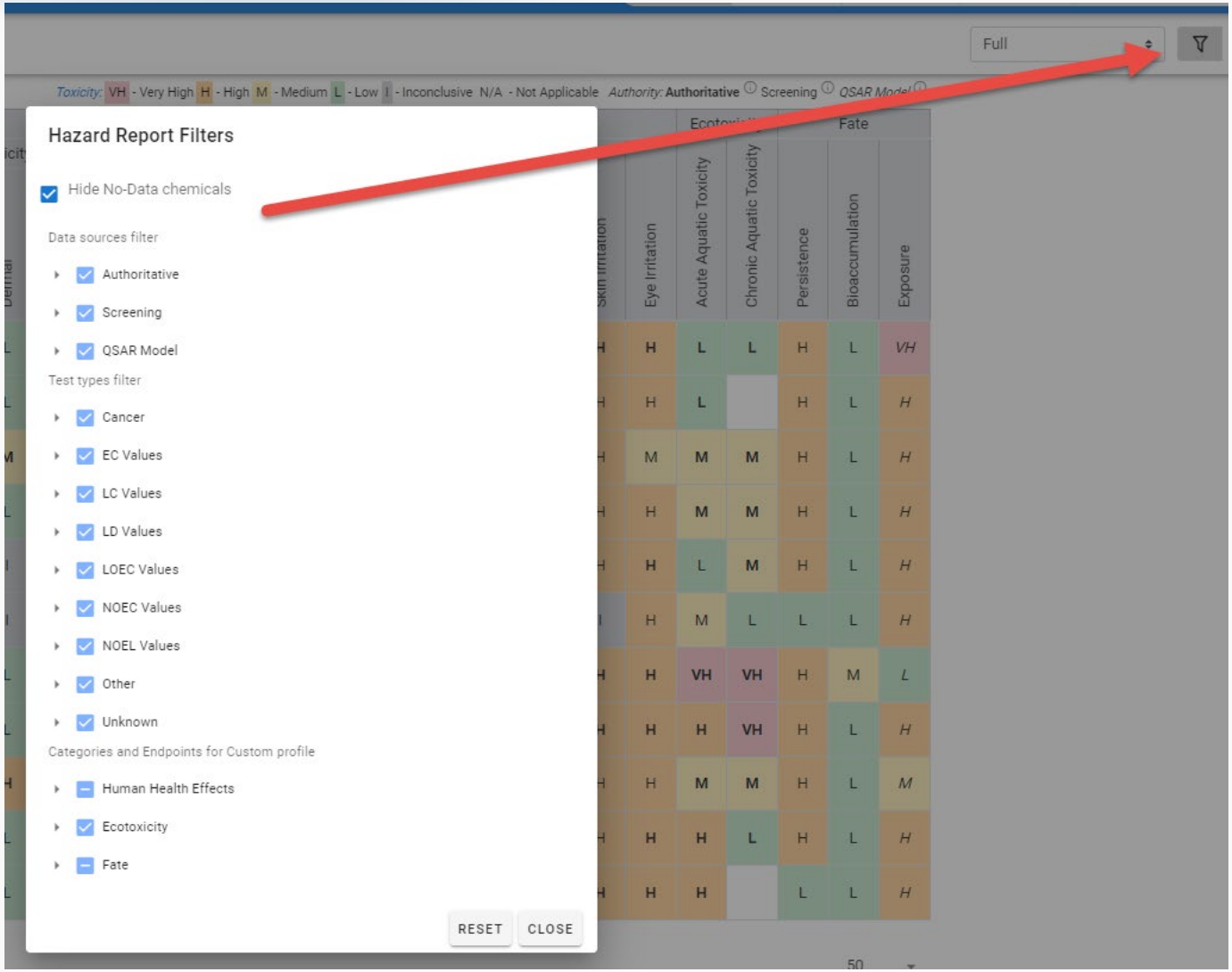


Filters

- Filter hazard ratings IN or OUT…select Endpoint – should be self explanatory

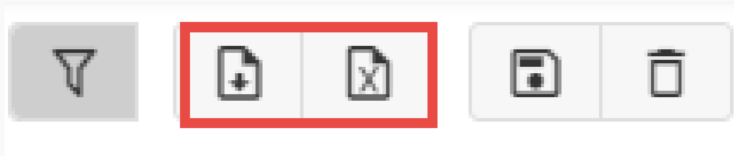


Filter out individual/multiple sources



Export SDF or Excel File

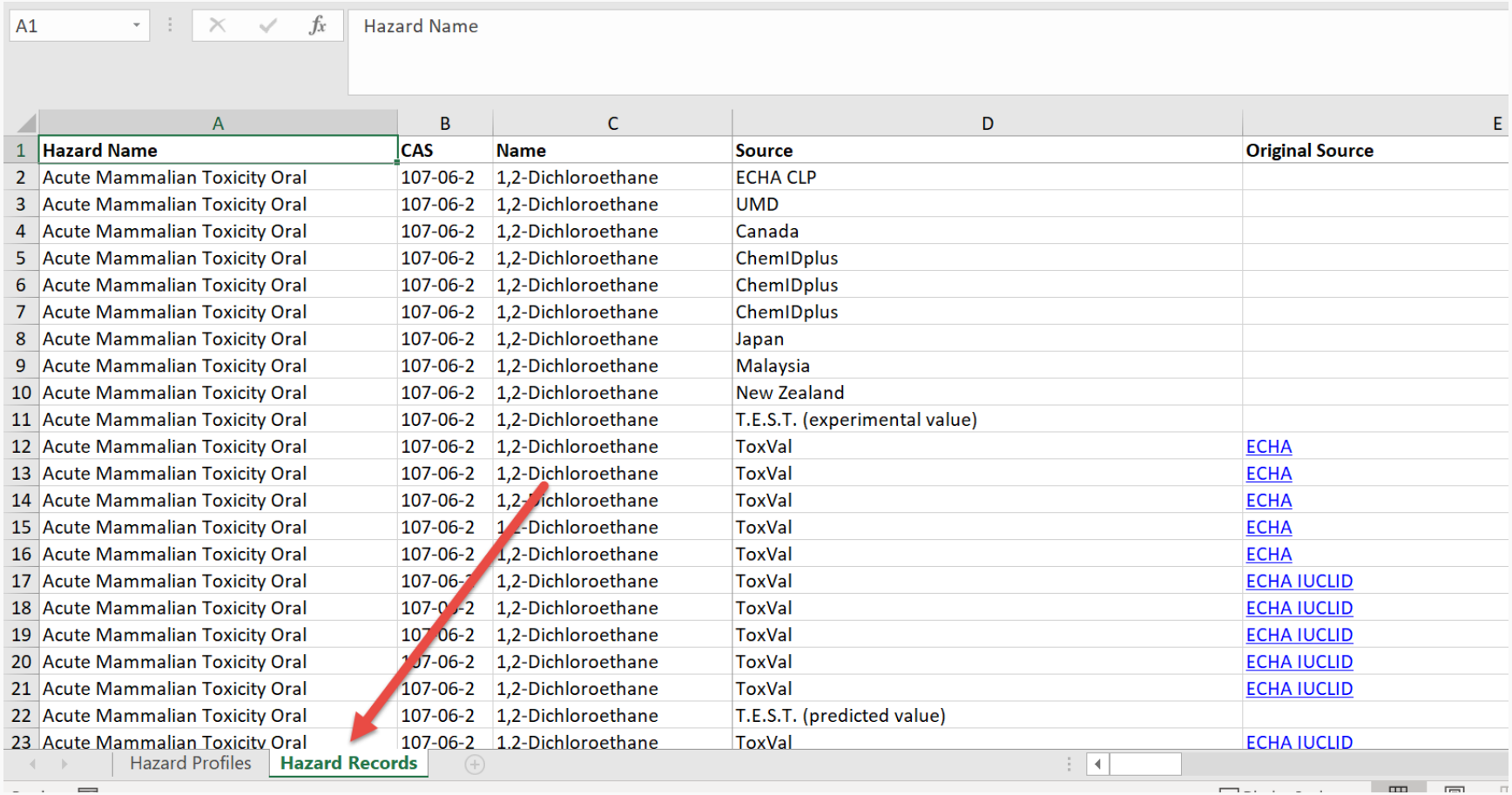
- Most useful form for your needs..Excel



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 - Very High	H - High		M - Medium		L - Low		I - Inconclusive		No Data			Authoritative		Screening		QSAR Model	
			Human Health Effects														Ecotoxicity		Fa	
			Acute Mammalian Toxicity								Neurotoxicity		Systemic Toxicity							
DTXSID	CAS	Name	Oral	Inhalation	Dermal	Carcinogenicity	Genotoxicity Mutagenicity	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
DTXSID6020438	107-06-2	1,2-Dichloroethane	M	H	L	VH	VH	L	H	L	H	H	M	M	M	H	H	L	L	H	l
DTXSID7024031	156-60-5	(E)-1,2-Dichloroethylene	M	L	L	I	L	I	I	L	I		M	H	I	H	H	L		H	l
DTXSID5021380	79-00-5	1,1,2-Trichloroethane	M	M	M	VH	L	L	I	L	H		H	H	I	H	M	M	M	H	l
DTXSID0020448	78-87-5	1,2-Dichloropropane	M	H	L	VH	VH	L	M	M			L	H	H	H	H	M	M	H	l
DTXSID1020437	75-34-3	1,1-Dichloroethane	M	M	I	VH	VH	L	I	L	I	H	L	M	I	H	H	L	M	H	l
DTXSID3020203	106-99-0	1,3-Butadiene	L	L	I	VH	VH	L	H	H			H	M	I	I	H	M	L	L	l
DTXSID6020430	95-50-1	1,2-Dichlorobenzene	M	H	L	I	VH	H	I	L	H		H	M	I	H	H	VH	VH	H	N
DTXSID0021383	79-01-6	Trichloroethylene	L	M	L	VH	VH	I	H	H	H	H	H	M	H	H	H	H	VH	H	l
DTXSID8020250	56-23-5	Carbon tetrachloride	H	H	H	VH	VH	H	M	L		H	H	H	H	H	H	M	M	H	l
DTXSID4020533	123-91-1	1,4-Dioxane	M	M	L	VH	VH	L	I	L	H	H	H	M	I	H	H	H	L	H	l
DTXSID6020856	872-50-4	N-Methyl-2-pyrrolidone	L	L	L	I	L	L	H	H	M		M	M	I	H	H	H		L	l

Check SECOND Worksheet



A1 | Hazard Name

	A	B	C	D	E
1	**Hazard Name**	**CAS**	**Name**	**Source**	**Original Source**
2	Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	ECHA CLP	
3	Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	UMD	
4	Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	Canada	
5	Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	ChemIDplus	
6	Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	ChemIDplus	
7	Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	ChemIDplus	
8	Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	Japan	
9	Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	Malaysia	
10	Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	New Zealand	
11	Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	T.E.S.T. (experimental value)	
12	Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	ToxVal	ECHA
13	Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	ToxVal	ECHA
14	Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	ToxVal	ECHA
15	Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	ToxVal	ECHA
16	Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	ToxVal	ECHA
17	Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	ToxVal	ECHA IUCLID
18	Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	ToxVal	ECHA IUCLID
19	Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	ToxVal	ECHA IUCLID
20	Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	ToxVal	ECHA IUCLID
21	Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	ToxVal	ECHA IUCLID
22	Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	T.E.S.T. (predicted value)	
23	Acute Mammalian Toxicity Oral	107-06-2	1,2-Dichloroethane	ToxVal	ECHA IUCLID

Hazard Profiles | Hazard Records

EPA United States Environmental Protection Agency

Chemical Transformation Database

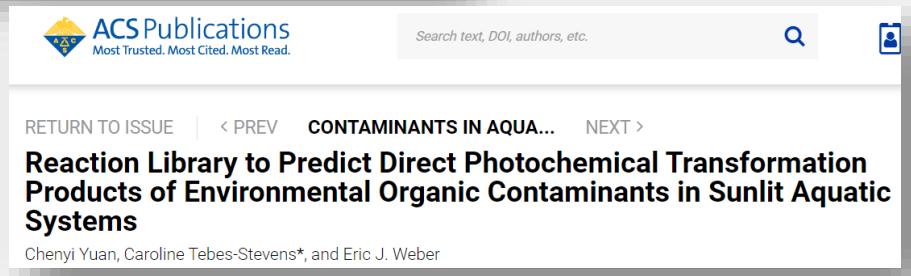
(Work in Progress)

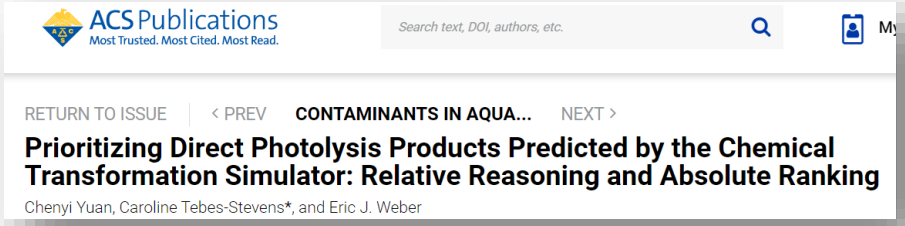
Chemical Transformation Database

- Building the database of reactions under the Chemical Transformation Simulator

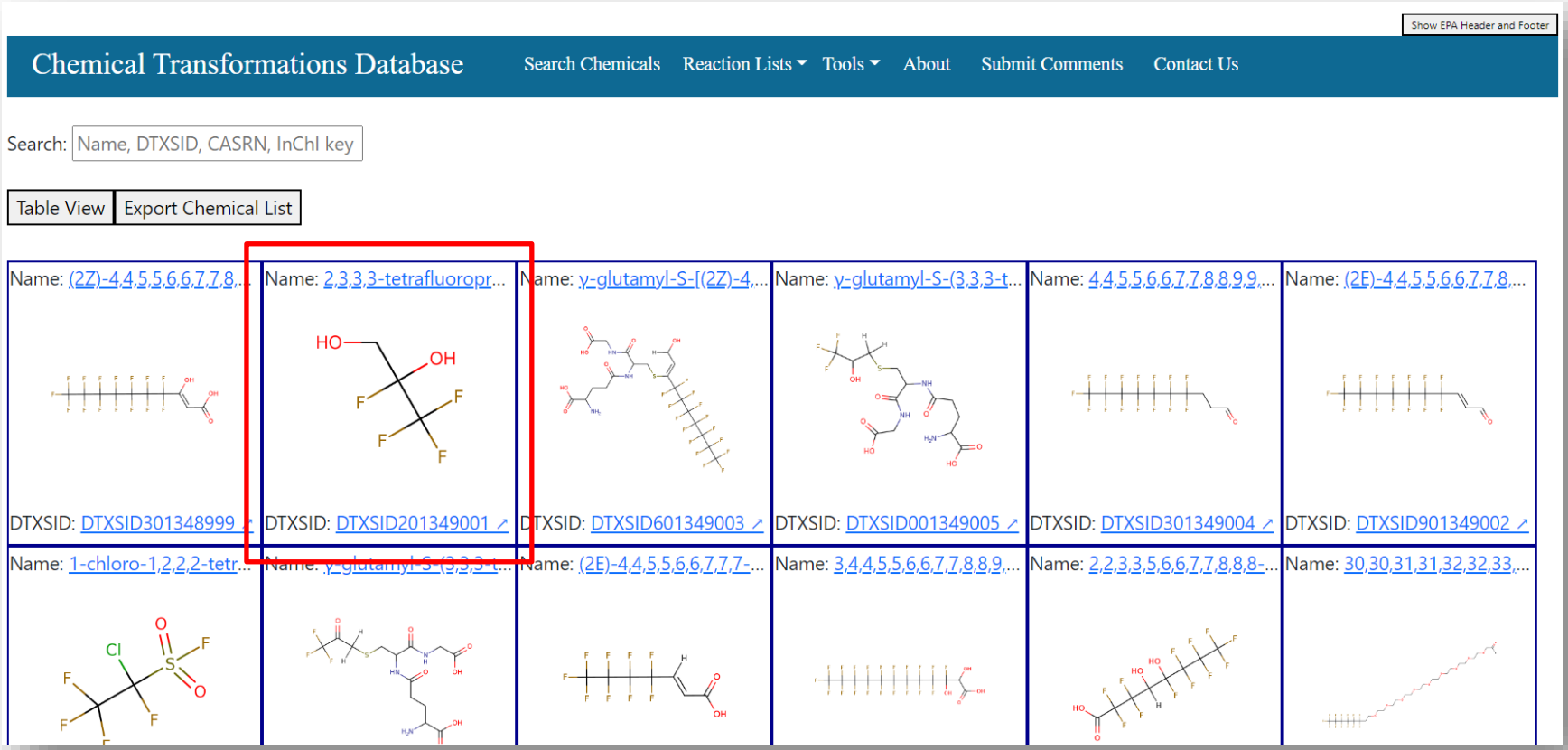
Chemical Transformation Database

- Building the database of reactions under the Chemical Transformation Simulator





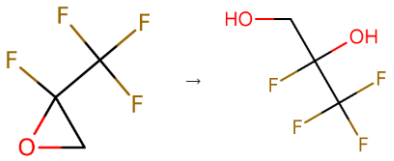
Chemical Transformation Database



Reaction, Original References etc

Chemical Transformations Database | Search Chemicals | Reaction Lists | Tools | About | Submit Comments | Contact Us

2-Fluoro-2-(trifluoromethyl)oxirane → 2,3,3,3-tetrafluoropropane-1,2-diol



Reaction Process:

Reaction Type: Hydrolysis

Reaction Scheme: Epoxide to diol PTP

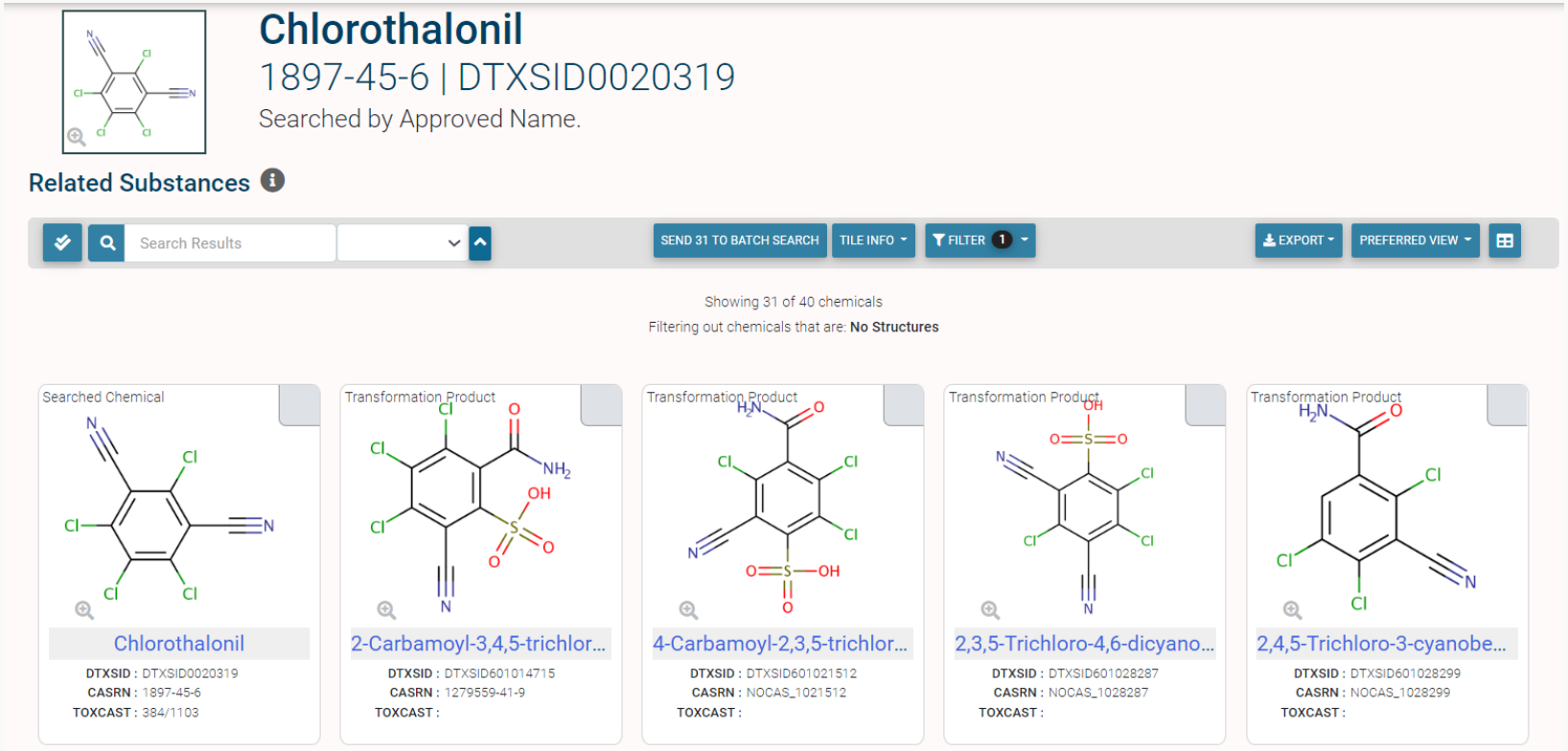
Reaction Details

T...	Half Life (days)	Reaction System	Metabolic	Environmental	Notes	Reference	Delete
		rat	1			Schuster et al., 2008	Delete

Export Reaction Details

What's Next?

- Adding Thousands of Parent-Product mappings from the Dashboard



EPA United States Environmental Protection Agency

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

0-9 | A | B | C | D | E | F | G | H | I | K | L | M | N | O | P | Q | R | S | T | V | Z

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

ECM – New and Old

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

- **MRID:** 44536511
- **Date:** 3/27/98
- **Matrix:** Soil
- **Registrant:** Dow Elanco
- **Analysis:** GC/MS
- **Limit of Quantitation (LOQ):** 0.2 µg/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!!!

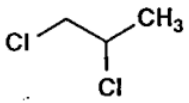
GRM.: 94.13
EFFECTIVE: July 26, 1995
SUPERSEDES: New

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

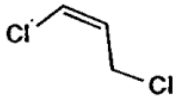
S. C. Dolder, C. E. Kubitschek and H. E. Dixon-White
North American Environmental Chemistry Laboratory
DowElanco
Indianapolis, Indiana 46268 - 1053

A. Scope

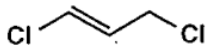
This method is applicable for the quantitative determination of residues of 1,2-dichloropropane (1,2-D) and *cis*- and *trans*-1,3-dichloropropene (1,3-D) in soil over the concentration range of 0.200-160,000 µg/kg with a validated limit of quantitation of 0.200 µg/kg for each compound.



1,2-D
CAS No. 78-87-5



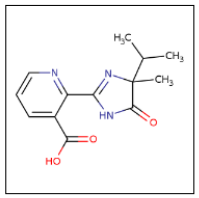
cis-1,3-D
CAS No. 10061-01-5



trans-1,3-D
CAS No. 10061-02-6

Embedding old Method PDFs

Search Results for "Imazapyr"



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

Spectrum Type	Source	Record Type	View
	Environmental Chemistry Methods	Method	PDF
	Environmental Chemistry Methods	Method	PDF
LC-MS+	MoNA	Spectrum	Spectrum
LC-MS+	MassBank EU	Spectrum	Spectrum
LC-MS+	MassBank EU	Spectrum	Spectrum
LC-MS+	MassBank EU	Spectrum	Spectrum
LC-MS+	MassBank EU	Spectrum	Spectrum
LC-MS+	MassBank EU	Spectrum	Spectrum

Imazapyr

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

US EPA - ECM for Imazapyr ... 1 / 8 90%

41891501

CYANAMID C3197 CONFIDENTIAL Page 5 of 22

SOP M1900
A. Khunachak/hm
09/05/89
Approved by:
J. M. Devine 09/05/89 Date

AMERICAN CYANAMID COMPANY
AGRICULTURAL RESEARCH DIVISION
CHEMICAL DEVELOPMENT
P. O. Box 400
Princeton, New Jersey 08540 USA

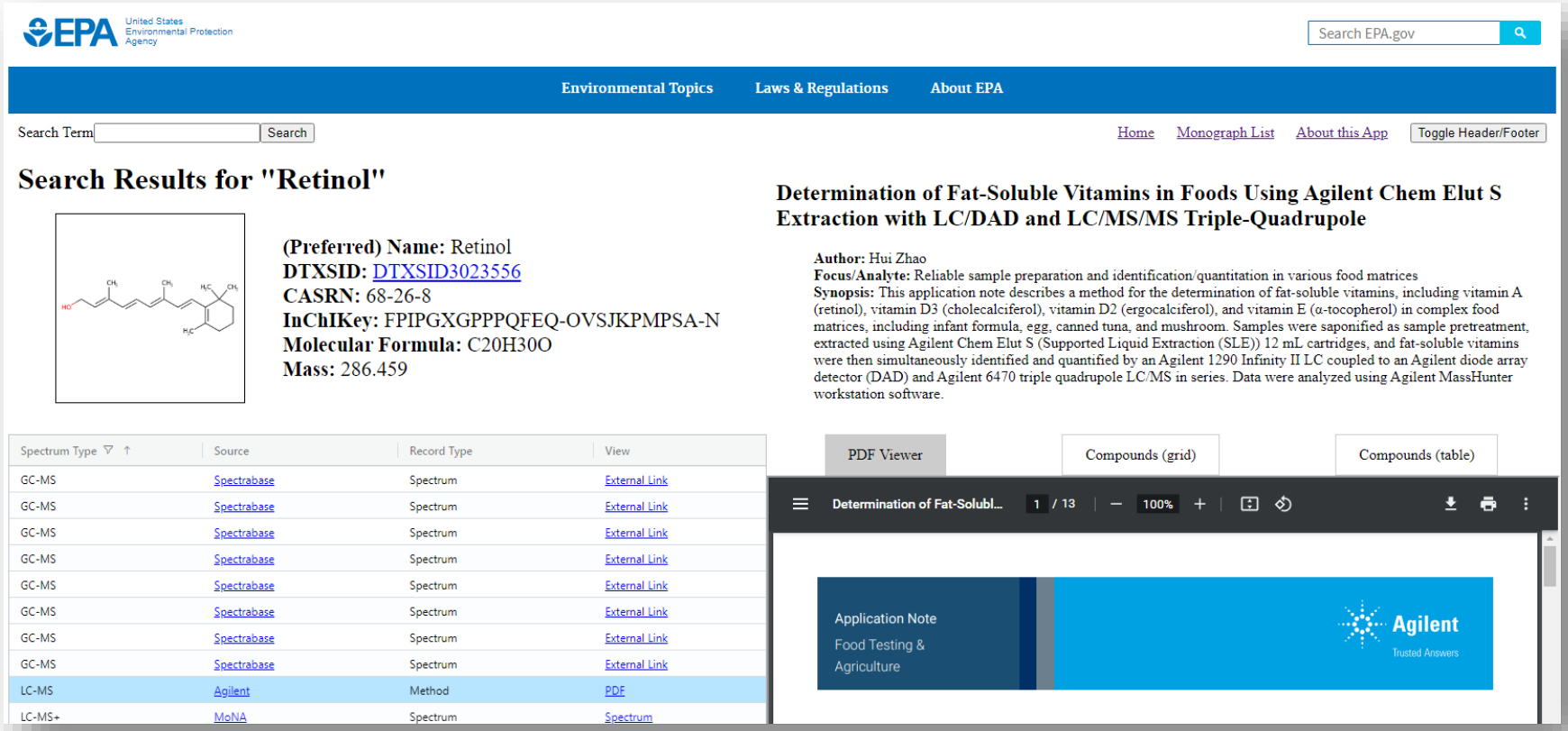
RECOMMENDED METHOD OF ANALYSIS

Imazapyr (CL 243,997): HPLC Method for the Determination of CL 243,997 Residues in Water

A. Principle

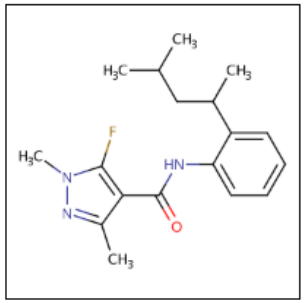
Residues of CL 243,997 are extracted from water by using a C18 solid phase extraction (SPE) cartridge. Additional cleanup and specificity are achieved by

Embedding New Method PDFs



Structure Tables/Tiles view

Search Results for "DTXSID9058107"



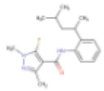
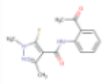
(Preferred) Name: Penflufen
DTXSID: DTXSID9058107
CASRN: 494793-67-8
InChIKey: GOFJDXZZHFNFLV-UHFFFAOYNA-N
Molecular Formula: C18H24FN3O
Mass: 317.408

Penflufen & Degradates

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

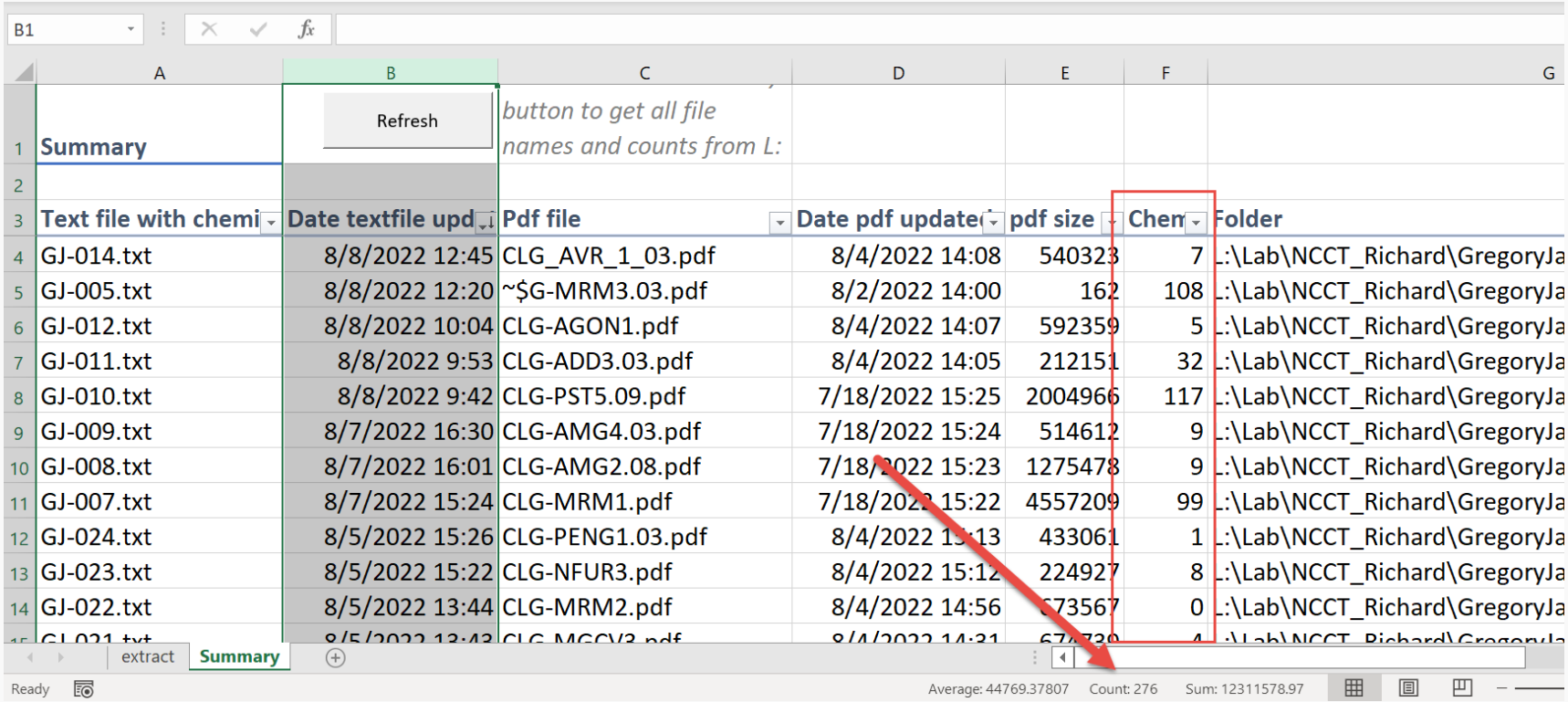
Spectrum Type ↑	Source	Record Type	Info...
LC/MS/MS	Environmental Chemistry Methods	Method (PDF)	
LC/MS/MS	Environmental Chemistry Methods	Method (PDF)	
LC/MS/MS	Environmental Chemistry Methods	Method (PDF)	
LC/MS/MS	Environmental Chemistry Methods	Method (PDF)	

PDF Viewer | Compounds (grid) | Compounds (table)

Structure	DTXSID	CASRN	Compound Name
	DTXSID9058107	494793-67-8	Penflufen
	DTXSID601024859	NOCAS_102485	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

	A	B	C	D	E	F	G
1	Summary	Refresh	button to get all file names and counts from L:				
2							
3	Text file with chemi	Date textfile upd	Pdf file	Date pdf update	pdf size	Chem	Folder
4	GJ-014.txt	8/8/2022 12:45	CLG_AVR_1_03.pdf	8/4/2022 14:08	540323	7	L:\Lab\NCCT_Richard\GregoryJa
5	GJ-005.txt	8/8/2022 12:20	~$G-MRM3.03.pdf	8/2/2022 14:00	162	108	L:\Lab\NCCT_Richard\GregoryJa
6	GJ-012.txt	8/8/2022 10:04	CLG-AGON1.pdf	8/4/2022 14:07	592359	5	L:\Lab\NCCT_Richard\GregoryJa
7	GJ-011.txt	8/8/2022 9:53	CLG-ADD3.03.pdf	8/4/2022 14:05	212151	32	L:\Lab\NCCT_Richard\GregoryJa
8	GJ-010.txt	8/8/2022 9:42	CLG-PST5.09.pdf	7/18/2022 15:25	2004966	117	L:\Lab\NCCT_Richard\GregoryJa
9	GJ-009.txt	8/7/2022 16:30	CLG-AMG4.03.pdf	7/18/2022 15:24	514612	9	L:\Lab\NCCT_Richard\GregoryJa
10	GJ-008.txt	8/7/2022 16:01	CLG-AMG2.08.pdf	7/18/2022 15:23	1275478	9	L:\Lab\NCCT_Richard\GregoryJa
11	GJ-007.txt	8/7/2022 15:24	CLG-MRM1.pdf	7/18/2022 15:22	4557209	99	L:\Lab\NCCT_Richard\GregoryJa
12	GJ-024.txt	8/5/2022 15:26	CLG-PENG1.03.pdf	8/4/2022 15:13	433061	1	L:\Lab\NCCT_Richard\GregoryJa
13	GJ-023.txt	8/5/2022 15:22	CLG-NFUR3.pdf	8/4/2022 15:12	224927	8	L:\Lab\NCCT_Richard\GregoryJa
14	GJ-022.txt	8/5/2022 13:44	CLG-MRM2.pdf	8/4/2022 14:56	573567	0	L:\Lab\NCCT_Richard\GregoryJa

extract | Summary

Ready | Average: 44769.37807 | Count: 276 | Sum: 12311578.97

Contact Information

- Antony Williams (Antony, without an H)

- williams.antony@epa.gov