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EPA United States Environmental Protection Agency

Introduction to the US EPA CompTox Chemicals Dashboard

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

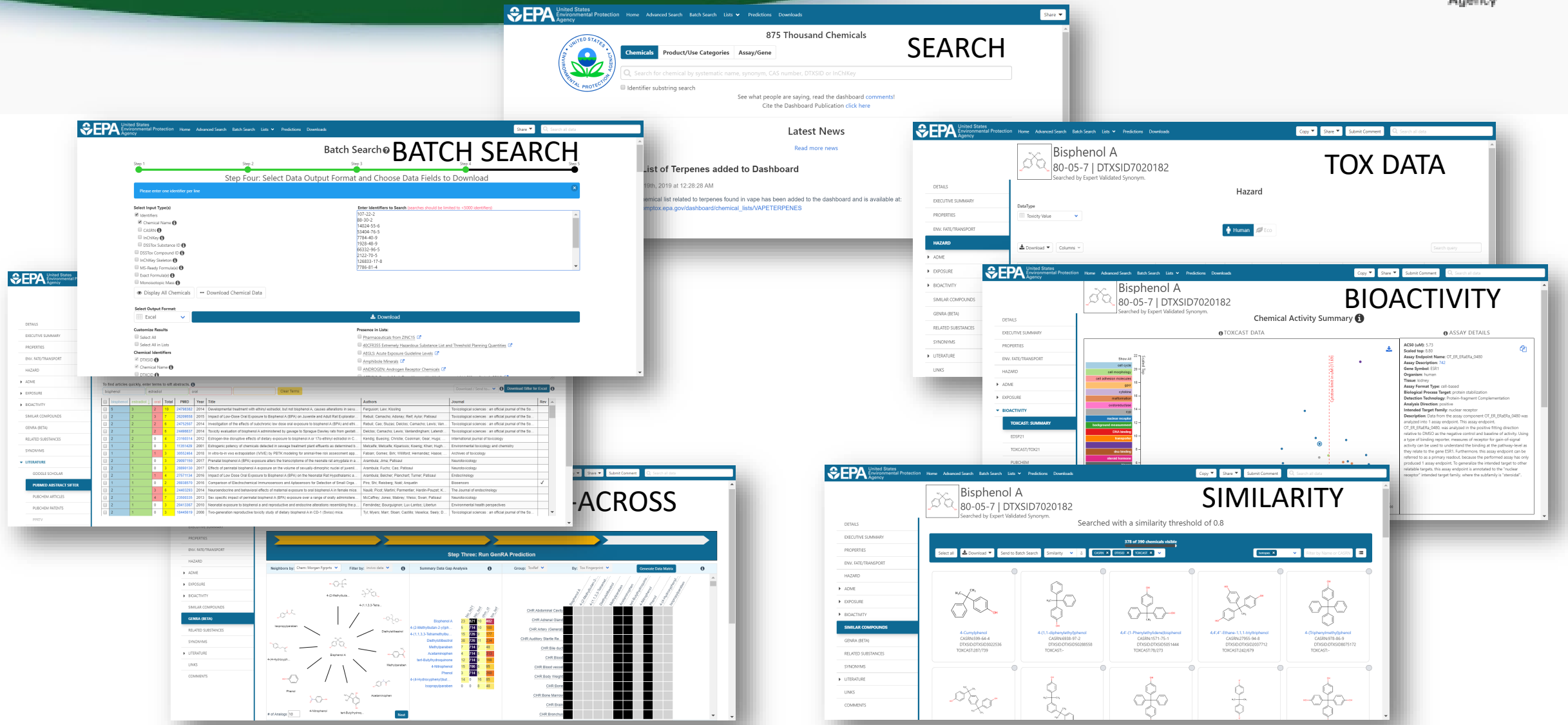
CompTox Chemicals Dashboard
https://comptox.epa.gov/dashboard

- A **publicly accessible website** delivering access:

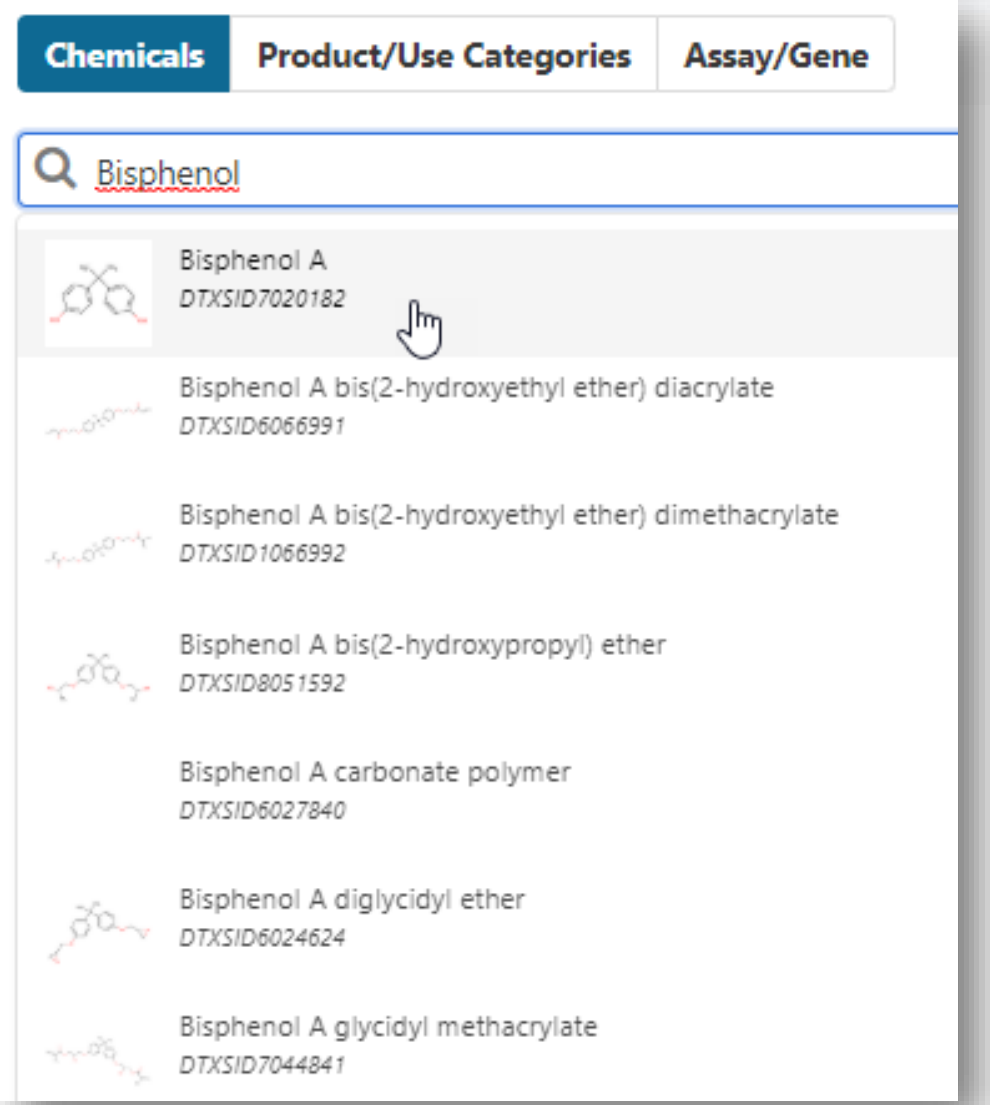
  - ~882,000 chemicals with related property data
  - Experimental and predicted physicochemical property data
  - Experimental Human and Ecological hazard data
  - Integration to “biological assay data” for 1000s of chemicals
  - Information regarding consumer products containing chemicals
  - Links to other agency websites and public data resources
  - “Literature” searches for chemicals using public resources
  - “Batch searching” for thousands of chemicals

CompTox Chemicals Dashboard

https://comptox.epa.gov/dashboard



BASIC Search

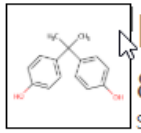


- Three searches from the home page
  - Chemicals (Names, CASRN, Substring)
  - Product/Use Categories
  - Assay Gene
- Searching millions of synonyms and includes Active, Deleted and Alternate CASRNs

Detailed Chemical Pages

EPA United States Environmental Protection Agency

EPA United States Environmental Protection Agency | Home | Advanced Search | Batch Search | Lists | Predictions | Downloads | Copy | Share | Submit Comment | Search all data

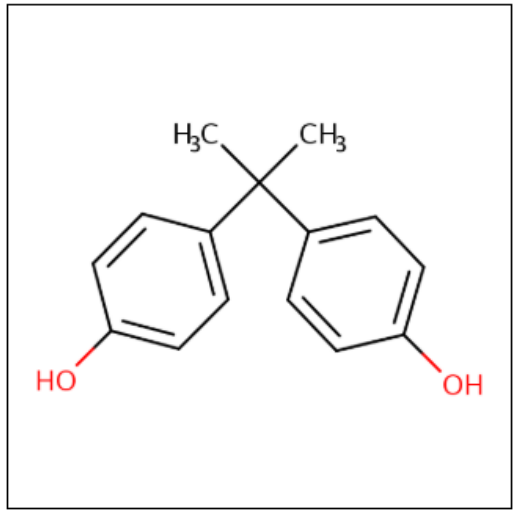


Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

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



Wikipedia

Bisphenol A (BPA) is an organic synthetic compound with the chemical formula $(CH_3)_2C(C_6H_4OH)_2$ belonging to the group of diphenylmethane derivatives and bisphenols, with two hydroxyphenyl groups. It is a colorless solid that is soluble in organic solvents, but poorly soluble in water (0.344 wt % at 83 °C).
BPA is a starting material for the synthesis of plastics, primarily certain polycarbonates
...
Read more

Intrinsic Properties

Molecular Formula: $C_{15}H_{16}O_2$ | Mol File | Find All Chemicals

Average Mass: 228.291 g/mol | Isotope Mass Distribution

Monoisotopic Mass: 228.11503 g/mol

Structural Identifiers

Linked Substances

Presence in Lists

Record Information

Quality Control Notes

Linked Substances: Mixtures and Components, Similar Compounds

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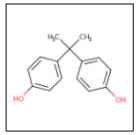
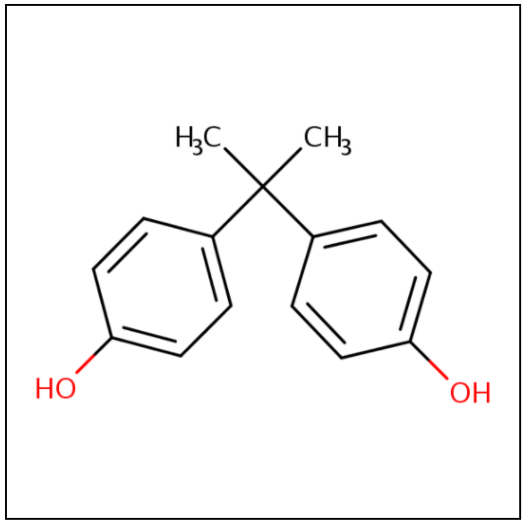


Bisphenol A

80-05-7 | DTXSID7020182

Searched by Expert Validated Synonym.



- **Wikipedia**
- **Quality Control Notes**
- **Intrinsic Properties**
- **Structural Identifiers**
- **Linked Substances**

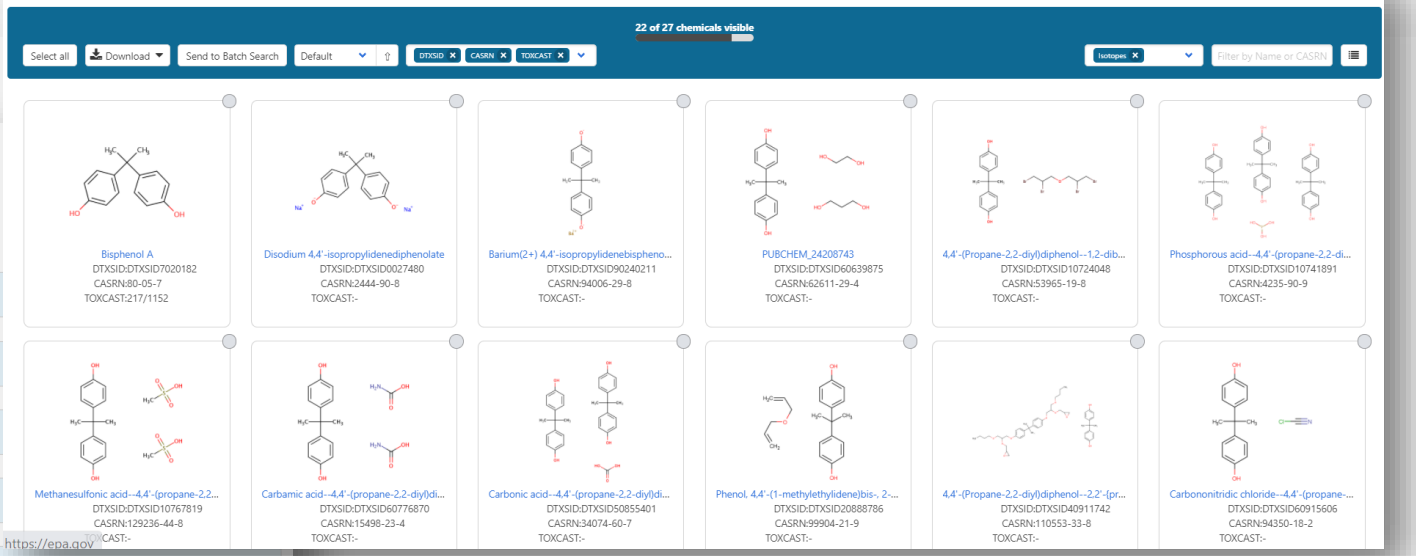
Same Connectivity: 6 records (based on first layer of InChI)

Mixtures, Components and Isotopomers: DTXCID30182: 27 records;

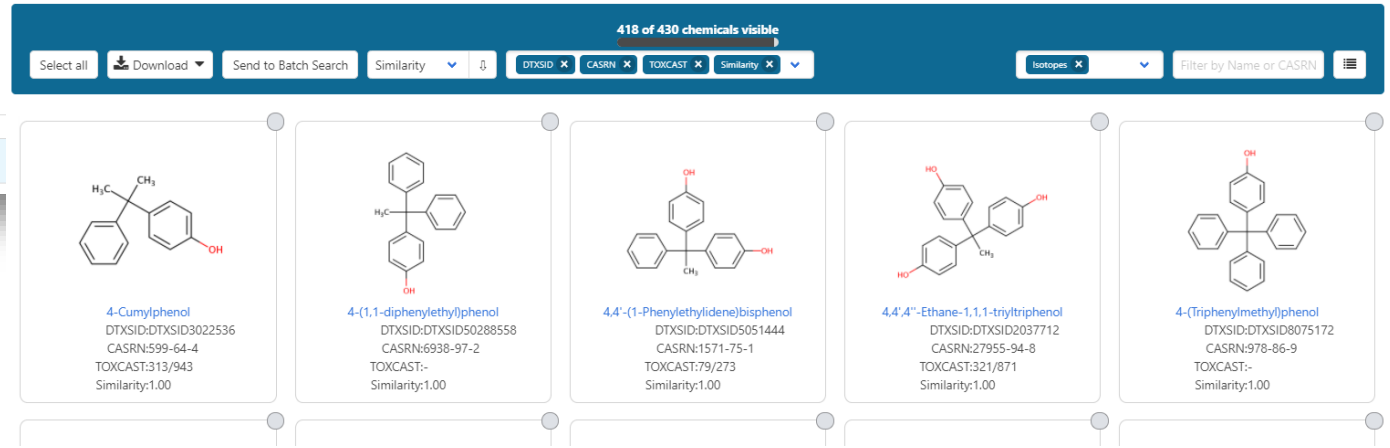
Similar Compounds: 430 records (based on Tanimoto coefficient >0.8)

- **Presence in Lists**

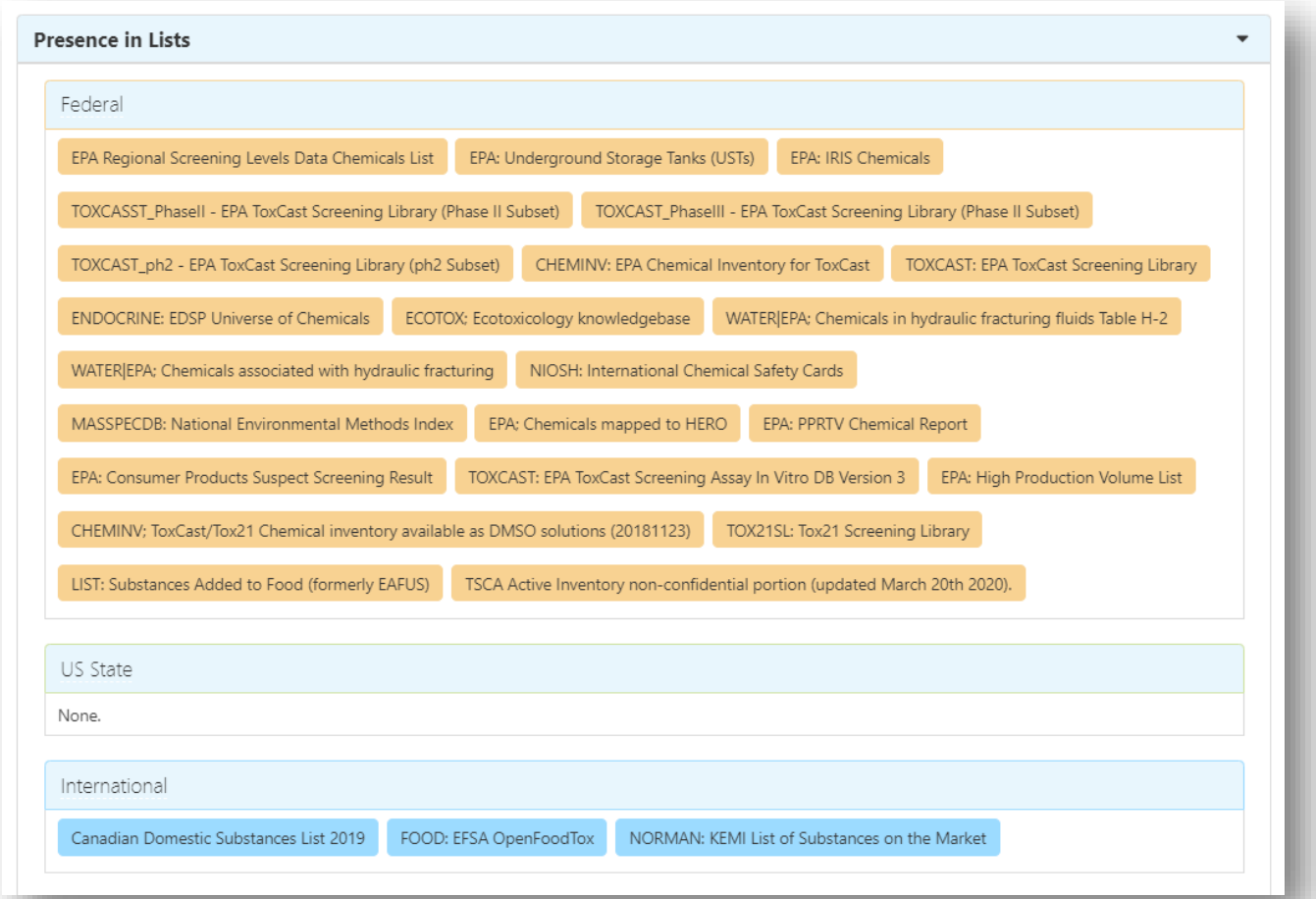
MS-Ready Mappings of Bisphenol A (Isotopes pre-filtered)



Searched with a similarity threshold of 0.8



Presence in Lists



- ~882,000 chemicals are associated with > 280 lists
- Lists are segregated into
  - Federal
  - US State
  - International
  - Other
- Chemicals can be present in multiple lists – with clickthrough

Lists of Lists of Chemicals
>280 lists and growing

EPA United States Environmental Protection Agency

EPA United States Environmental Protection Agency | Home | Advanced Search | Batch Search | Lists | Predictions | Downloads | Share | Search all data

Lists of Chemicals
List of Assays

Select List

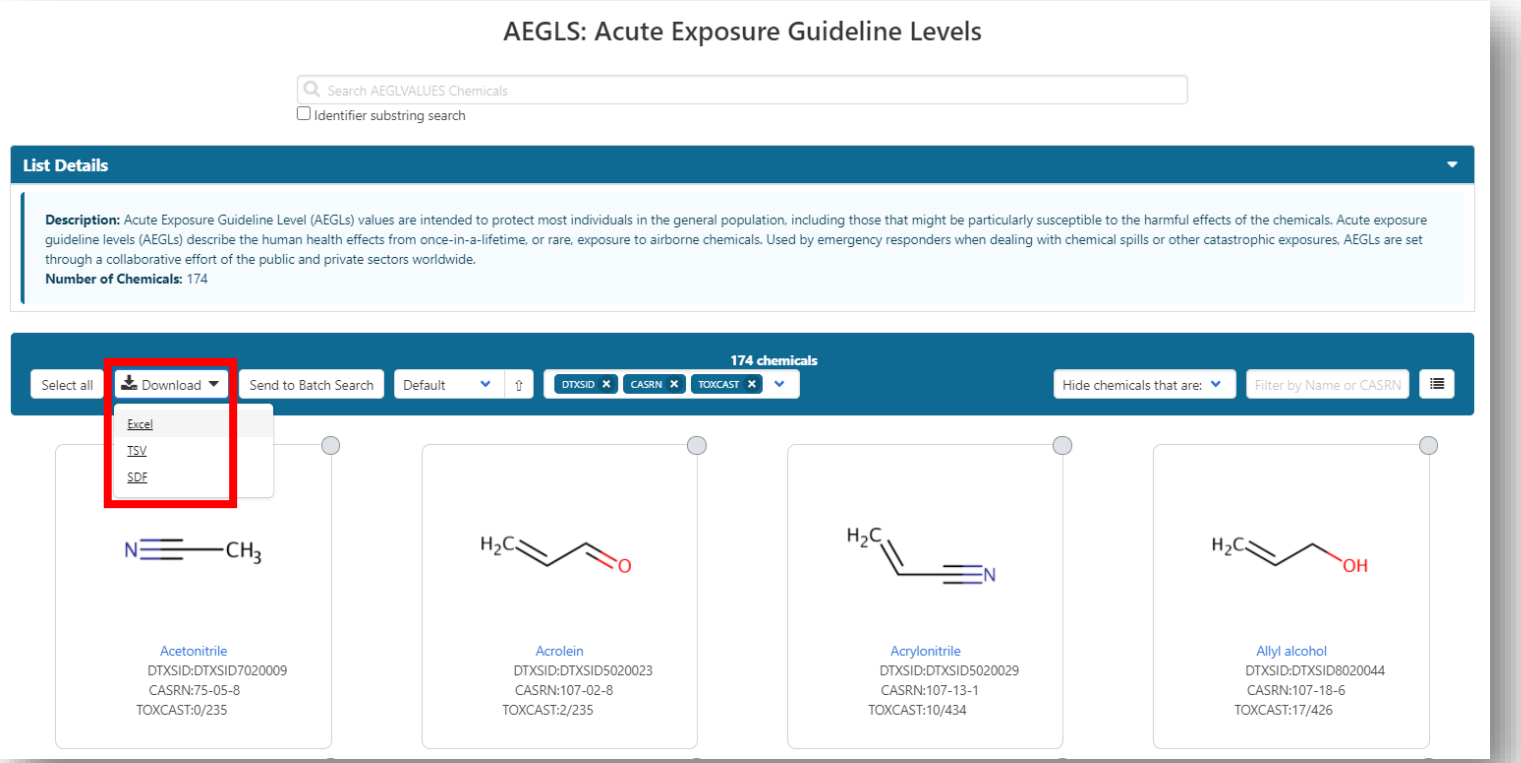
Download | Columns | 10 | Search query | Copy page URL

List Acronym	List Name	Last Updated	Number of Chemicals	List Description
40CFR1164	40CFR116.4 Designation of Hazardous Substances (Above Ground Storage Tanks)	2020-06-25	331	Hazardous Substance List (40CFR116.4): related to Above Ground Storage Tanks
40CFR355	40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities	2018-01-05	354	Extremely Hazardous Substance List and Threshold Planning Quantities; Emergency Planning and Release Notification Requirements; Final Rule. (52 FR 13378)
ACSREAG	LIST: ACS Reagent Chemicals	2017-04-14	405	The ACS Committee on Analytical Reagents sets purity specifications for almost 500 reagent chemicals and over 500 standard-grade reference materials.
AEGLVALUES	AEGLS: Acute Exposure Guideline Levels	2018-04-20	174	Acute exposure guideline levels (AEGLs) describe the human health effects from once-in-a-lifetime, or rare, exposure to airborne chemicals.
ALGALTOX	LIST: Algal Toxins	2018-05-04	55	A list of Algal Toxins of potential interest
AMINOACIDS	CATEGORY: Amino acids	2019-02-04	20	Amino acids are organic compounds containing amine (-NH2) and carboxyl (-COOH) functional groups, along with a side chain (R group) specific to each amino acid.
AMPHIBOLES	LIST: Amphiboles	2019-03-26	23	Amphiboles are an important group of inosilicate minerals.
ANTIBIOTICS	CATEGORY|PHARMACEUTICALS: Antibiotics	2019-11-16	170	List of antibiotics and related compounds
ANTIMICROBIALS	CATEGORY|WIKILIST|ANTIMICROBIALS: List of Antimicrobials from Wikipedia	2020-10-11	289	A list of antimicrobials extracted from Wikipedia.
AOPSTRESSORS	List of Adverse Outcome Pathway Stressors	2020-06-05	349	List of Adverse Outcome Pathway Stressors from the AOP Database

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

Showing 1 to 10 of 281 records

List of Chemicals
Example: Acute Exposure Guideline Levels



- Chemical List Examples
  - Disinfection by-products
  - EPA Pesticide Search DB
  - Consumer Products DB
  - Chemicals in Biosolids
  - ATSDR Toxicological Profiles
  - Canadian Domestic Substances
  - Chemical Inventory for ToxCast
  - EFSA OpenFoodTox
  - EDSP Universe of Chemicals
  - Hydraulic Fracturing Chemicals

Quality

- Five full time curators register and curate data to elevate quality

Record Information

Citation: U.S. Environmental Protection Agency. CompTox Chemicals Dashboard. https://comptox.epa.gov/dashboard/DTXSID0020022 (accessed October 18, 2020), 5-(2-Chloro-4-(trifluoromethyl)phenoxy)-2-nitrobenzoic acid

Data Quality:

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

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

Level 3: Programmatically curated from high quality EPA source, unique chemical ic

Level 4: Programmatically curated from ChemID, unique chemical identifiers have r

Level 5: Programmatically curated from ACToR or PubChem, unique chemical ident

Computational Toxicology 12 (2019) 100096

Contents lists available at ScienceDirect

Computational Toxicology

journal homepage: www.elsevier.com/locate/comtox

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

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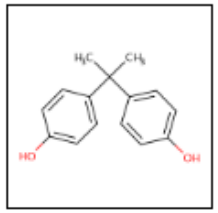
Properties, Fate and Transport



Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

Property

Summary

Summary

Download

Columns

Property	Experimental average	Predicted average	Experimental median	Predicted median
LogKow: Octanol-Water	3.32 (1)	3.30		3.39
Melting Point	155 (7)	140	156	144
Boiling Point	200 (1)	360		355
Water Solubility	8.55e-4 (3)	8.78e-4	5.26e-4	7.56e-4
Vapor Pressure	-	6.83e-7		1.51e-7
Flash Point	-	190		190
Surface Tension	-	46.0		
Index of Refraction	-	1.60		
Molar Refractivity	-	68.2		

Properties, Fate and Transport e.g. Solubility

Download Experimental Data

Source	Result
PhysPropNCCT	5.26e-4
Tetko et al. J. Chem. Inf. and Comp. Sci. 41.6 (2001): 1488-1493	1.51e-3
Kovdienko, et. al. Molecular informatics 29.5 (2010): 394-406.	5.25e-4

Source	Result	Calculation Details
EPISUITE	7.56e-4	Not Available
NICEATM	1.31e-3	Not Available
TEST	1.24e-3	TEST Report
OPERA	5.44e-4	OPERA Model Report [Inside AD]
OPERA2	5.35e-4	Not Available

OPERA Models

United States Environmental Protection Agency

Journal
SAR and QSAR in Environmental Research
Volume 27, 2016 - Issue 11: 17th International Conference on QSAR in Environmental and Health Sciences (QSAR 2016) - Part II. Guest Editors: C.G. Barber and G.J. Myatt

1,711 Views
47 CrossRef citations to date
21 Altmetric

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Articles

An automated curation pr addressing chemical erro inconsistencies in public c QSAR modelling[$]

K. Mansouri, C. M. Grulke, A. M. Richard, R. S. Judson & A. J. Wi

Pages 911-937 | Received 03 Sep 2016, Accepted 24 Oct 2016, Published onli

Download citation | https://doi.org/10.1080/1062936X.2016.12

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Kamel Mansouri, Chris M. Grulke, Richard S. Judson & Antony J. Wi

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Research article | Open Access | Published: 18 September 2019

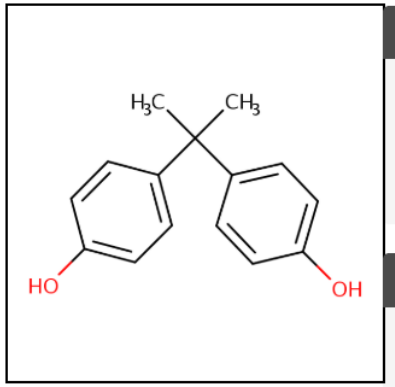
Open-source QSAR models for pKa prediction using multiple machine learning approaches

Kamel Mansouri, Neal F. Cariello, Alexandru Korotcov, Valery Tkachenko, Chris M. Grulke, Catherine S. Sprankle, David Allen, Warren M. Casey, Nicole C. Kleinstreuer & Antony J. Williams

Journal of Cheminformatics **11**, Article number: 60 (2019) | Cite this article

9334 Accesses | **8** Citations | **20** Altmetric | Metrics

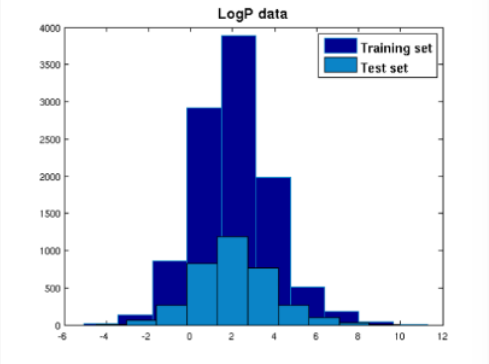
Properties, Fate and Transport
e.g. logP



Model Results

Predicted value: 3.35
Global applicability domain: Inside
Local applicability domain index: 0.877
Confidence level: 0.748

Model Performance

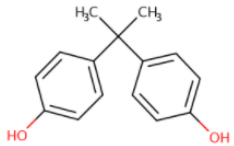


QMRF

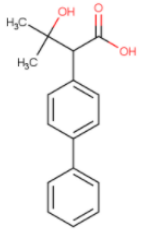
5-fold CV (75%)	
Q2	RMSE
0.850	0.690

od.epa.gov/dashboard/advanced_search/index

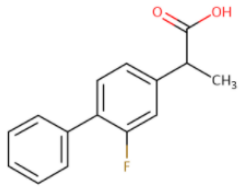
Nearest Neighbors from the Training Set



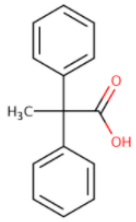
Bisphenol A
Measured:3.32
Predicted: 3.32



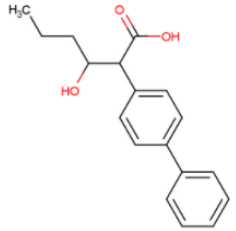
BUTANOIC ACID,2-(4-BIPHENYLYL)-3-HYDROXY-3-METHY
Measured:3.25
Predicted: 3.25



Flurbiprofen
Measured:4.16
Predicted: 4.16



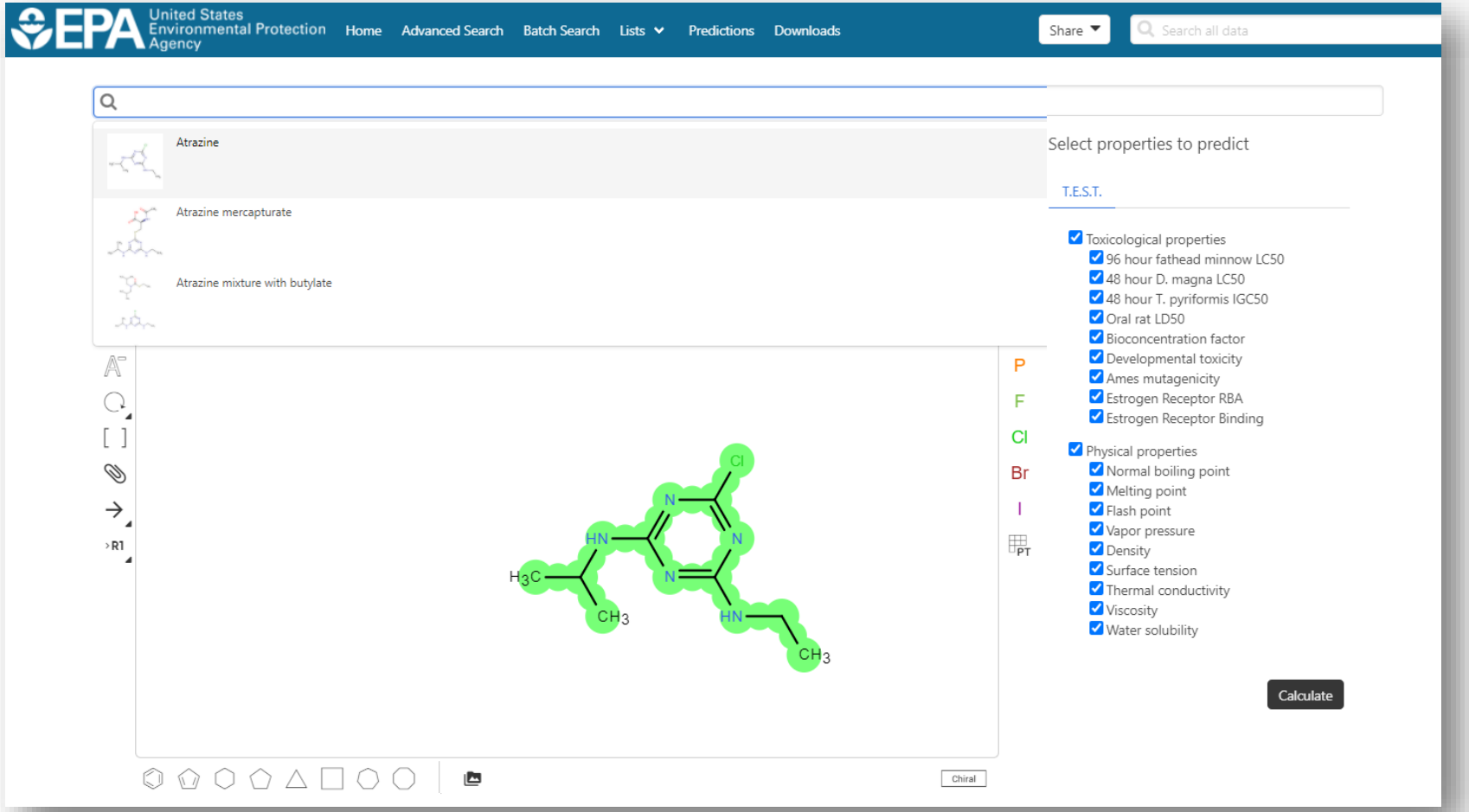
2,2-Diphenylpropionic acid
Measured:2.69
Predicted: 2.69



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

Predictions for New Chemicals

https://comptox.epa.gov/dashboard/predictions/index



Predictions for New Chemicals

https://comptox.epa.gov/dashboard/predictions/index

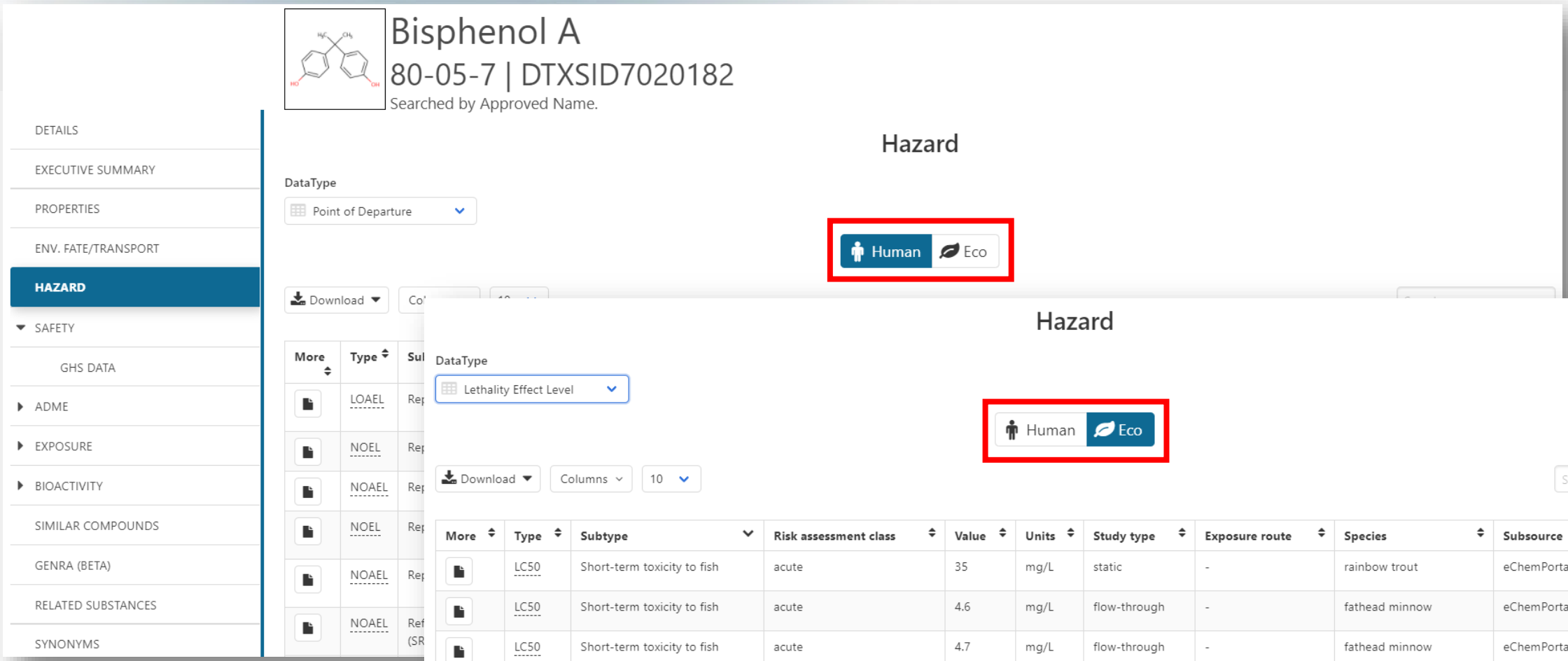
EPA United States Environmental Protection Agency

Provider: T.E.S.T.

Download Summary

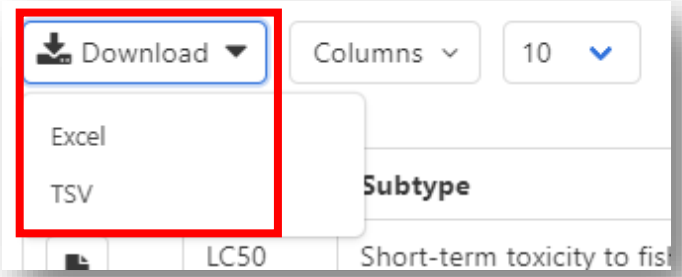
Property	Experimental Value	Consensus	Hierarchical clustering	Single model	Group contribution	Nearest neighbor
96 hour fathead minnow LC50		3.969 -Log10(mol/L) 22.469 mg/L	3.936 -Log10(mol/L) 24.234 mg/L	3.742 -Log10(mol/L) 37.882 mg/L	4.135 -Log10(mol/L) 15.355 mg/L	4.064 -Log10(mol/L) 18.079 mg/L
48 hour D. magna LC50		3.791 -Log10(mol/L) 33.887 mg/L	3.568 -Log10(mol/L) 56.592 mg/L	4.243 -Log10(mol/L) 11.976 mg/L	3.832 -Log10(mol/L) 30.824 mg/L	3.521 -Log10(mol/L) 63.123 mg/L
48 hour T. pyriformis IGC50			2.986 -Log10(mol/L) 216.359 mg/L			
Oral rat LD50		2.439 -Log10(mol/kg) 761.182 mg/kg	2.355 -Log10(mol/kg) 924.254 mg/kg			2.524 -Log10(mol/kg) 626.882 mg/kg
Bioconcentration factor		0.847 Log10 7.038	0.906 Log10 8.051	0.690 Log10 4.903	0.820 Log10 6.607	0.974 Log10 9.409
Developmental toxicity		true	true	true		
Ames mutagenicity		false	true			false
Estrogen Receptor RBA						
Estrogen Receptor Binding		false	false	false	false	
Normal boiling point		315.9 °C	318.0 °C		345.4 °C	284.3 °C
Melting point		114.0 °C	105.0 °C		79.4 °C	157.7 °C
Flash point		176.1 °C	180.1 °C		172.5 °C	175.7 °C
Vapor pressure		-6.072 Log10(mmHg) 8.464*10^-7 mmHg	-6.164 Log10(mmHg) 6.851*10^-7 mmHg		-5.679 Log10(mmHg) 2.093*10^-6 mmHg	-6.374 Log10(mmHg) 4.23*10^-7 mmHg

Hazard Data (Human and Eco)

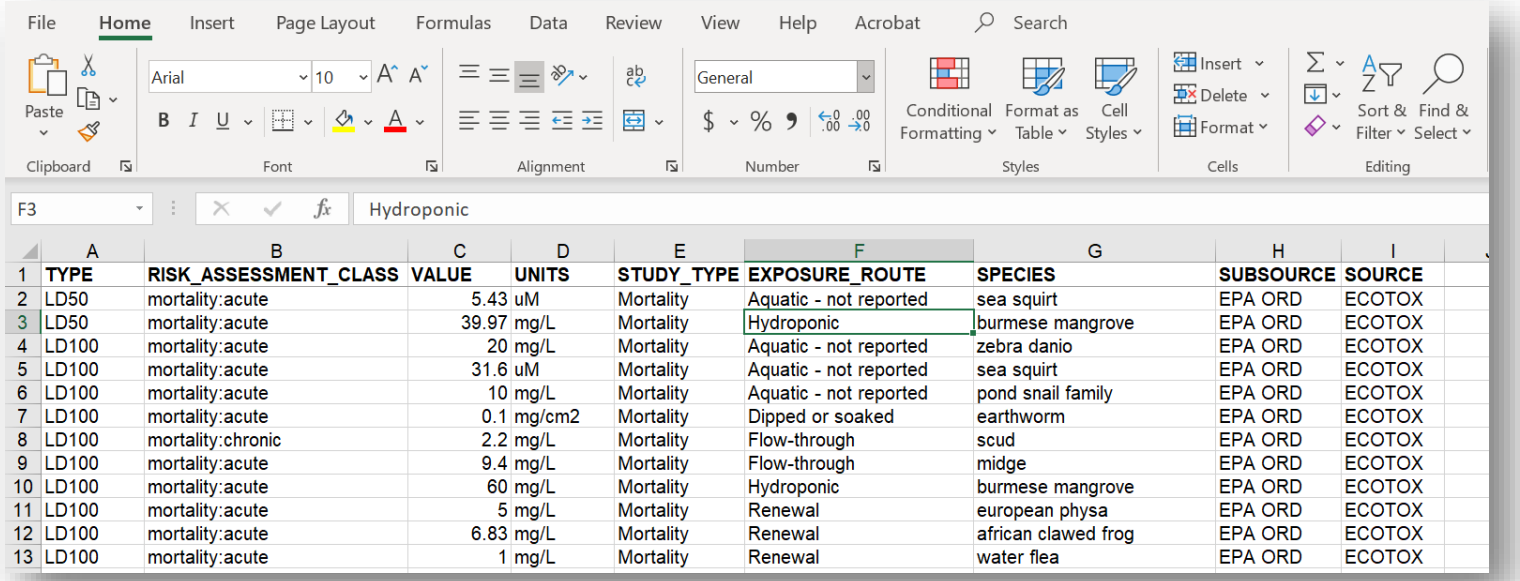


Hazard Data

- Data are harvested from > 30 data sources and provides both human and ecological data for >50,000 chemicals



- ***General Feature*** – anywhere you see a table you can download the data…



	A	B	C	D	E	F	G	H	I
1	TYPE	RISK_ASSESSMENT_CLASS	VALUE	UNITS	STUDY_TYPE	EXPOSURE_ROUTE	SPECIES	SUBSOURCE	SOURCE
2	LD50	mortality:acute	5.43	uM	Mortality	Aquatic - not reported	sea squirt	EPA ORD	ECOTOX
3	LD50	mortality:acute	39.97	mg/L	Mortality	Hydroponic	burmese mangrove	EPA ORD	ECOTOX
4	LD100	mortality:acute	20	mg/L	Mortality	Aquatic - not reported	zebra danio	EPA ORD	ECOTOX
5	LD100	mortality:acute	31.6	uM	Mortality	Aquatic - not reported	sea squirt	EPA ORD	ECOTOX
6	LD100	mortality:acute	10	mg/L	Mortality	Aquatic - not reported	pond snail family	EPA ORD	ECOTOX
7	LD100	mortality:acute	0.1	mg/cm2	Mortality	Dipped or soaked	earthworm	EPA ORD	ECOTOX
8	LD100	mortality:chronic	2.2	mg/L	Mortality	Flow-through	scud	EPA ORD	ECOTOX
9	LD100	mortality:acute	9.4	mg/L	Mortality	Flow-through	midge	EPA ORD	ECOTOX
10	LD100	mortality:acute	60	mg/L	Mortality	Hydroponic	burmese mangrove	EPA ORD	ECOTOX
11	LD100	mortality:acute	5	mg/L	Mortality	Renewal	european physa	EPA ORD	ECOTOX
12	LD100	mortality:acute	6.83	mg/L	Mortality	Renewal	african clawed frog	EPA ORD	ECOTOX
13	LD100	mortality:acute	1	mg/L	Mortality	Renewal	water flea	EPA ORD	ECOTOX

Safety Data

- Safety Data (Global Harmonization System (GHS)) from PubChem

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

GHS Data

Print Page

PUBCHEM > BISPHENOL A > LABORATORY CHEMICAL SAFETY SUMMARY (LCSS) > GHS CLASSIFICATION

CID 6623

Bisphenol A

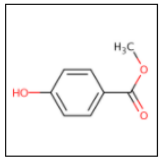
GHS Classification

Showing 6 of 6

Pictogram(s)	Corrosive Irritant Health Hazard
Signal	Danger
GHS Hazard Statements	H317: May cause an allergic skin reaction [Warning Sensitization, Skin] H318: Causes serious eye damage [Danger Serious eye damage/eye irritation] H335: May cause respiratory irritation [Warning Specific target organ toxicity, single exposure; Respiratory tract irritation] H360F: May damage fertility [Danger Reproductive toxicity]
Precautionary Statement Codes	P201, P202, P261, P271, P272, P280, P281, P302+P352, P304+P340, P305+P351+P338, P308+P313, P310, P312, P321, P333+P313, P363, P403+P233, P405, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)

Sources of Exposure to Chemicals (More later – Kristin Isaacs)

EPA United States Environmental Protection Agency



Methylparaben

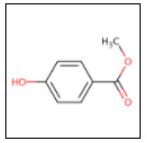
99-76-3 | DTXSID4022529

Searched by DSSTox Substance Id.

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- SAFETY
- ADME
- EXPOSURE
  - PRODUCT & USE CATEGORIES
  - CHEMICAL WEIGHT FRACTION
  - CHEMICAL FUNCTIONAL USE
  - TOXICS RELEASE INVENTORY

Product and Use Categories (PUCs)

Download | Columns | 10 | Search query



Methylparaben

99-76-3 | DTXSID4022529

Searched by DSSTox Substance Id.

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- SAFETY
- ADME
- EXPOSURE
  - PRODUCT & USE CATEGORIES
  - CHEMICAL WEIGHT FRACTION
  - CHEMICAL FUNCTIONAL USE
  - TOXICS RELEASE INVENTORY
  - MONITORING DATA

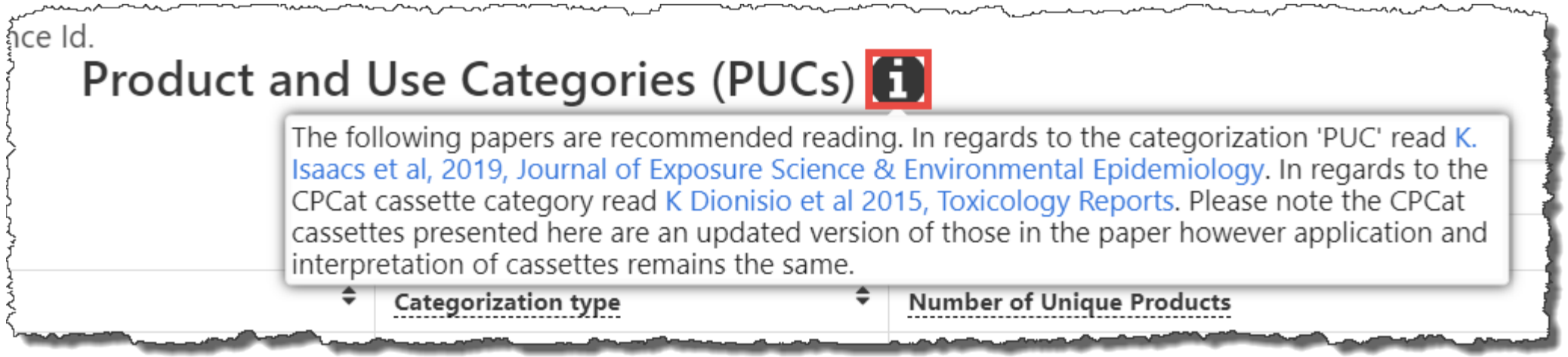
Chemical Weight Fractions

Download | Columns | 25 | Search query

Product Name	Product Use Category	Minimum Weight Fraction	Maximum Weight Fraction	Data Type	Source
YOUTOPIA- PET SHAMPOO	all pets: pet shampoo			MSDS	CPCPdb
YLP Lip Gloss Solid F4203-06006-A12	make-up and related: lip gloss			MSDS	CPCPdb
ylp lip gloss liquid multiple colors 2	make-up and related: lip gloss			MSDS	CPCPdb
YLP Lip Gloss Liquid F4204-06001-A47	make-up and related: lip gloss			MSDS	CPCPdb
YLP Lip Gloss Liquid F4204-06001-A21	make-up and related: lip gloss			MSDS	CPCPdb
wondermask p peelable mask_ 2211 bulk	Not Yet Categorized:	0.00	1.00e-2	MSDS	SIRI
waterlss skn cleansr w/plastc scrubr_sbs-33	Not Yet Categorized:			MSDS	SIRI
water for injection_ bacteriostatic	Not Yet Categorized:			MSDS	SIRI
Water Based Nail Polish - 196C	nails: nail polish			other	CPCPdb
Washable Ink	Not Yet Categorized:			MSDS	CPCPdb
Vitamin Cream	facial cleansing and moisturizing: face cream/moisturizer			MSDS	CPCPdb

General Feature
On-hover Informational Icons

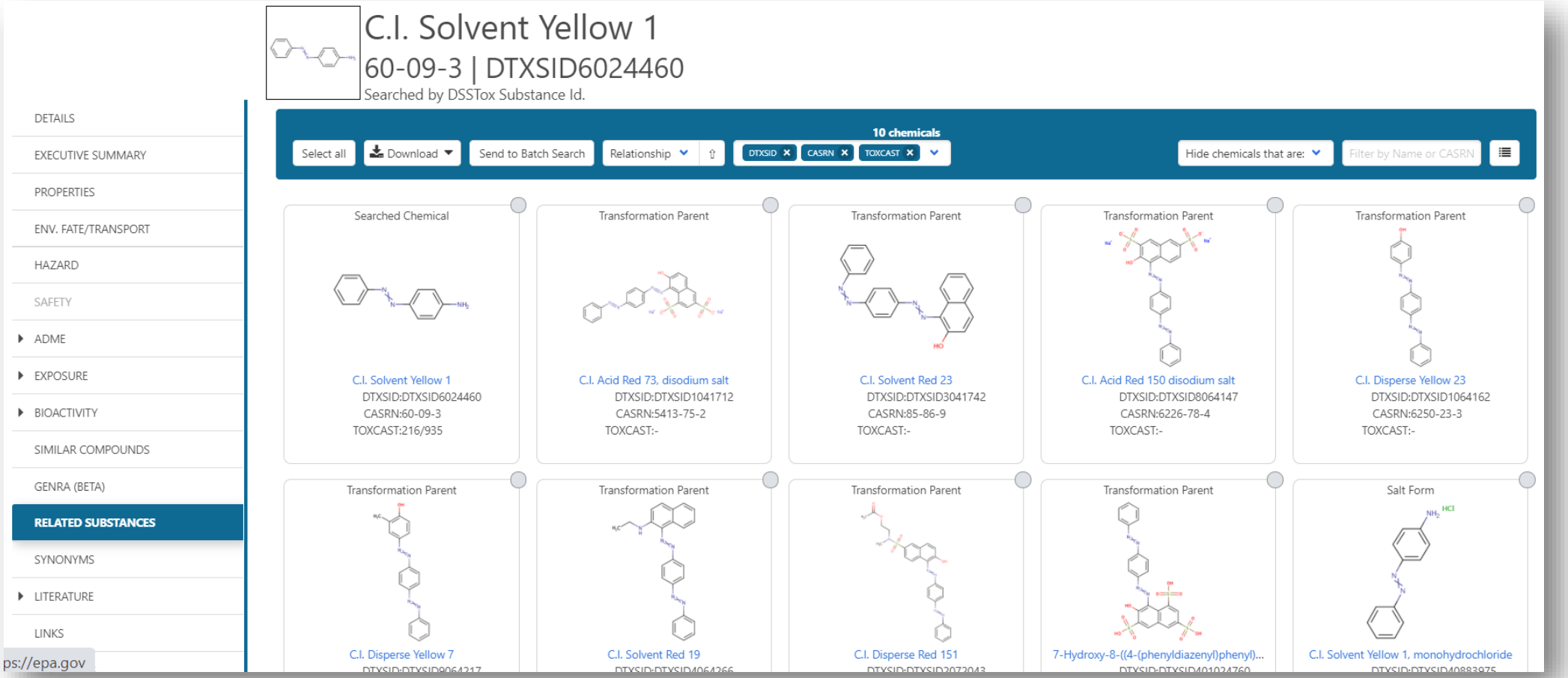
- Watch out for the on-hover informational icons to gather info



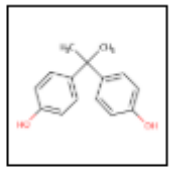
- Descriptive text or video about the data, associated publications etc.

Related Substances
e.g. Aromatic amine to Azo Dyes

- Related substances – Parent to Transformation product: metabolites, degradants; Monomer to polymer;



Identifiers to Support Searches



Bisphenol A

80-05-7 | DTXSID7020182

Searched by Approved Name.

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

Synonyms

Download | 25 | Search query

Synonym	Quality
Bisphenol A	**Valid**
4,4'-(Propane-2,2-diyl)diphenol	**Valid**
Phenol, 4,4'-(1-methylethylidene)bis-	**Valid**
80-05-7 Active CAS-RN	**Valid**
BPA	**Valid**
4,4'-Propane-2,2-diyldiphenol	**Valid**
Phenol, 4,4'-(1-methylethylidene)bis-	**Valid**
4-06-00-06717 Beilstein Registry Number	Beilstein
(4,4'-Dihydroxydiphenyl)dimethylmethane	*Good*
2,2-Bis(4'-hydroxyphenyl) propane	*Good*
2,2'-Bis(4-hydroxyphenyl)propane	*Good*
2,2-BIS-(4-HYDROXY-PHENYL)-PROPANE	*Good*
2,2-Bis(4-hydroxyphenyl)propane	*Good*
2,2-Bis(p-hydroxyphenyl)propane	*Good*
2,2-Di(4-Hydroxyphenyl) Propane	*Good*

Identifiers to Support Searches

- Identifiers include systematic names, trade names, CASRNs (Active, Alternate and Deleted)

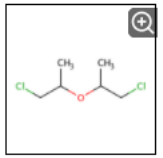
Synonym	Quality
beta,beta'-Bis(p-hydroxyphenyl)propane	Other
beta,beta-Di-(p-hydroxyphenyl)propane	Other
beta-Di-(p-hydroxyphenyl)propane	Other
beta-Di-p-hydroxyphenylpropane	Other
137885-53-1 Deleted CAS-RN	Deleted
146479-75-6 Deleted CAS-RN	Deleted
27360-89-0 Deleted CAS-RN	Deleted
28106-82-3 Deleted CAS-RN	Deleted
37808-08-5 Deleted CAS-RN	Deleted

<< < 1 2 3 4 5 6 > >>

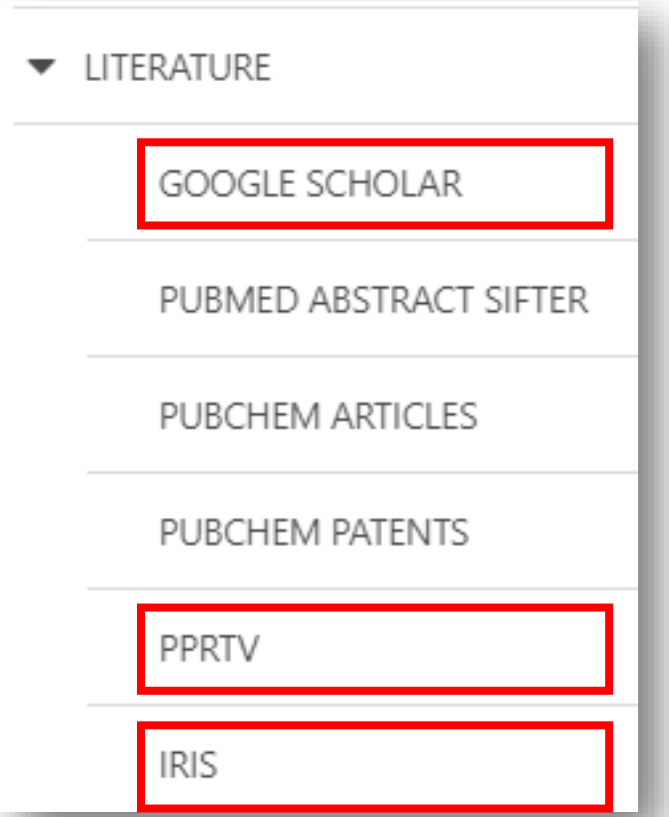
Showing 126 to 134 of 134 records

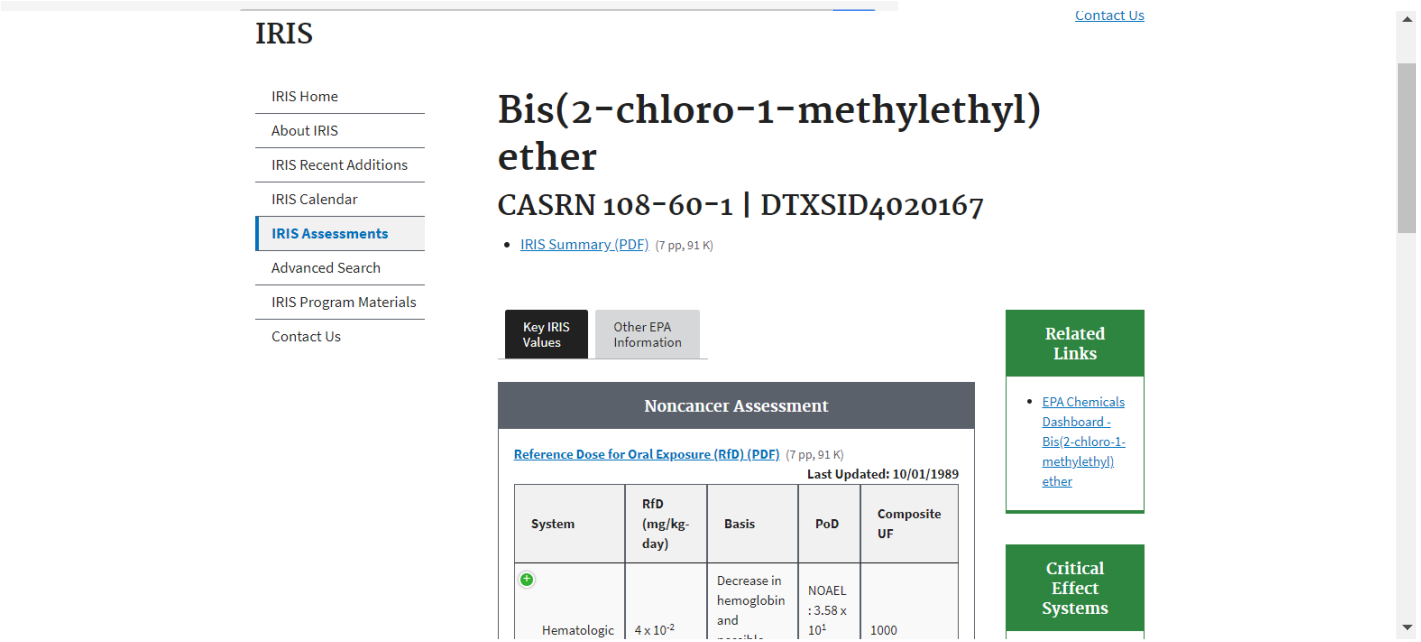
Identifiers are used in the app

- Identifiers are used to feed and link into “Literature”



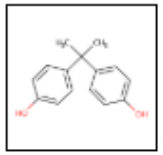
bis(2-Chloro-1-methylethyl) ether
108-60-1 | DTXSID4020167





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

EPA United States Environmental Protection Agency



Bisphenol A

80-05-7 | DTXSID7020182

Searched by Approved Name.

- DETAILS
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- BIOACTIVITY
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE
- **LINKS**
- COMMENTS

General

- EPA Substance Registry Service
- Household Products Database
- Chemical Entities of Biological Interest (ChEBI)
- PubChem
- Chemspider
- CPCat
- DrugBank
- HMDB
- Wikipedia
- MSDS Lookup
- ChEMBL
- Chemical Vendors
- CalEPA Office of Environmental Health Hazard Assessment
- NIOSH Chemical Safety Cards
- ToxPlanet
- ACS Reagent Chemicals
- Wikidata
- ChemHat: Hazards and Alternatives Toolbox
- Wolfram Alpha
- ScrubChem
- ECHA Brief Profile

Toxicology

- ACToR
- DrugPortal
- CCRIS
- ChemView
- CTD
- eChemPortal
- Gene-Tox
- HSDB
- ToxCast Dashboard 2
- LactMed
- International Toxicity Estimates for Risk
- ATSDR Toxic Substances Portal
- Superfund Chemical Data matrix
- NIOSH IDLH Values
- ACToR PDF Report
- Toxics Release Inventory
- CREST
- National Air Toxics Assessment

Publications

- Toxline
- Environmental Health Perspectives
- NIEHS
- National Toxicology Program
- Google Books
- Google Scholar
- Google Patents
- PPRTVWEB
- PubMed
- IRIS Assessments
- EPA HERO
- NIOSH Skin Notation Profiles
- NIOSH Pocket Guide
- RSC Publications
- BioCaddie DataMed
- Springer Materials
- Federal Register
- Regulations.gov
- Bielefeld Academic Search Engine
- CORE Literature Search

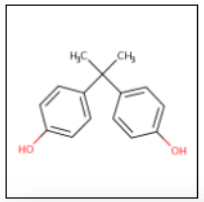
Analytical

- FOR-IDENT
- NEMI: National Environmental Methods Index
- RSC Analytical Abstracts
- Tox21 Analytical Data
- MONA: MassBank North America
- mzCloud
- NIST IR Spectrum
- NIST MS Spectrum

Prediction

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

External Links



Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

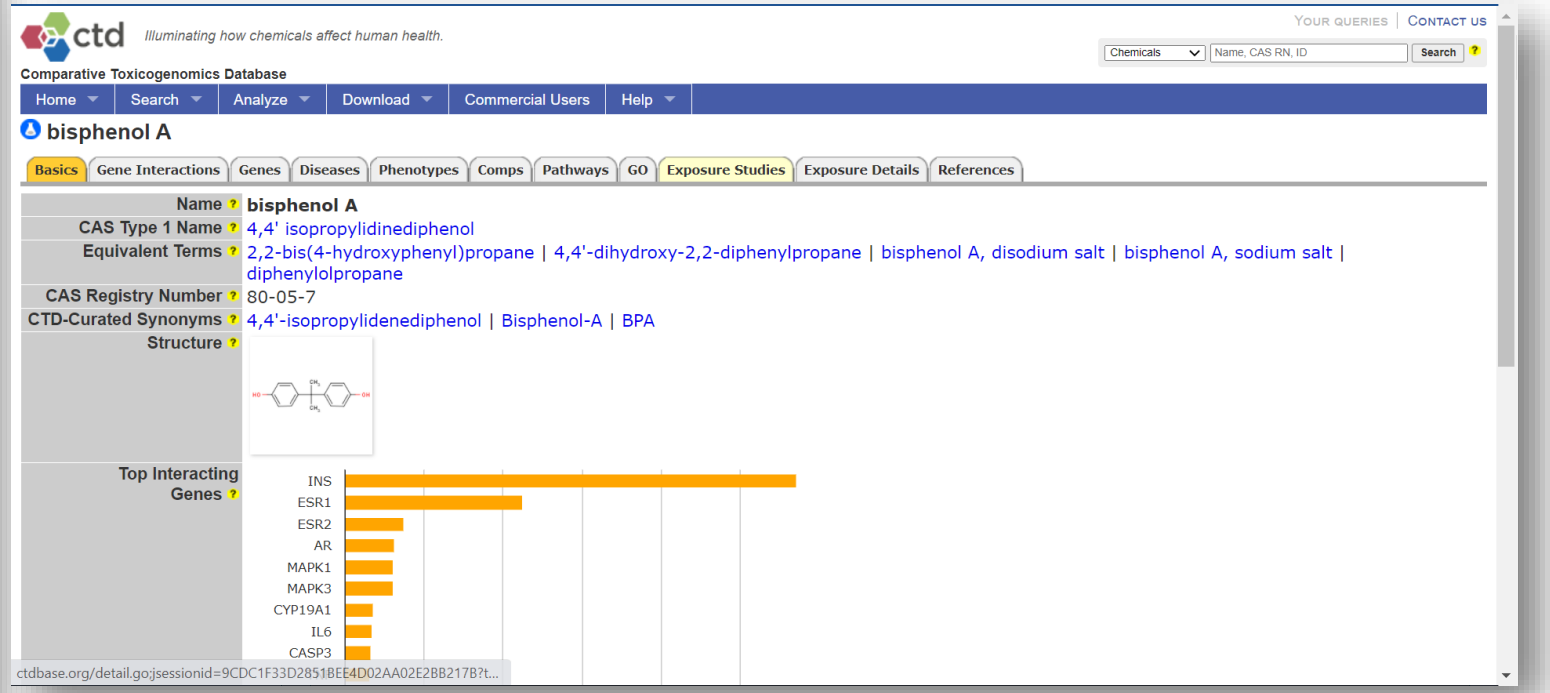
General

- EPA Substance Registry Service
- PubChem
- Chemspider
- CPCat
- DrugBank
- Wikipedia
- MSDS Lookup
- ChEMBL
- ToxPlanet
- ACS Reagent Chemicals
- ChemHat: Hazards and Alternatives Toolbox

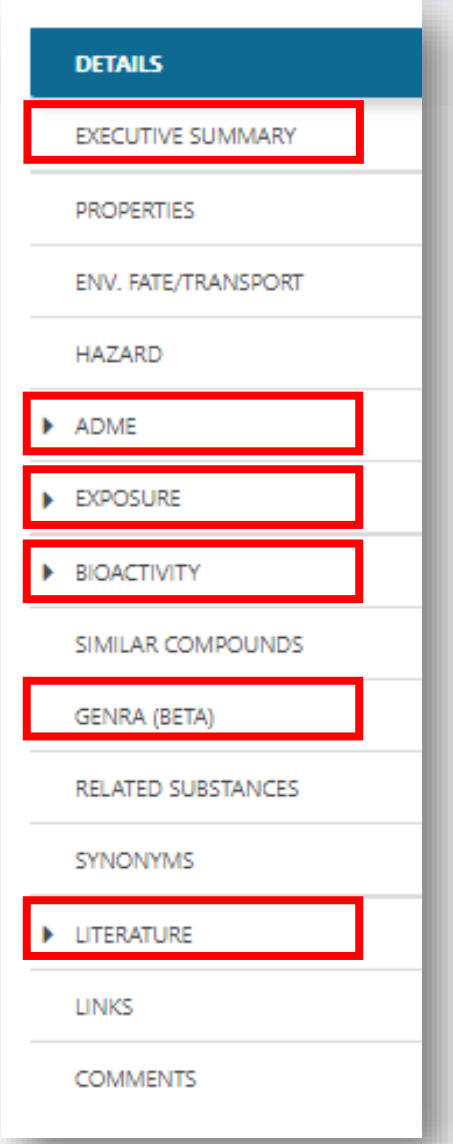
Toxicology

- ACToR
- DrugPortal
- CCRIS
- ChemView
- CTD
- eChemPortal
- Gene-Tox
- HSDB
- ToxCast Dashboard 2
- ACToR PDF Report
- CREST
- National Air Toxics Assessment

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



More details will be covered on…



- ADME:IVIVE will be covered by John Wambaugh
- Exposure will be covered by Kristin Isaacs
- Bioactivity will be covered by Katie Paul-Friedman
- GenRA will be covered by Grace Patlewicz
- Literature:Abstract Sifter will be covered by Nancy Baker

- …and much of this data will show up in the Executive Summary for a chemical substance

Executive Summary
Summary view of relevant data

EPA United States Environmental Protection Agency

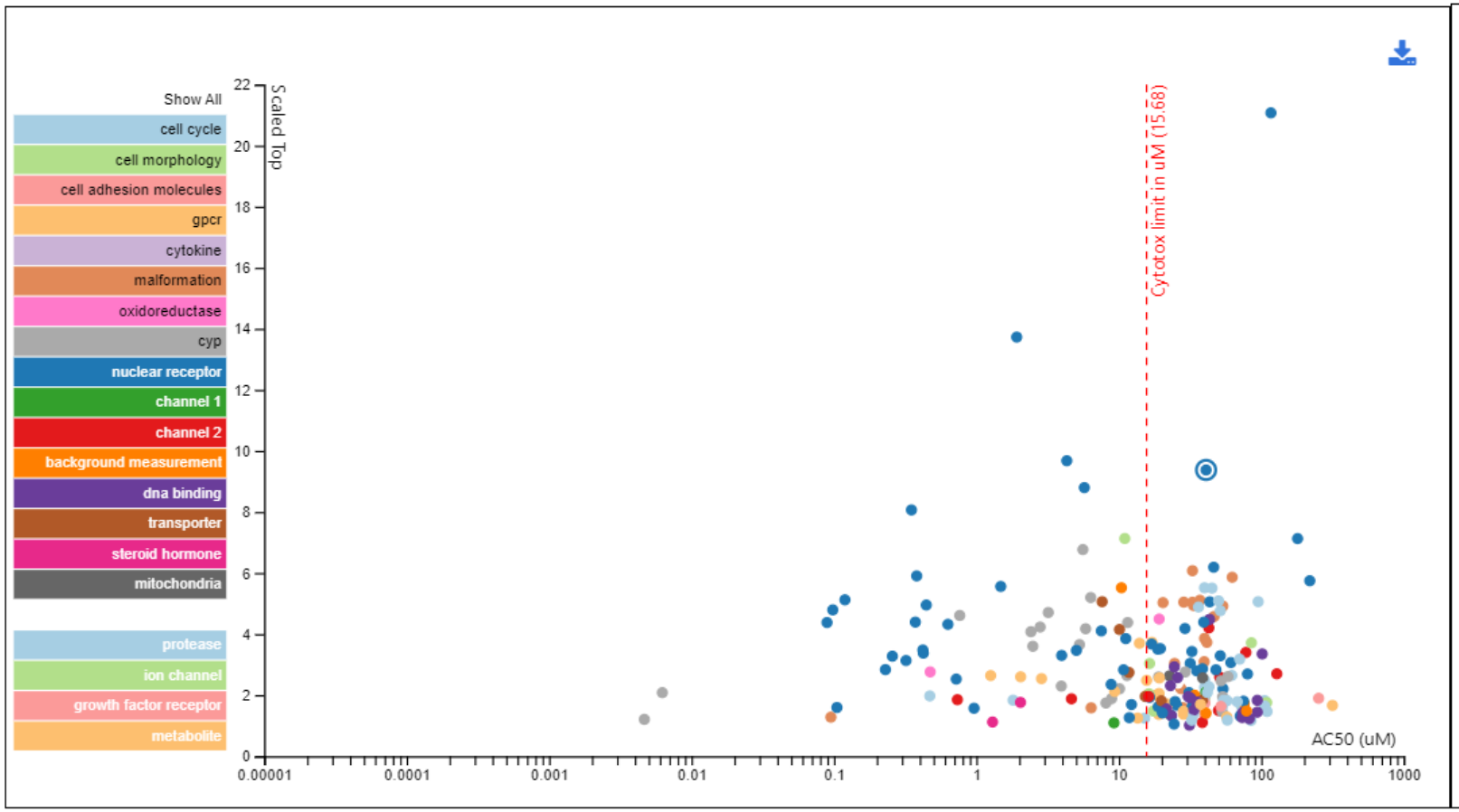
Quantitative Risk Assessment Values

IRIS values available

Endocrine System

Endocrine Disruption Potential. Significant Estrogen and Androgen Receptor activity seen. Chemical was positive

TOXCAST DATA



ASSAY DETAILS

AC50 (uM): 40.99
Scaled top: 9.38
Assay Endpoint Name: ACEA_AR_antagonist_80hr
Gene Symbol: AR
Organism: human
Tissue: prostate
Assay Format Type: cell-based
Biological Process Target: cell proliferation
Detection Technology: RT-CES
Analysis Direction: NA
Intended Target Family: nuclear receptor
Description: Data from the assay component ACEA_AR_agonist_80hr was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of growth reporter, measures of the cells for gain-of-signal activity can be used to understand the signaling at the pathway-level as they relate to the gene AR. Furthermore, this assay endpoint can be referred to as a primary readout, because this assay has produced multiple assay endpoints where this one serves a signaling function. To generalize the intended target to other relatable targets, this assay endpoint is annotated to the "nuclear receptor" intended target family, where the subfamily is "steroidal".

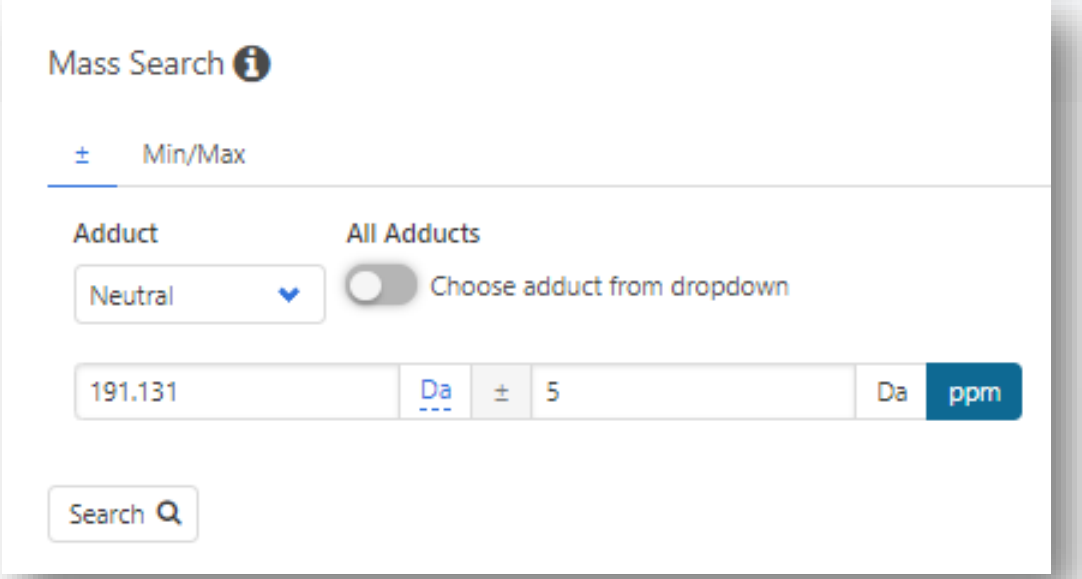
Developmental Toxicology

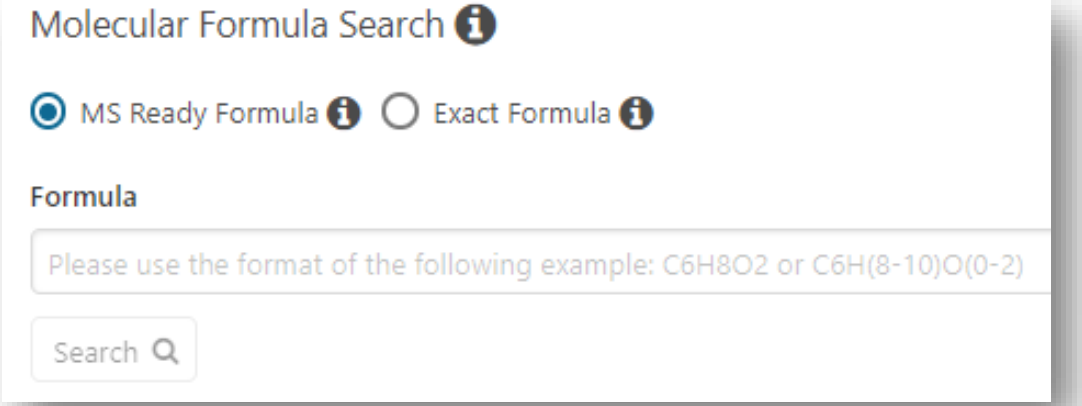
Developmental toxicity PODs available

logP log(BCF) log(VP)

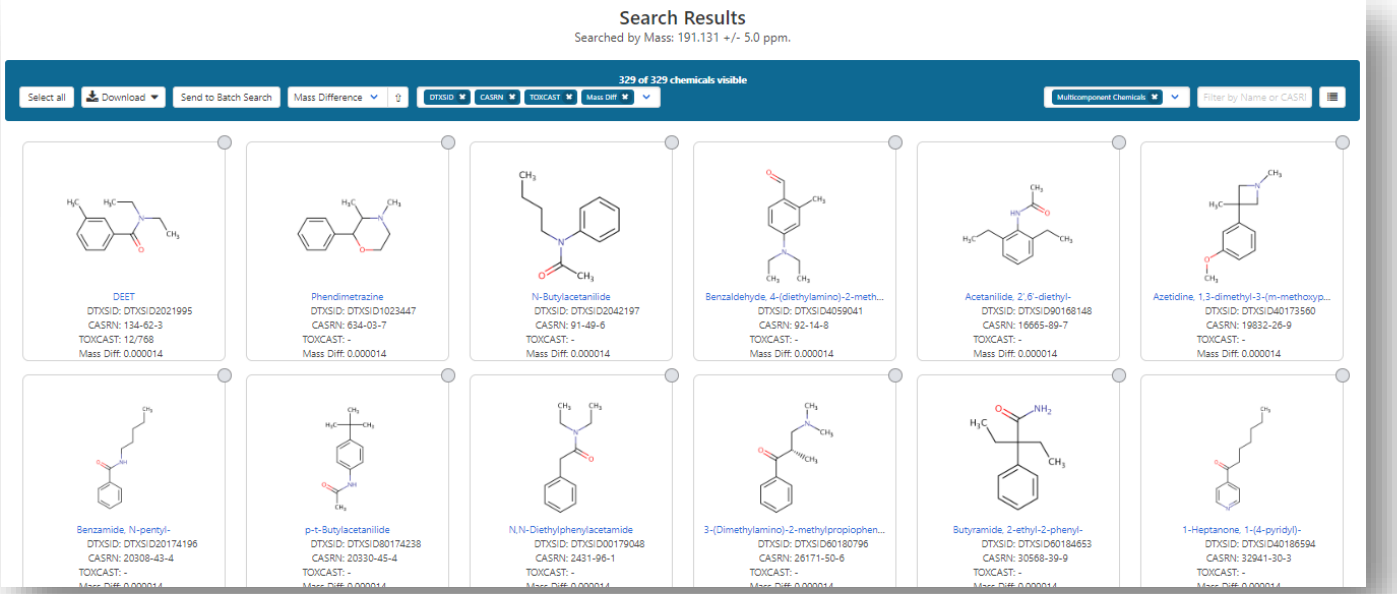
Advanced Searching: Mass and Formula

Advanced Searches
Mass and **Formula** Searches





Supports our suspect screening and non-targeted analysis mass spectrometry research efforts



Batch Searching

Access data *en masse* for thousands of chemicals….

EPA United States Environmental Protection Agency

EPA United States Environmental Protection Agency | Home | Advanced Search | Batch Search | Lists | Predictions | Downloads | Share | Search all data

Batch Search

Step 1 — Step 2 — Step 3 — Step 4 — Step 5

Step Three: Select Download Data or Display Chemicals

Please enter one identifier per line

Select Input Type(s)

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

Enter Identifiers to Search (One per line. Searches should be limited to <5000 identifiers.)

```
Sodium azide
O,O-Dimethyl S-[(4-oxo-1,2,3-benzotriazin-3(4H)-yl)methyl] phosphorodithioate
(Trichloromethyl)benzene
100-44-7
(Chloromethyl)benzene
98-07-7
111-44-4
1-Chloro-2-(2-chloroethoxy)ethane
Chloro(chloromethoxy)methane
2-(Butan-2-yl)-4,6-dinitrophenol
```

Display All Chemicals | Download Chemical Data

Select Output Format and Content

United States Environmental Protection Agency

Step Four: Select Data Output Format and Choose Data Fields to Download

Select Output Format:

Excel

Download

Customize Results

- [ ] Select All
- [ ] Select All in Lists

Chemical Identifiers

- [x] DTXSID
- [x] Chemical Name
- [ ] DTXCID
- [ ] CAS-RN
- [ ] InChIKey
- [ ] IUPAC Name

Structures

- [ ] Mol File
- [ ] SMILES
- [ ] InChI String
- [ ] MS-Ready SMILES
- [ ] QSAR-Ready SMILES

Intrinsic And Predicted Properties

- [ ] Molecular Formula
- [ ] Average Mass
- [ ] Monoisotopic Mass
- [ ] TEST Model Predictions
- [ ] OPERA Model Predictions

Metadata

- [ ] Curation Level Details
- [ ] NHANES/Predicted Exposure
- [ ] Data Sources
- [ ] Include ToxVal Data Availability
- [ ] Assay Hit Count
- [ ] Number of PubMed Articles
- [ ] PubChem Data Sources
- [ ] CPDat Product Occurrence Count
- [ ] IRIS
- [ ] PPRTV
- [ ] Wikipedia Article
- [ ] QC Notes
- [ ] Include links to ACToR reports - SLOW! (BETA)

Presence in Lists:

- [ ] 40CFR116.4 Designation of Hazardous Substances (Above Ground Storage Tanks)
- [ ] 40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities
- [ ] AEGLS: Acute Exposure Guideline Levels
- [ ] ANDROGEN: Androgen Receptor Chemicals
- [ ] ARTICLE; Bench-Mark Dose Human Health Assessment List (Wignall et al., 2014)
- [ ] ARTICLE: Collaborative Estrogen Receptor Activity Prediction Project (CERAPP)
- [ ] ARTICLE: Collaborative Estrogen Receptor Activity Prediction Project (COMPARA)
- [ ] ATSDR Toxicological Profiles
- [ ] ATSDR: Minimal Risk Levels (MRLs) for Hazardous Substances
- [ ] ATSDR: Toxic Substances Portal Chemical List
- [ ] California Office of Environmental Health Hazard Assessment
- [ ] Canadian Domestic Substances List 2019
- [ ] CATEGORY: Amino acids
- [ ] CATEGORY: Color Index dyes
- [ ] CATEGORY: Flame Retardants

Batch Search CASRNs

EPA United States Environmental Protection Agency

Batch Search

Step 1 — Step 2 — Step 3 — Step 4 — Step 5

Step Four: Select Data Output Format and Choose Data Fields to Download

Please enter one identifier per line

Chemical Identifiers
- [x] DTXSID
- [x] Chemical Name
- [ ] DTXCID
- [x] CAS-RN
- [x] InChIKey
- [x] IUPAC Name

Structures
- [ ] Mol File
- [ ] SMILES
- [ ] InChI String
- [x] MS-Ready SMILES
- [ ] QSAR-Ready SMILES

Intrinsic And Predicted Properties
- [x] Molecular Formula
- [ ] Average Mass
- [ ] Monoisotopic Mass
- [ ] TEST Model Predictions
- [x] OPERA Model Predictions

Metadata
- [ ] Curation Level Details
- [ ] NHANES/Predicted Exposure
- [ ] Data Sources
- [x] Include ToxVal Data Availability
- [x] Assay Hit Count
- [x] Number of PubMed Articles

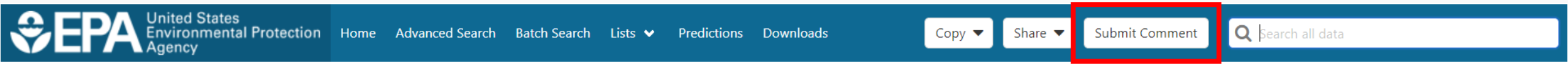
	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	INPUT	FOUND_BY	DTXSID	PREFERRE	CASRN	INCHIKEY	IUPAC_NAI	MOLECULA	TOXVAL_D	TOXCAST_	TOXCAST_	MS_READY	NUMBER_C	IRIS_LINK	PPRTV_LIN	ATMOSPHE	BIOCONCE
2	534-52-1	CAS-RN	DTXSID10	2-Methyl-4,6	534-52-1	ZXVONLUN	2-Methyl-4,6	C7H6N2O5	Y	27.56	261/947	CC1=C(O)C	179	-	Y	1.571E-12	2.88959
3	115-21-9	CAS-RN	DTXSID70	Ethyl silicon	115-21-9	ZOYFEXPF	Trichloro(eth	C2H5Cl3Si	Y	-	-	-	-	-	-	8.289E-12	13.9658
4	111-44-4	CAS-RN	DTXSID90	Bis(2-chloro	111-44-4	ZNSMNVML	1-Chloro-2-(	C4H8Cl2O	Y	1.12	10/891	ClCCOCCCl	12	Y	-	2.647E-12	9.99608
5	2763-96-4	CAS-RN	DTXSID50	Muscimol	2763-96-4	ZJQHPWUV	5-(Aminome	C4H6N2O2	Y	-	-	NCC1=CC((	4308	-	-	1.179E-10	5.05695
6	1464-53-5	CAS-RN	DTXSID00	2,2'-Bioxiran	1464-53-5	ZFIVKAOQE	2,2'-Bioxiran	C4H6O2	Y	-	-	C1OC1C1C	363	-	-	4.383E-12	1.27107
7	22224-92-6	CAS-RN	DTXSID30	Fenamiphos	22224-92-	ZCJPOPBZI	Ethyl 3-meth	C13H22NO3	Y	10.8	105/972	CCOP(=O)(	58	Y	-	1.66E-11	2.3394
8	359-06-8	CAS-RN	DTXSID40	Fluoroacetyl	359-06-8	ZBHDTYQJ	Fluoroacetyl	C2H2ClFO	Y	-	-	FCC(Cl)=O	-	-	-	3.513E-13	4.49379
9	5344-82-1	CAS-RN	DTXSID40	1-(o-Chloro	5344-82-1	YZUKKTCD	N-(2-Chloro	C7H7ClN2S	Y	-	-	NC(=S)NC1	-	-	-	2.482E-11	9.95206
10	7446-18-6	CAS-RN	DTXSID10	Thallium (I)	7446-18-6	YTQVHRVI	Dithallium(1-	O4STl2	Y	-	-	-	34	Y	Y	-	-
11	62207-76-5	CAS-RN	DTXSID40	Bis(3-fluoro	62207-76-	YRZXYIHD	-	C16H14CoF	Y	-	-	-	-	-	-	-	-
12	66-81-9	CAS-RN	DTXSID60	Cycloheximi	66-81-9	YPHMISFO	4-{(2R)-2-[(	C15H23NO4	Y	32.27	294/911	CC1CC(C)C	18709	-	-	1.756E-11	2.81761
13	106-96-7	CAS-RN	DTXSID30	Propargyl br	106-96-7	YORCIIVHL	3-Bromopro	C3H3Br	Y	-	-	BrCC#C	-	-	-	1.069E-11	10.4968
14	315-18-4	CAS-RN	DTXSID70	Mexacarbat	315-18-4	YNEVBPNZ	4-(Dimethyla	C12H18N2C	Y	5.11	12/235	CNC(=O)OC	27	-	-	1.447E-11	26.2914
15	110-00-9	CAS-RN	DTXSID60	Furan	110-00-9	YLQBMQCI	Furan	C4H4O	Y	0.0	0/235	O1C=CC=C	919	Y	-	4.019E-11	5.01648
16	3037-72-7	CAS-RN	DTXSID20	4-(diethoxyn	3037-72-7	YHFFINXFN	4-[Diethoxy(	C9H23NO2S	Y	-	-	-	-	-	-	5.95E-12	6.71292
17	75-44-5	CAS-RN	DTXSID00	Phosgene	75-44-5	YGYAWVD	Carbonyl dic	CCl2O	Y	-	-	ClC(Cl)=O	489	Y	-	9.994E-16	13.0711
18	2032-65-7	CAS-RN	DTXSID30	Methiocarb	2032-65-7	YFBPRJGD	3,5-Dimethy	C11H15NO2	Y	18.14	88/485	CNC(=O)OC	65	-	-	1.446E-11	34.1692
19	2778-04-3	CAS-RN	DTXSID20	Endothion	2778-04-3	YCAGGFXS	S-[(5-Metho	C9H13O6PS	Y	-	-	COC1=COC	-	-	-	4.355E-11	1.18341
20	12108-13-3	CAS-RN	DTXSID90	(Methylcyclo	12108-13-	YASXMYPV	Tricarbonyl(	C9H7MnO3	Y	2.56	11/430	-	68	-	-	-	-
21	7803-51-2	CAS-RN	DTXSID20	Phosphine	7803-51-2	XYFCBTPG	Phosphane	H3P	Y	-	-	-	928	Y	-	-	-
22	107-18-6	CAS-RN	DTXSID80	Allyl alcohol	107-18-6	XXROGKLT	Prop-2-en-1	C3H6O	Y	3.99	17/426	OCC=C	627	Y	Y	2.592E-11	4.03901
23	108-05-4	CAS-RN	DTXSID30	Vinyl acetate	108-05-4	XTXRWKRV	Ethenyl acet	C4H6O2	Y	1.7	4/235	CC(=O)OC=	206	Y	-	2.5E-11	5.52157
24	19624-22-7	CAS-RN	DTXSID10	Pentaborane	19624-22-	XPIBKKWN	-	B5H9	Y	-	-	-	-	-	-	-	-
25	75-74-1	CAS-RN	DTXSID00	Tetramethyl	75-74-1	XOOGZRUE	Tetramethyl	C4H12Pb	Y	-	-	C[Pb](C)(C)	24	-	-	-	-

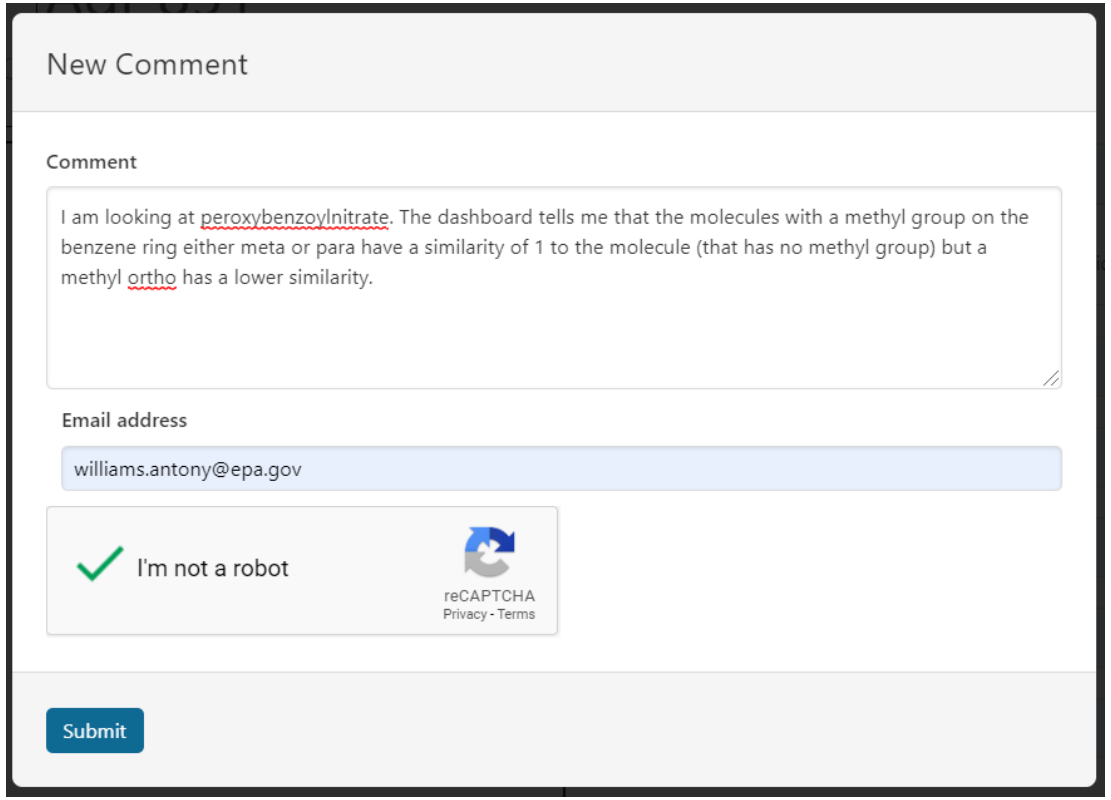
Worksheet1

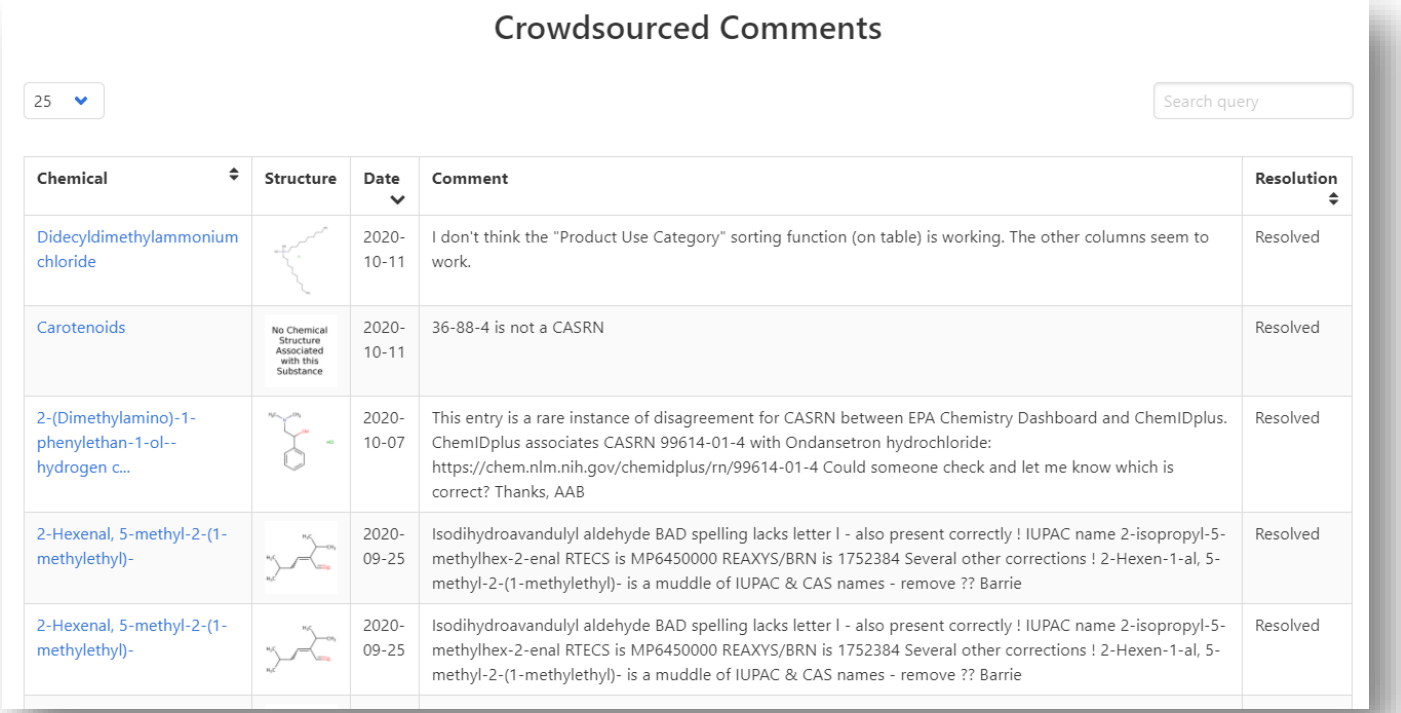
How Can You Help?

How can you help?

- Please submit comments for curation and feedback. We will respond.







Crowdsourced Comments

25

Search query

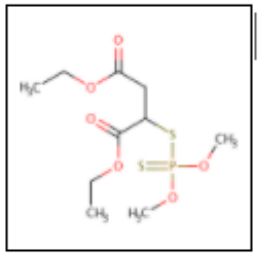
Chemical	Structure	Date	Comment	Resolution
Didecyldimethylammonium chloride		2020-10-11	I don't think the "Product Use Category" sorting function (on table) is working. The other columns seem to work.	Resolved
Carotenoids	No Chemical Structure Associated with this Substance	2020-10-11	36-88-4 is not a CASRN	Resolved
2-(Dimethylamino)-1-phenylethan-1-ol--hydrogen c...		2020-10-07	This entry is a rare instance of disagreement for CASRN between EPA Chemistry Dashboard and ChemIDplus. ChemIDplus associates CASRN 99614-01-4 with Ondansetron hydrochloride: https://chem.nlm.nih.gov/chemidplus/rn/99614-01-4 Could someone check and let me know which is correct? Thanks, AAB	Resolved
2-Hexenal, 5-methyl-2-(1-methylethyl)-		2020-09-25	Isodihydroavandulyl aldehyde BAD spelling lacks letter l - also present correctly ! IUPAC name 2-isopropyl-5-methylhex-2-enal RTECS is MP6450000 REAXYS/BRN is 1752384 Several other corrections ! 2-Hexen-1-al, 5-methyl-2-(1-methylethyl)- is a muddle of IUPAC & CAS names - remove ?? Barrie	Resolved
2-Hexenal, 5-methyl-2-(1-methylethyl)-		2020-09-25	Isodihydroavandulyl aldehyde BAD spelling lacks letter l - also present correctly ! IUPAC name 2-isopropyl-5-methylhex-2-enal RTECS is MP6450000 REAXYS/BRN is 1752384 Several other corrections ! 2-Hexen-1-al, 5-methyl-2-(1-methylethyl)- is a muddle of IUPAC & CAS names - remove ?? Barrie	Resolved

Prototypes in Progress

New AnalyticalQC Database

- The analytical QC data on the dashboard is based on a snapshot from ~5 years ago
- The Tox21 browser has continued to be updated with new data including NMR data
- New database is presently in construction hosting ALL QC data

Example of unsynchronized data



Malathion

121-75-5 | DTXSID4020791

Searched by Approved Name.

ToxCast/Tox21

QC Data ID	Grade	Description
Tox21_111175	Pass	Purity>90% and MW confirmed
Tox21_111175_1	Pass	Purity>90% and MW confirmed
Tox21_400048	Pass	Purity>90% and MW confirmed

QC Grade

T0	A	MW Confirmed, Purity > 90%
T4	F	CAUTION, Incorrect MW Biological Activity Unreliable

QC Grade

T0	Z	MW Confirmed, No Purity Info
T4	ND	Not Determined Analytical analysis is in progress

QC Grade

T0	D	CAUTION, Purity <50%
T4	D	CAUTION, Purity <50%

AnalyticalQC Database

- Single database integrating all analytical data at a substance level
- Hyperlinked to all individual spectral report files

DTXSID4020791

121-75-5

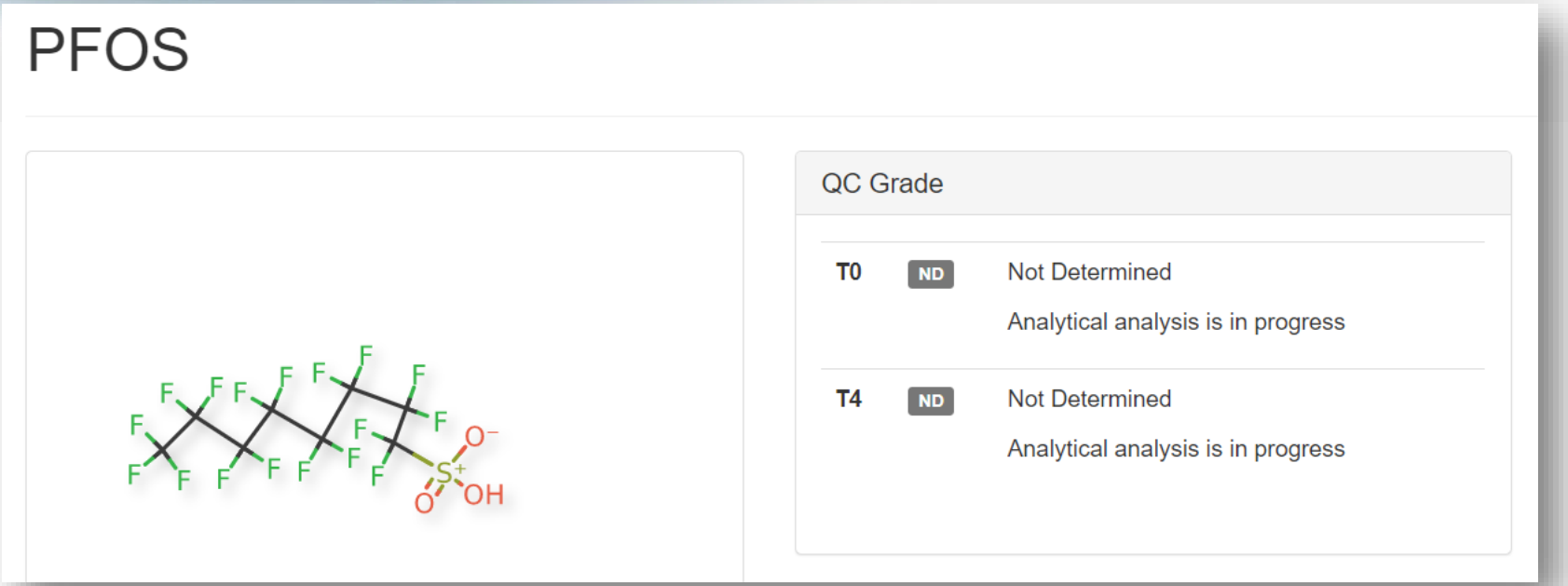
Malathion

Show 25 entries Copy Excel CSV

Search:

FileDate	ExpDate	SampleId	PubChemSid	PubChemCid	Tox21Id	filename	study	Timepoint	batch	well	grade	purity	PassFail	comment
2015-02-23	2014-07-29	NCGC00091902-08	144214009	4004	400048	Tox21_400048-12_04_LCMS.pdf	OPANS LCMS	T4	Batch5-SP123647	L19	Z	MW Confirmed, No Purity Info	Fail	
2015-02-23	2014-07-30	NCGC00091902-08	144214009	4004	400048	Tox21_400048-13_04_LCMS.pdf	OPANS LCMS	T4	Batch5-SP123647	P20	Z	MW Confirmed, No Purity Info	Fail	
2019-02-13	2016-11-01	NCGC00091902-05	144204726	4004	111175	Tox21_111175_04_NMR.pdf	OPANS NMR	T4		A7	F	Impure	Fail	CAUTION, Incorrect MW
2014-11-07	2011-09-10	NCGC00091902-08	144214009	4004	400048	Tox21_400048_00_LCMS1.pdf	OPANS LCMS	T0	Batch2-SP109801	H24	D	<50%	Fail	
2015-02-23	2014-07-26	NCGC00091902-08	144214009	4004	400048	Tox21_400048-4_04_LCMS.pdf	OPANS LCMS	T4	Batch5-SP123646	C24	D	<50%	Fail	
2015-02-23	2014-07-27	NCGC00091902-08	144214009	4004	400048	Tox21_400048-5_04_LCMS.pdf	OPANS LCMS	T4	Batch5-SP123646	H20	D	<50%	Fail	
2015-02-23	2014-08-02	NCGC00091902-08	144214009	4004	400048	Tox21_400048-3_04_LCMS.pdf	OPANS LCMS	T4	Batch5-SP123649	D24	D	<50%	Fail	
2015-02-23	2014-09-04	NCGC00091902-08	144214009	4004	400048	Tox21_400048_04_LCMS.pdf	OPANS LCMS	T4	Batch5-SP123651	K5	D	<50%	Fail	
2015-02-23	2014-09-29	NCGC00091902-08	144214009	4004	400048	Tox21_400048-1_04_LCMS.pdf	OPANS LCMS	T4	Batch5-SP123653	C12	D	<50%	Fail	
2015-02-23	2014-09-30	NCGC00091902-08	144214009	4004	400048	Tox21_400048-2_04_LCMS.pdf	OPANS LCMS	T4	Batch5-SP123653	P11	D	<50%	Fail	
2014-10-24		NCGC00091902-05	144204726	4004	111175	Tox21_111175_00_GCMS1.pdf	NIST GCMS	T0			A	MW Confirmed, Purity>90%	Pass	

“Analysis in Progress”



- Some chemicals remain “analysis in progress” after many years
- We have examined the data for many of these and the issue is in the analysis method. Examples are: Retention time is longer than run time, cannot get HNMR spectra for chemicals without H

PROTOTYPE Hazard Comparison Dashboard

United States Environmental Protection Agency

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 one location. 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.

Hazard Comparison Dashboard Hazard Predict Search Standardizer

Hazard Comparison | None | Export

169 / 169

Legend: VH - Very High, H - High, M - Medium, L - Low, I - Inconclusive **Authoritative**, Screening, *QSAR Model*

- Skipped (1)
- Filters (0)
- Sorting (0)
- Products (0)
- Structure

CAS Name	Human Health Effects															Ecotoxicity		Fate	
	Acute Mammalian Toxicity								Neurotoxicity		Systemic Toxicity								
	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
75-05-8 Acetonitrile	M	M	M	I	L	*L*	I	L	M										
107-02-8 Acrolein	VH	VH	H	H	H	*L*	L	L											
107-13-1 Acrylonitrile	H	H	H	VH	H	*L*	H	H	H										
107-18-6 Allyl alcohol	H	H	H	H	L	H	I	I											
62-53-3 Aniline	H	H	H	VH	H	*L*	M	L	H										

Springer Link

Original Paper | Published: 21 January 2020

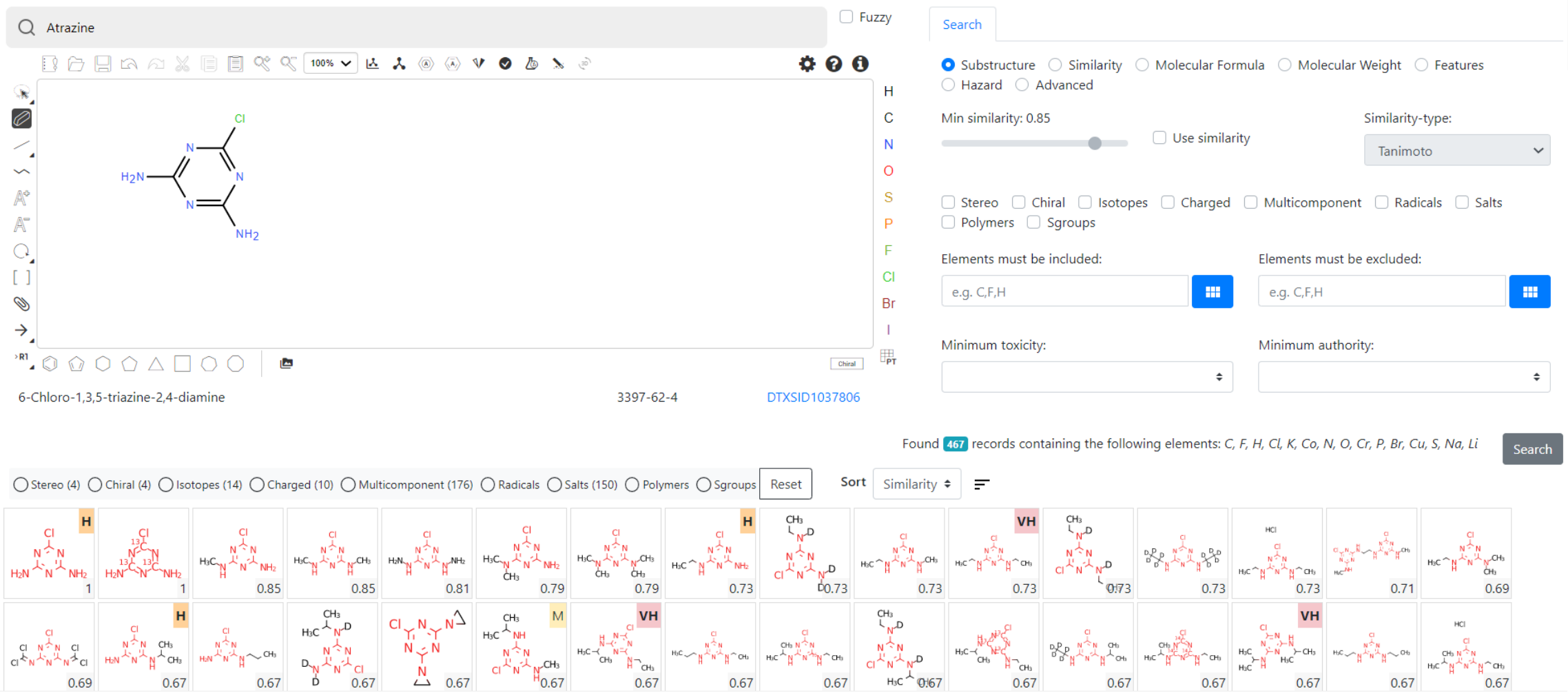
An automated framework for compiling and integrating chemical hazard data

Leora Vegosen & Todd M. Martin

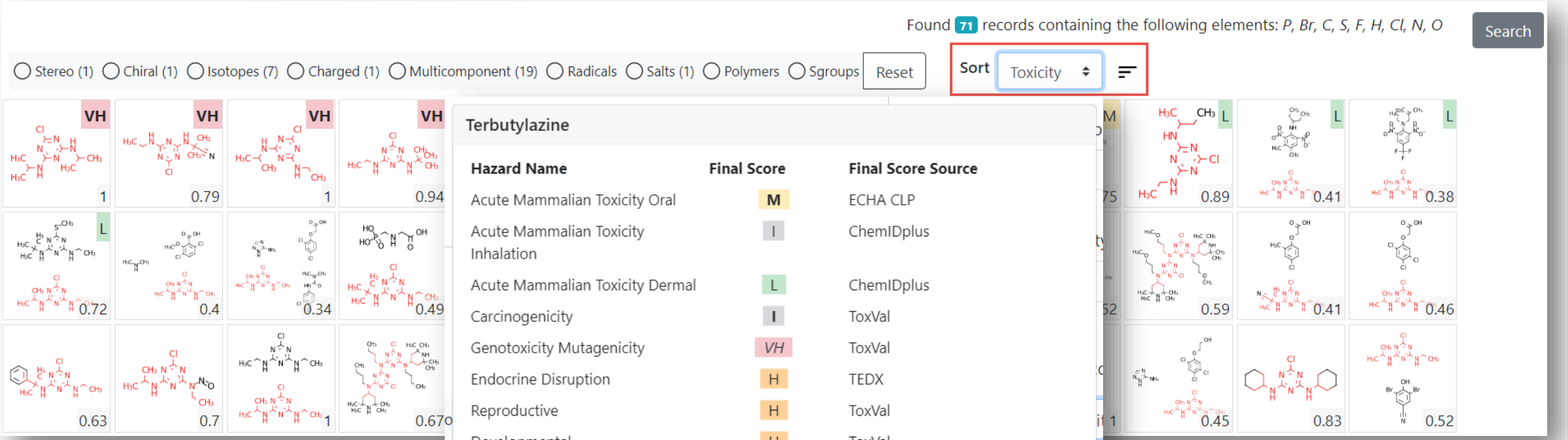
Clean Technologies and Environmental Policy **22**, 441–458(2020) | Cite this article

163 Accesses | Metrics

PROTOTYPE Structure/Substructure/Similarity Search available



Hit Sets based on Show and Sort on Toxicity

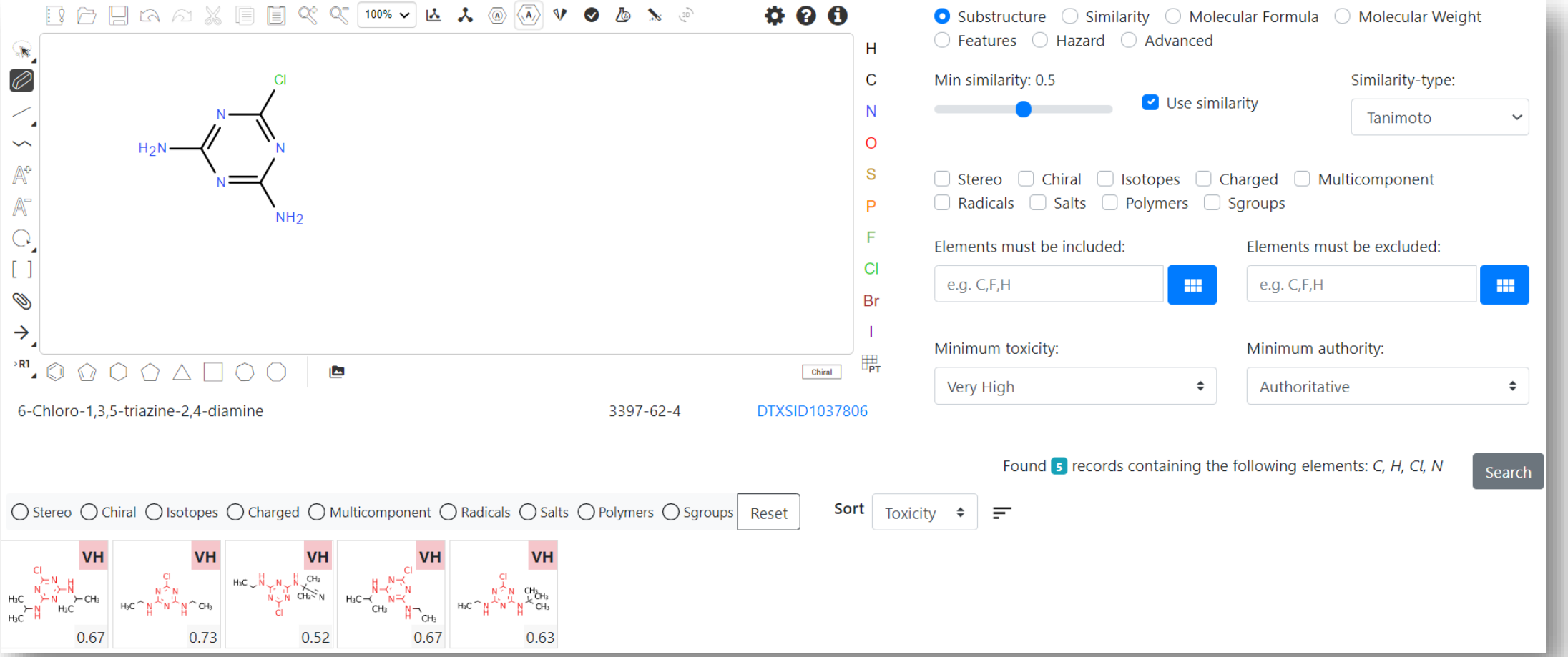


Terbutylazine

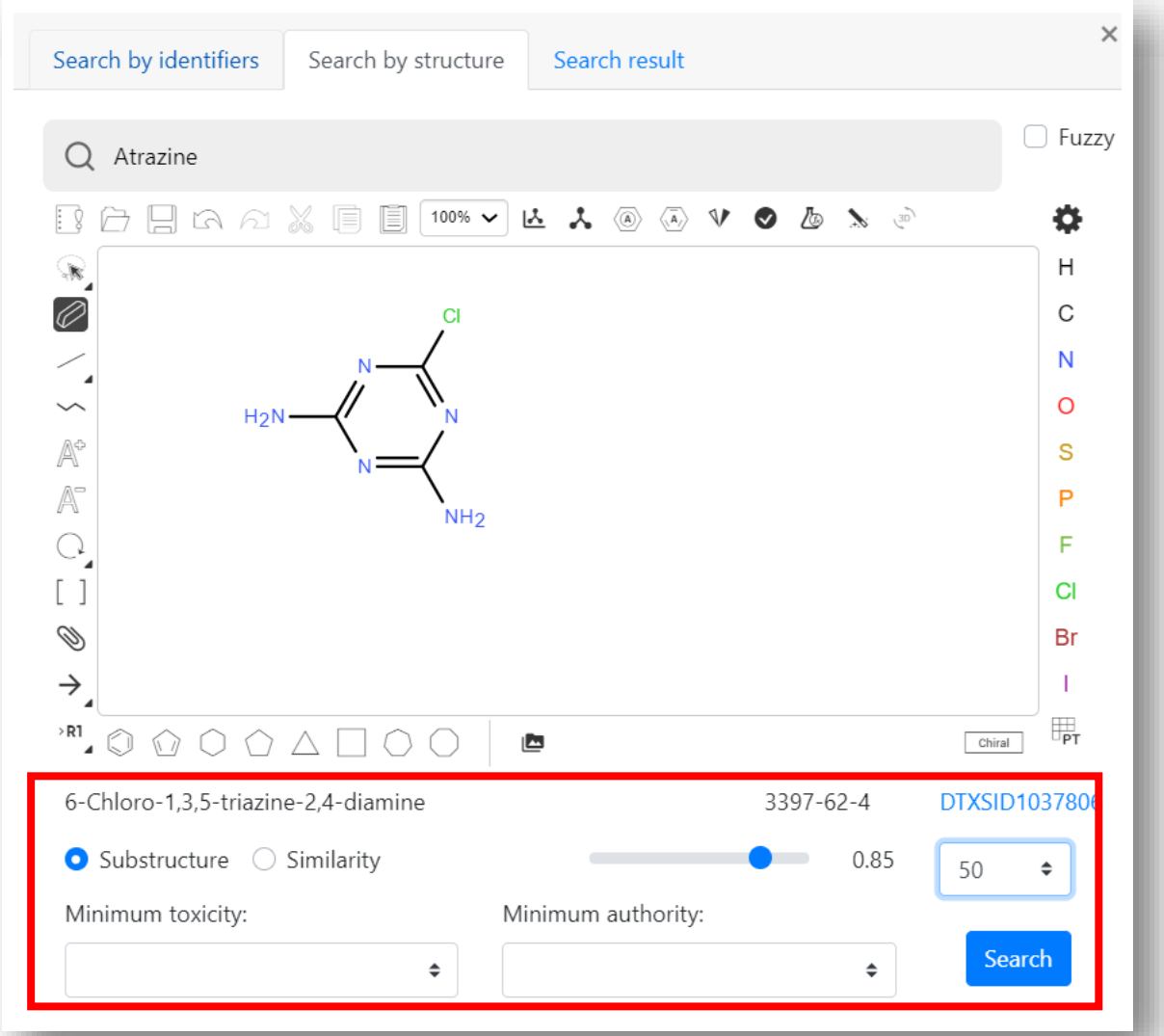
Hazard Name	Final Score	Final Score Source
Acute Mammalian Toxicity Oral	M	ECHA CLP
Acute Mammalian Toxicity Inhalation	I	ChemIDplus
Acute Mammalian Toxicity Dermal	L	ChemIDplus
Carcinogenicity	I	ToxVal
Genotoxicity Mutagenicity	VH	ToxVal
Endocrine Disruption	H	TEDX
Reproductive	H	ToxVal
Developmental	H	ToxVal
Neurotoxicity Repeat Exposure	H	ToxVal
Neurotoxicity Single Exposure	ND	
Systemic Toxicity Repeat Exposure	M	ECHA CLP
Systemic Toxicity Single Exposure	ND	
Skin Sensitization	H	Denmark
Skin Irritation	H	Denmark
Eye Irritation	ND	
Acute Aquatic Toxicity	VH	ECHA CLP
Chronic Aquatic Toxicity	VH	ECHA CLP
Persistence	H	ToxVal

Substructure + “Very High Toxicity” from Authoritative Sources

EPA United States Environmental Protection Agency

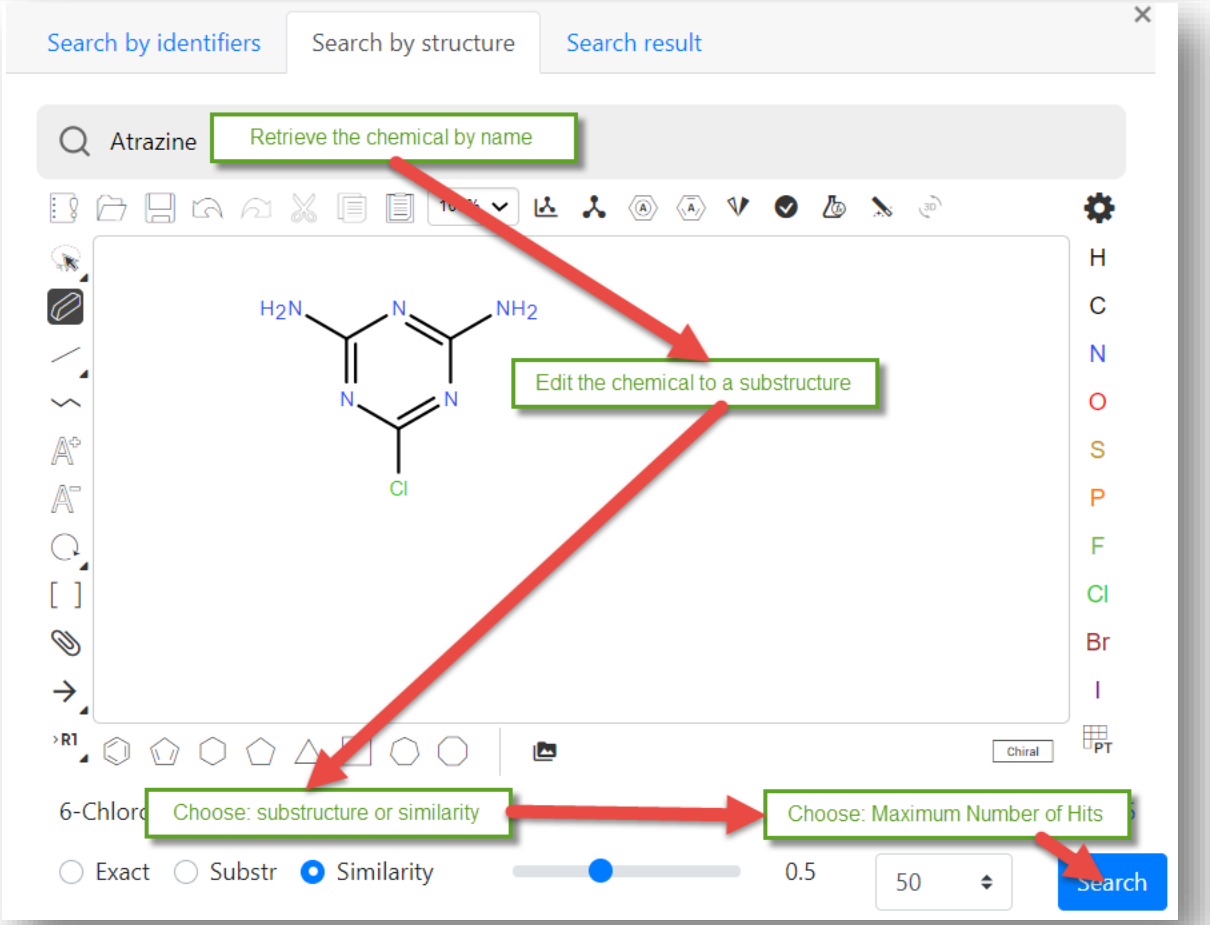


Substructure/similarity search in HCD

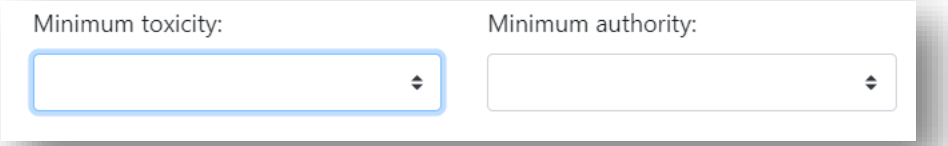


- In HCD search based on substructure and similarity
- Search results can be used as input to HCD
- Then the application can:
  - Run Hazard Comparison
  - Filter based on “available experimental data”

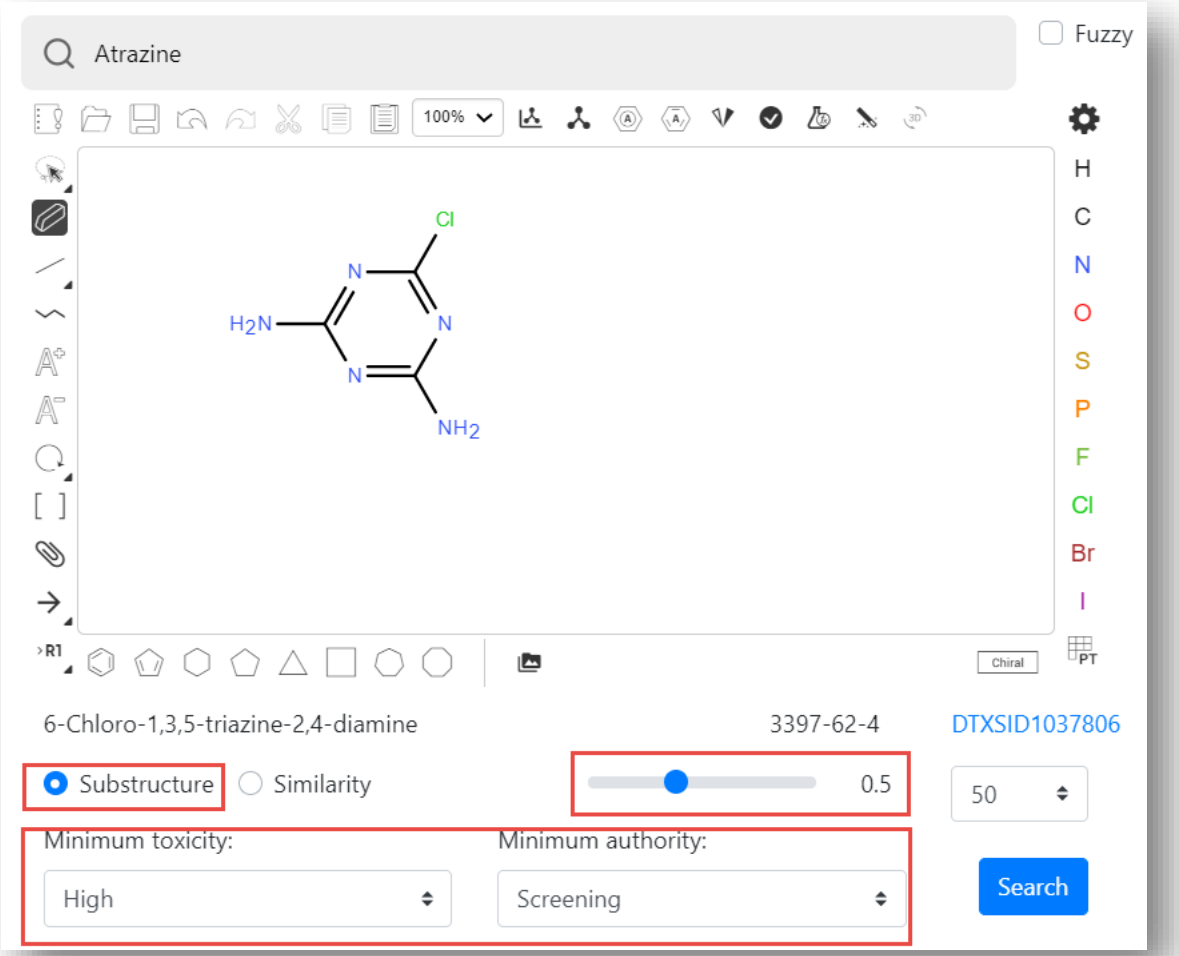
Choices to Create a Set of Hits

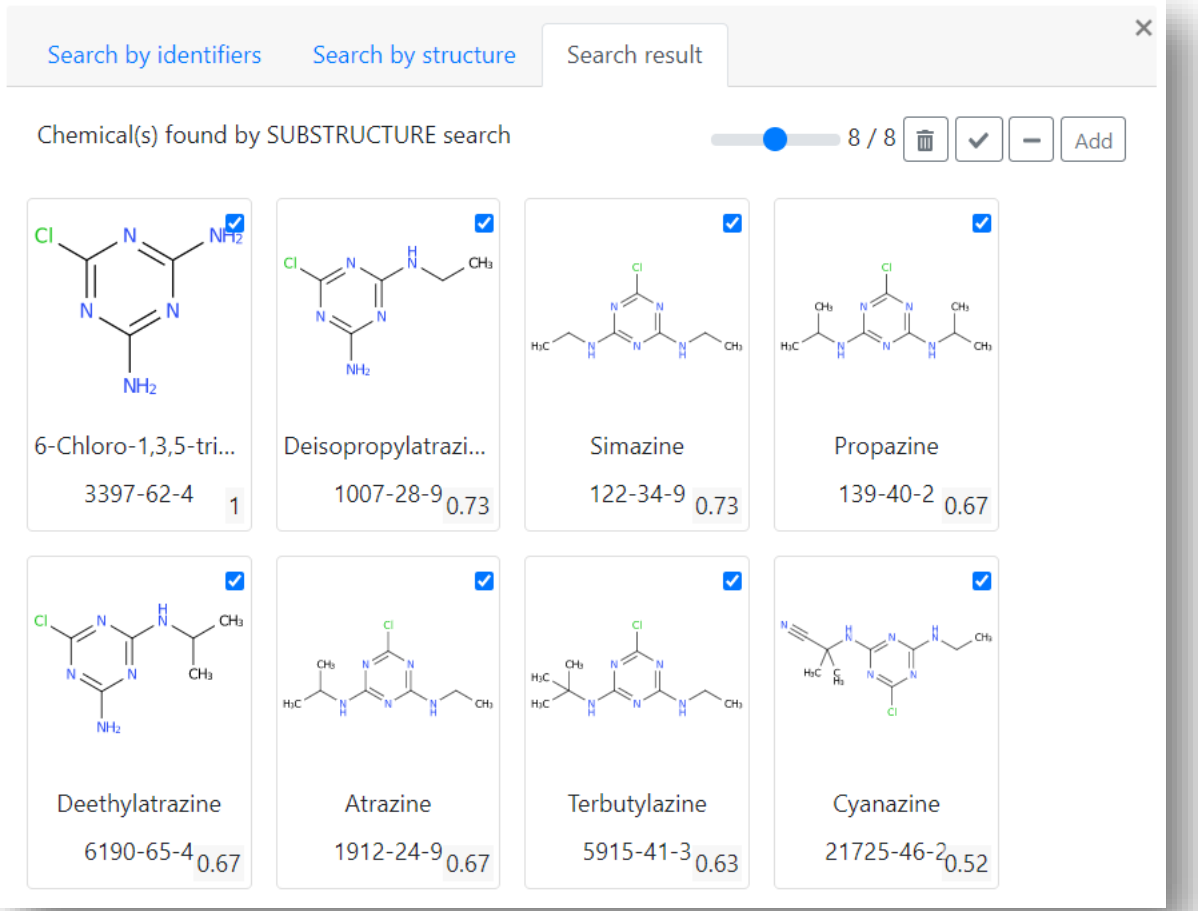


- Looking for a set of chemicals to add to HCD
  - Select structure by name or draw structure
  - Edit the chemical if necessary
  - Choose substructure or similarity
  - Choose number of hits
  - Choose Toxicity “thresholds”



Choose substructure, similarity, thresholds





Choose substructure, similarity, thresholds

Hazard Comparison | None | Export

8 / 8

Legend: VH - Very High, H - High, M - Medium, L - Low, I - Inconclusive **Authoritative**, Screening, *QSAR Model*

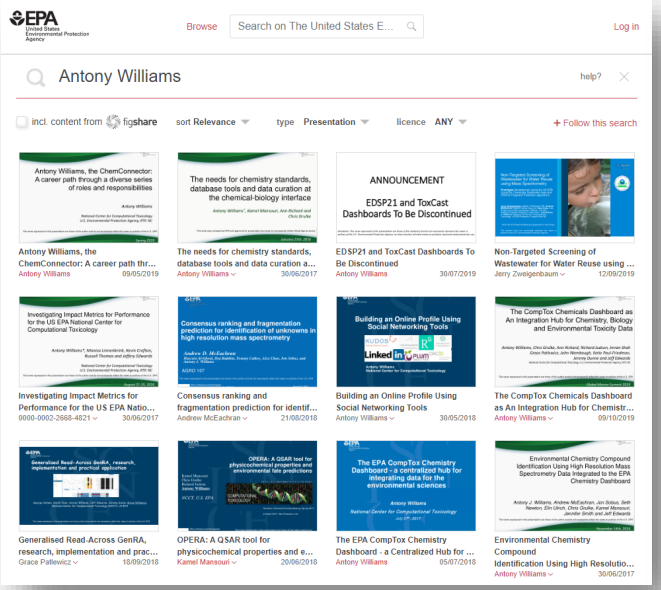
- [ ] Skipped (0)
- [ ] Filters (0)
- [x] Sorting (0)
- [ ] Products (0)
- [ ] Structure

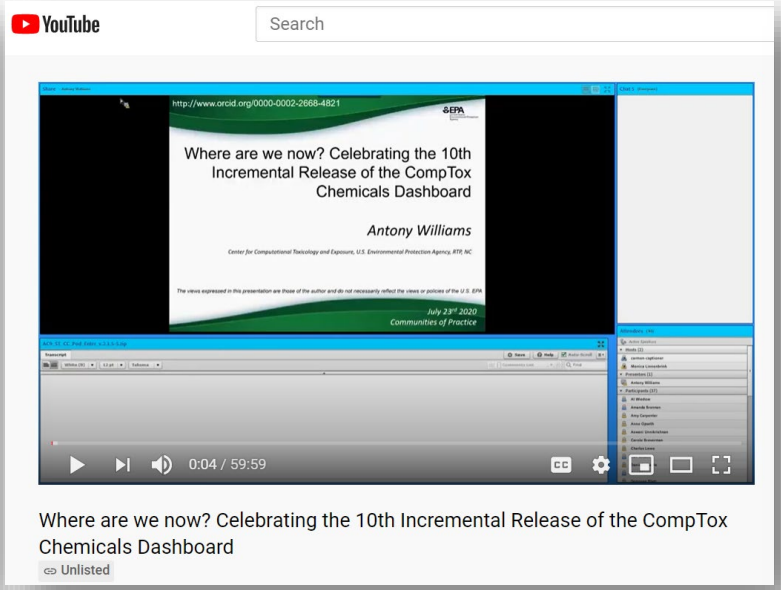
CAS Name	Human Health Effects															Ecotoxicity		Fate	
	Acute Mammalian Toxicity								Neurotoxicity		Systemic Toxicity								
	Oral	Inhalation	Dermal	Carcinogenicity	Genotoxicity Mutagenicity	Endocrine Disruption	Reproductive	Developmental	Repeat Exposure	Single Exposure	Repeat Exposure	Single Exposure	Skin Sensitization	Skin Irritation	Eye Irritation	Acute Aquatic Toxicity	Chronic Aquatic Toxicity	Persistence	Bioaccumulation
6190-65-4 Deethylatrazine	*M*	I	I	I	L	H	M	**H**		I	H	I	I	I	I	**H**	**VH**		*L*
1007-28-9 Deisopropylatrazine	*M*				L	H		**H**								**H**		*H*	*L*
21725-46-2 Cyanazine	**M**	H	M	**VH**	*L*	H	M	**H**			H	M			H	**VH**	**VH**	H	L
3397-62-4 6-Chloro-1,3,5-tri...	*M*				L	*L*		**H**			H					**H**	*H*		*L*
122-34-9 Simazine	M	H	L	**VH**	L	H	H	**H**	H		**H**	M	I	H	H	**VH**	**VH**	*H*	L
139-40-2 Propazine	M	M	L	**H**	L	H	M	**H**	I	I	H	I	I	M	H	**VH**	**VH**	*H*	*L*
1912-24-9 Atrazine	M	H	L	**VH**	L	H	H	**H**	H	M	**M**		**H**	L	M	**VH**	**VH**	H	VH
5915-41-3 Terbutylazine	**M**	I	L	**I**	*VH*	H	H	H	H		**M**		*H*	*H*		**VH**	**VH**	*H*	L

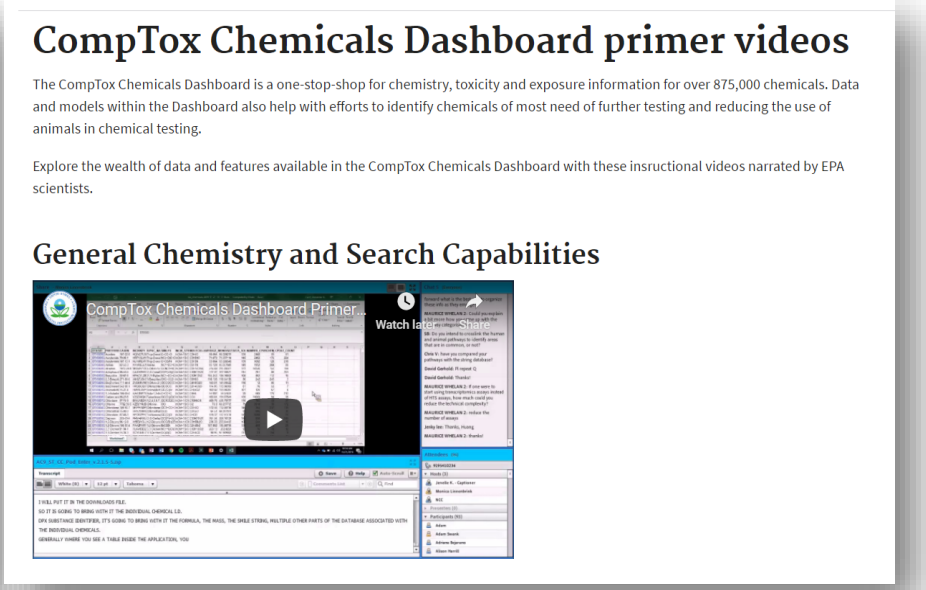
Online Materials

You want to know more…

- Lots of resources available
  - Presentations: https://tinyurl.com/w5hqs55
  - Communities of Practice Videos: https://rb.gy/qsbno1
  - Manual: https://rb.gy/4fgydc
  - Latest News: https://comptox.epa.gov/dashboard/news_info



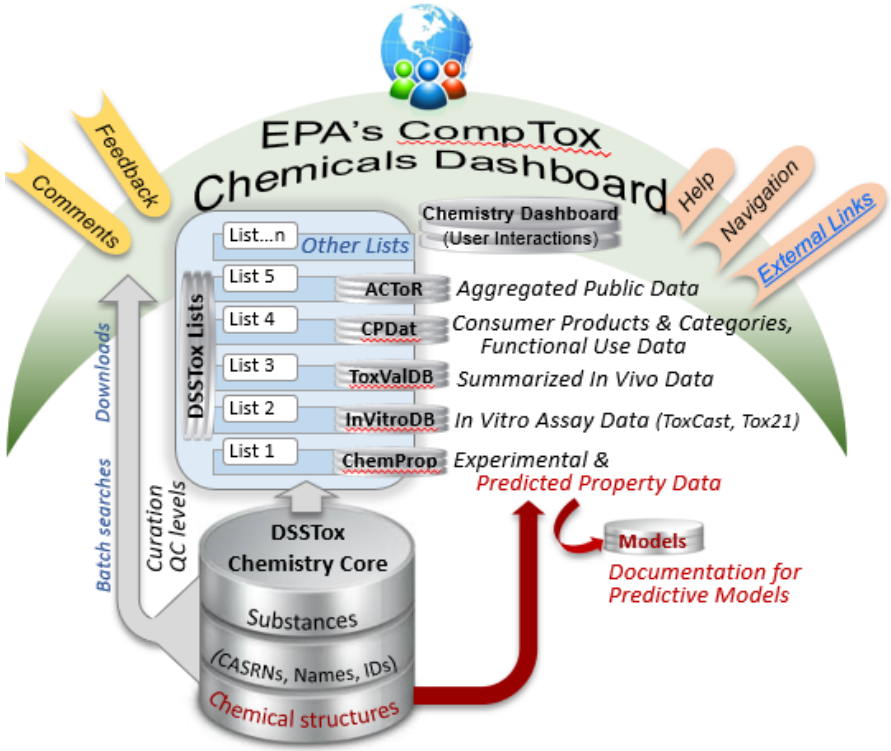




Conclusion

- Dashboard access to data for ~882,000 chemicals (and growing)
- Data aggregation for ALL data sources continues unabated
- Flexible search capabilities continue to expand release-to-release
- Expansion of new modules continues with prototype development
- The application is being totally rearchitected at present to also develop a Public API

- …and now for the deeper dives into the relevant sub-tabs and modules…



Acknowledgments

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

- Thank you NURA for hosting us

EPA's Center for Computational Toxicology and Exposure