http://www.orcid.org/0000-0002-2668-4821

EPA United States Environmental Protection Agency

Physicians Committee for Responsible Medicine

NURA™

Introduction to the US EPA CompTox Chemicals Dashboard

Antony John Williams

williams.antony@epa.gov

Center for Computational Toxicology and Exposure, US-EPA, RTP, NC

October 23rd 2020

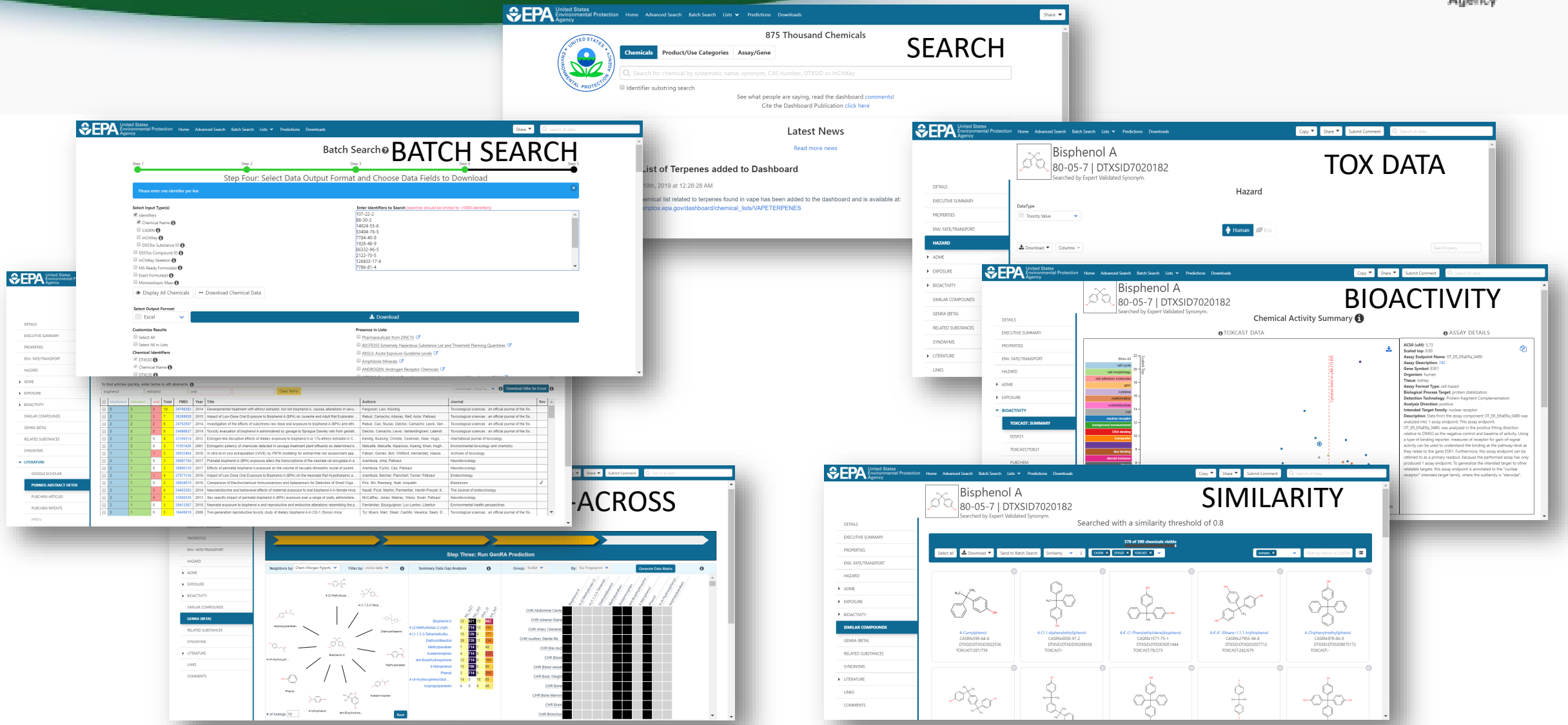
CompTox Chemicals Dashboard
https://comptox.epa.gov/dashboard

EPA United States Environmental Protection Agency

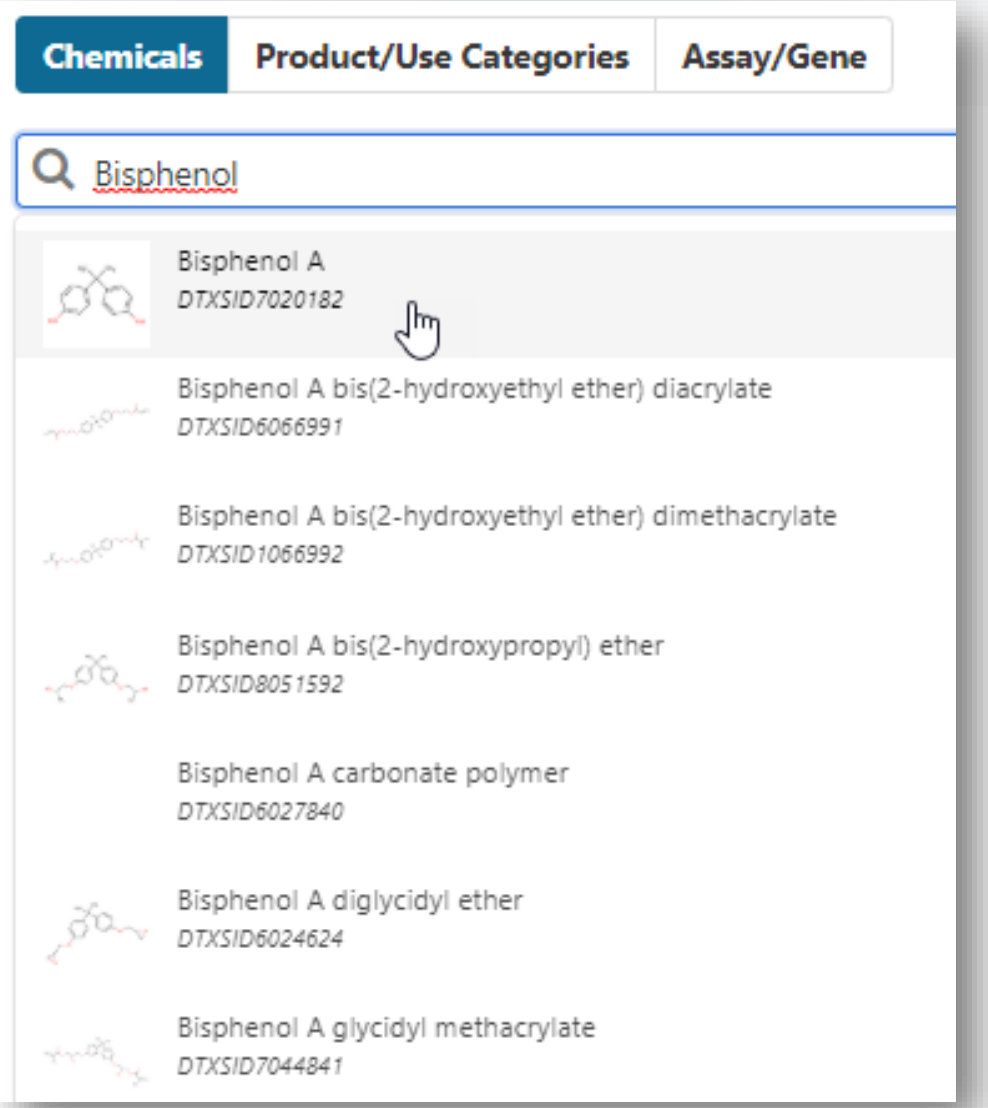
- A **publicly accessible website** delivering access:
  - ~882,000 chemicals with related property data
  - Experimental and predicted physicochemical property data
  - Experimental Human and Ecological hazard data
  - Integration to “biological assay data” for 1000s of chemicals
  - Information regarding 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

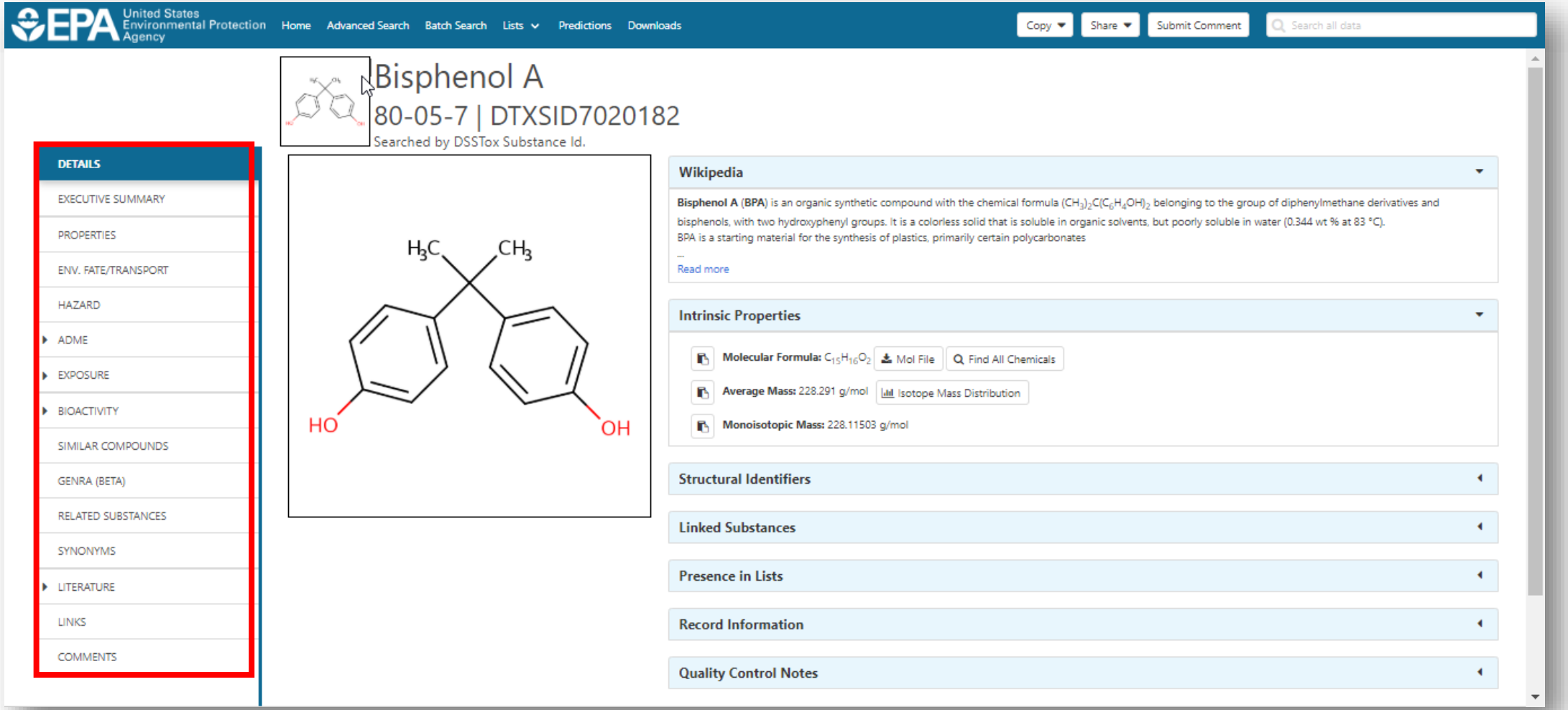


BASIC Search

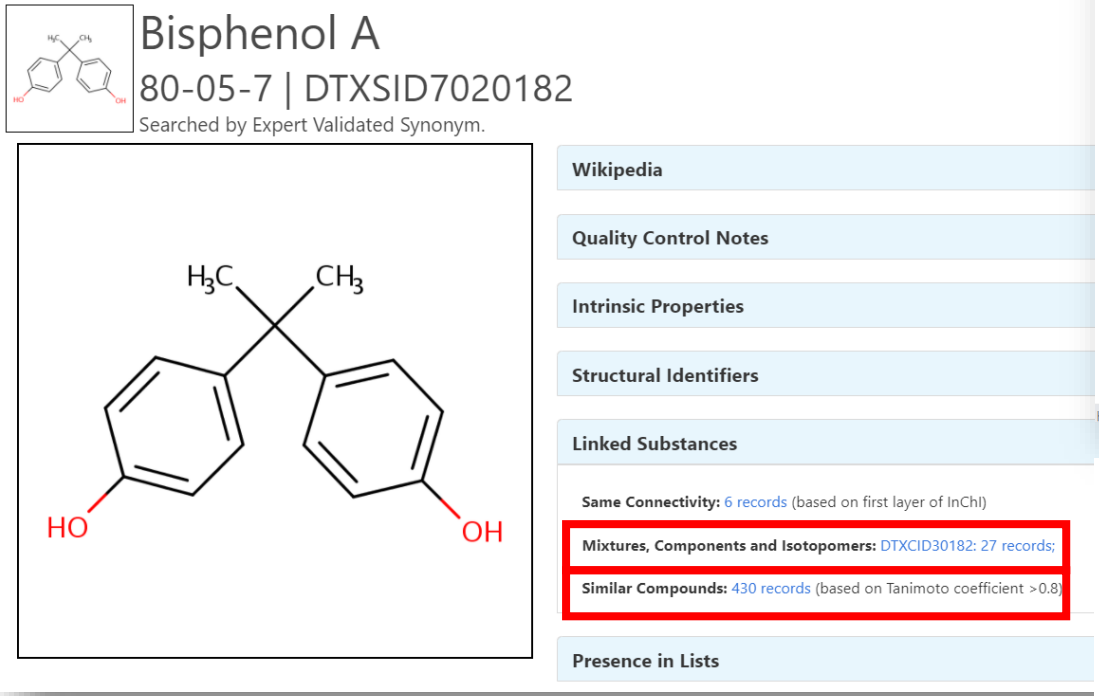


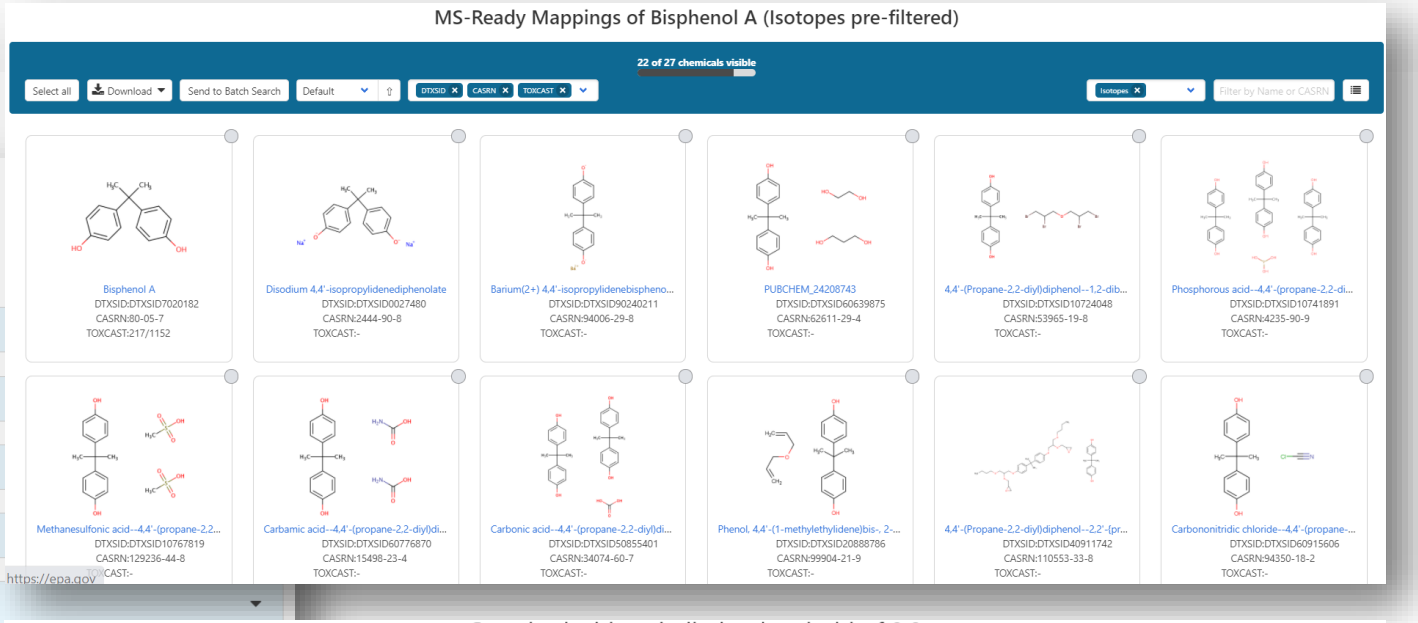
- Three searches from the home page
  - Chemicals (Names, CASRN, Substring)
  - Product/Use Categories (Kristin…)
  - Assay Gene (Katie…)
- Searching millions of synonyms and includes Active, Deleted and Alternate CASRNs

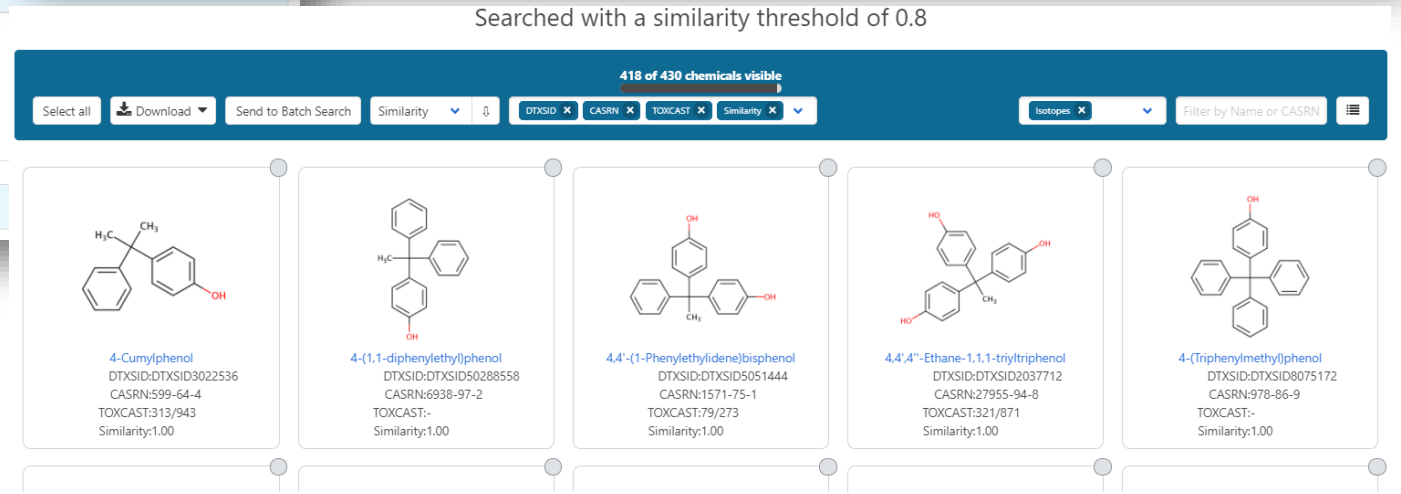
Detailed Chemical Pages



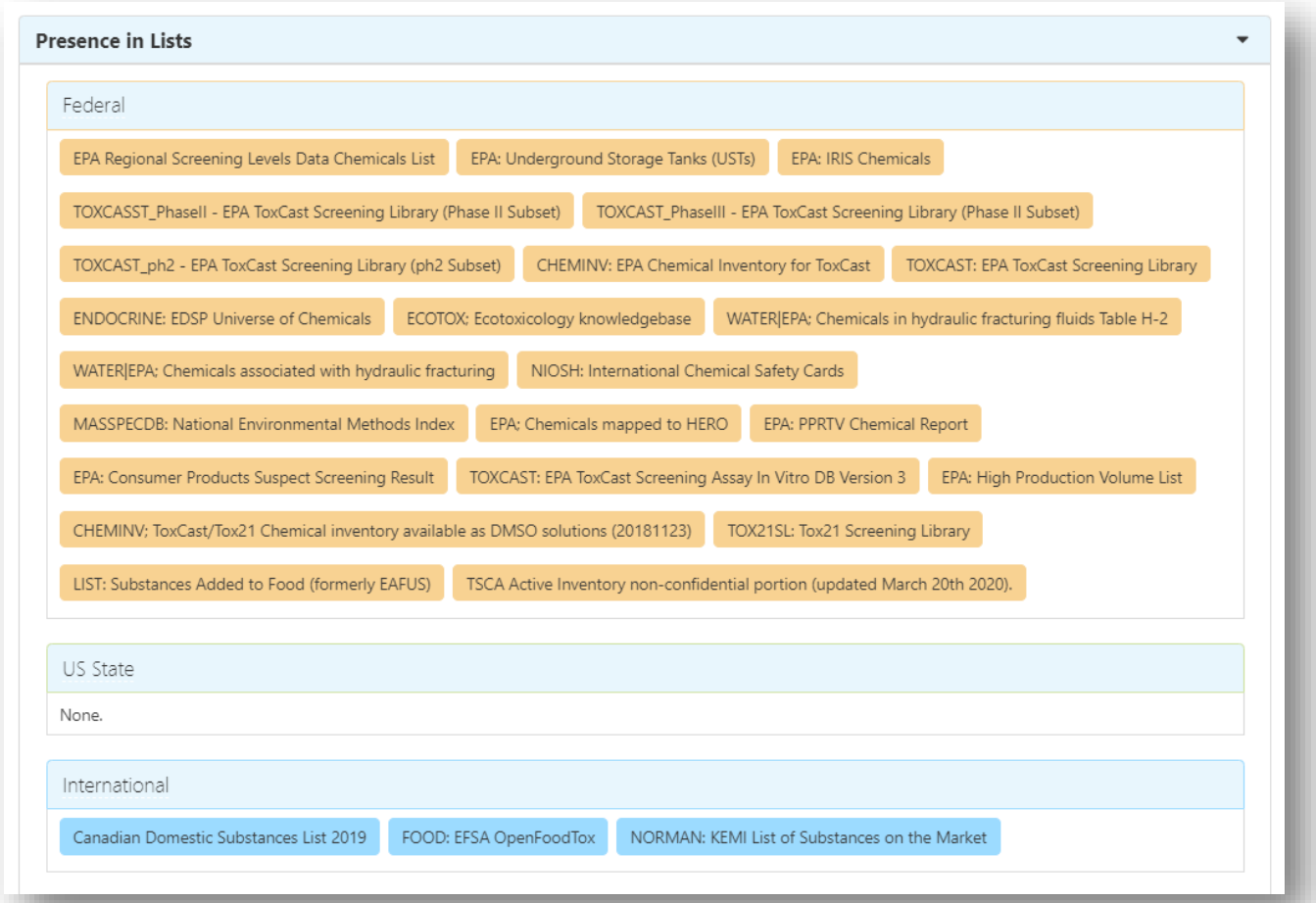
Linked Substances: Mixtures and Components, Similar Compounds





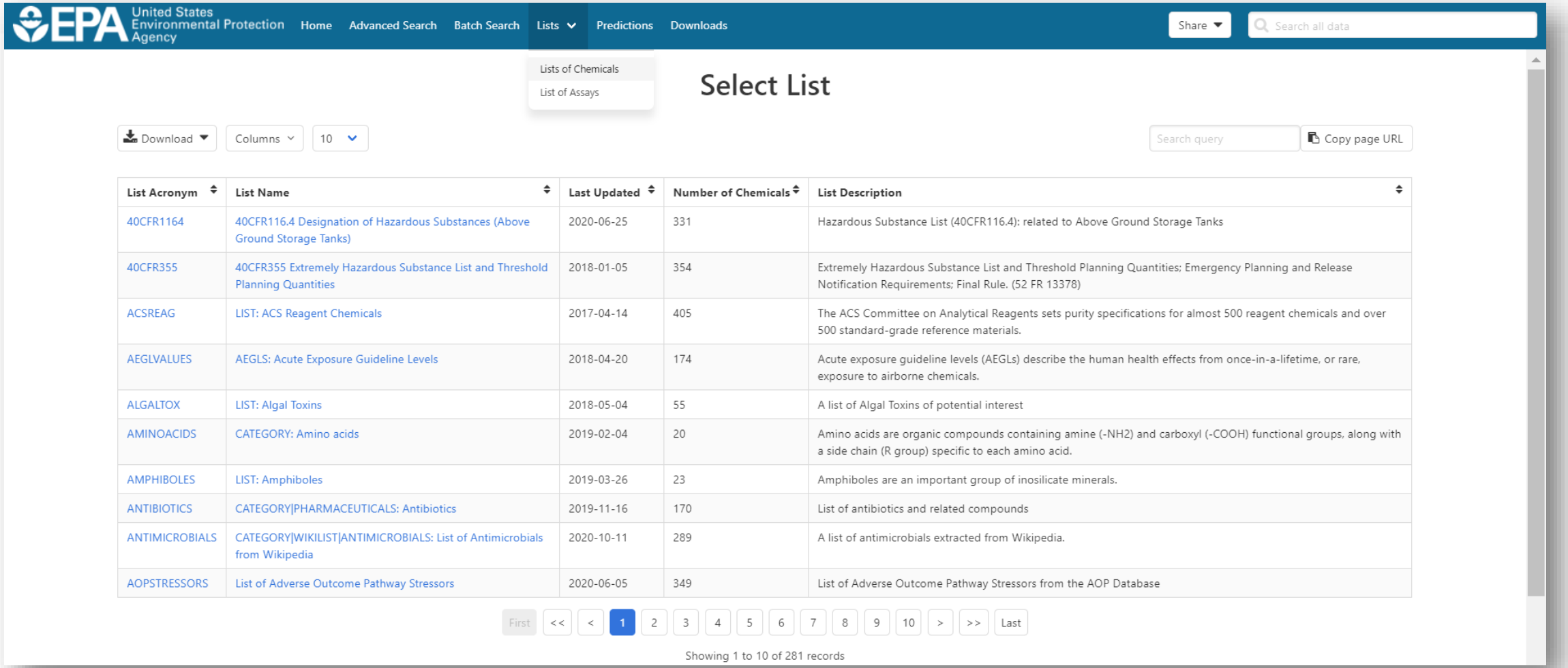


Presence in Lists

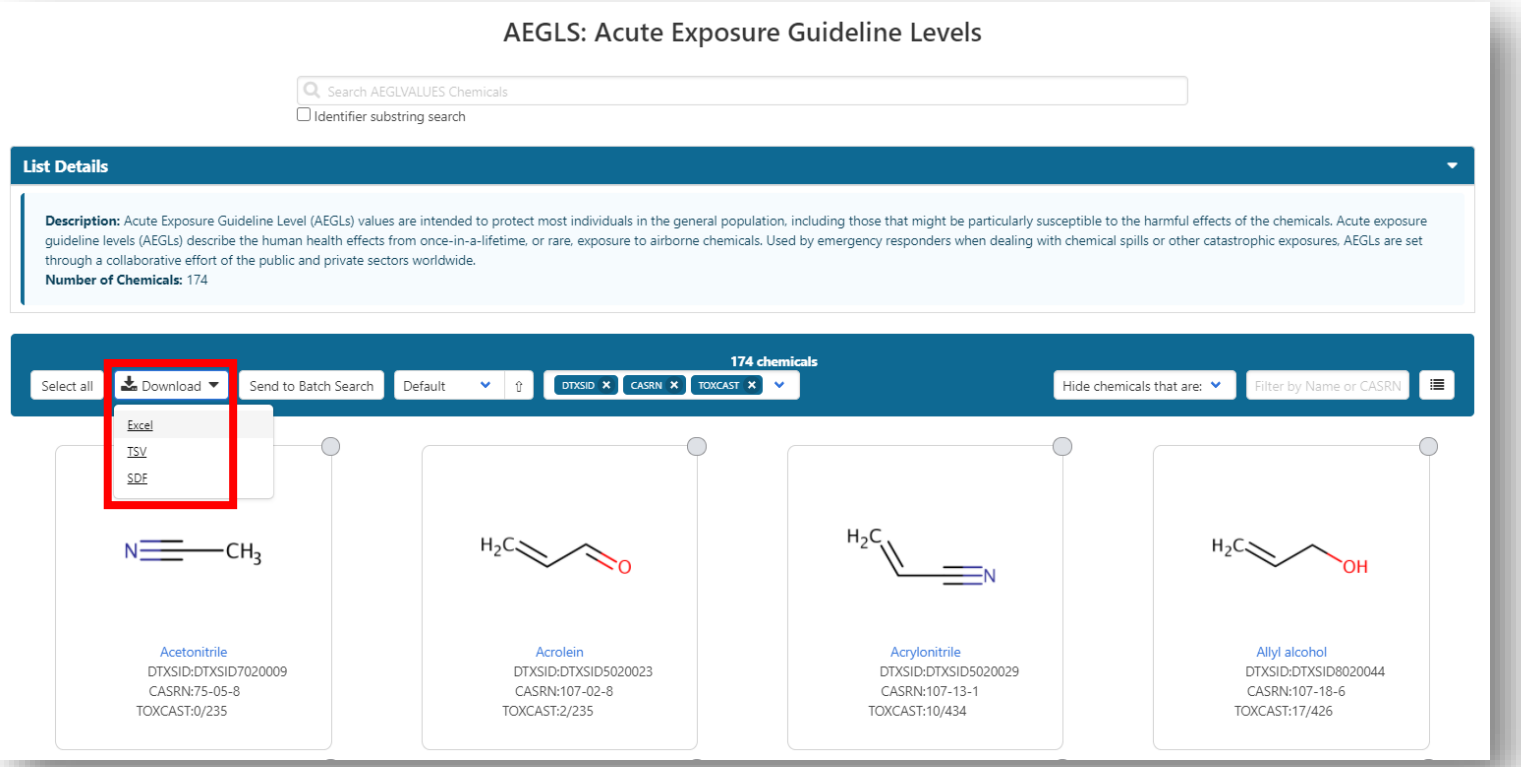


- ~882,000 chemicals are associated with > 280 lists
- Lists are segregated into
  - Federal
  - US State
  - International
  - Other
- Chemicals can be present in multiple lists – with clickthrough

Lists of Lists of Chemicals
>280 lists and growing



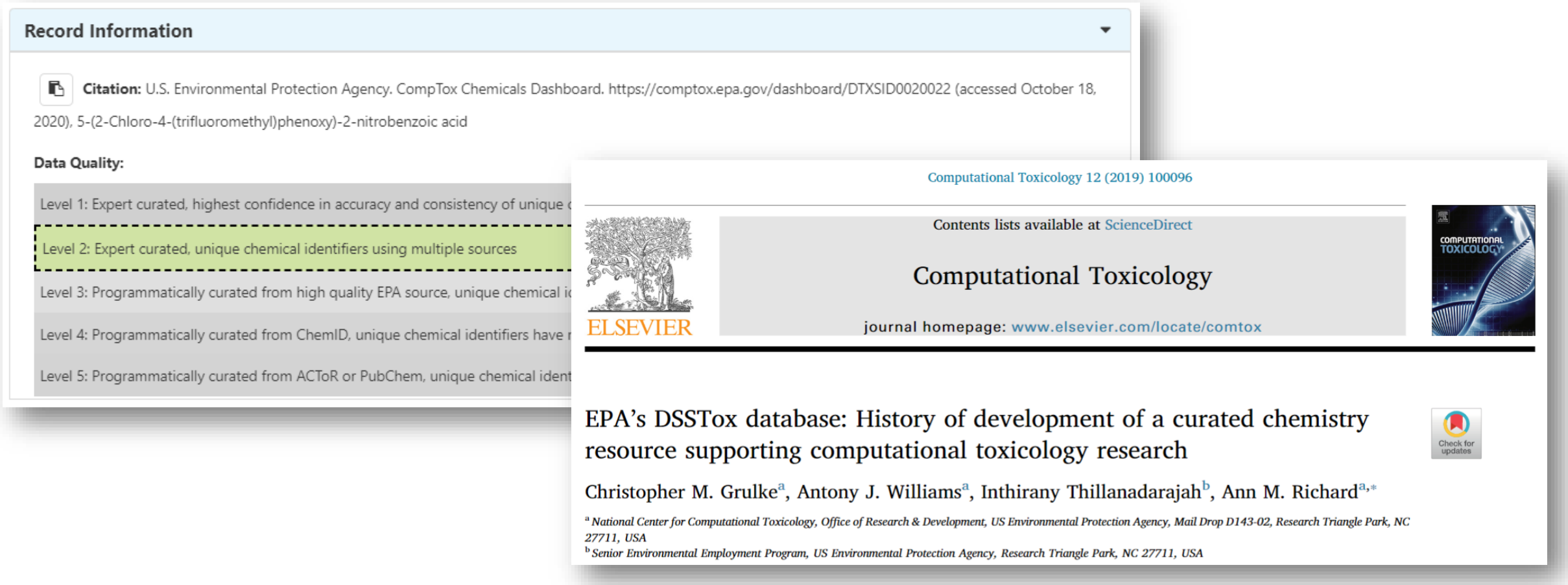
List of Chemicals
Example: Acute Exposure Guideline Levels



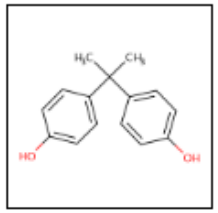
- Chemical List Examples
  - Disinfection by-products
  - EPA Pesticide Search DB
  - Consumer Products DB
  - Chemicals in Biosolids
  - ATSDR Toxicological Profiles
  - Canadian Domestic Substances
  - Chemical Inventory for ToxCast
  - EFSA OpenFoodTox
  - EDSP Universe of Chemicals
  - Hydraulic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

Quality

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



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

EPA United States Environmental Protection Agency

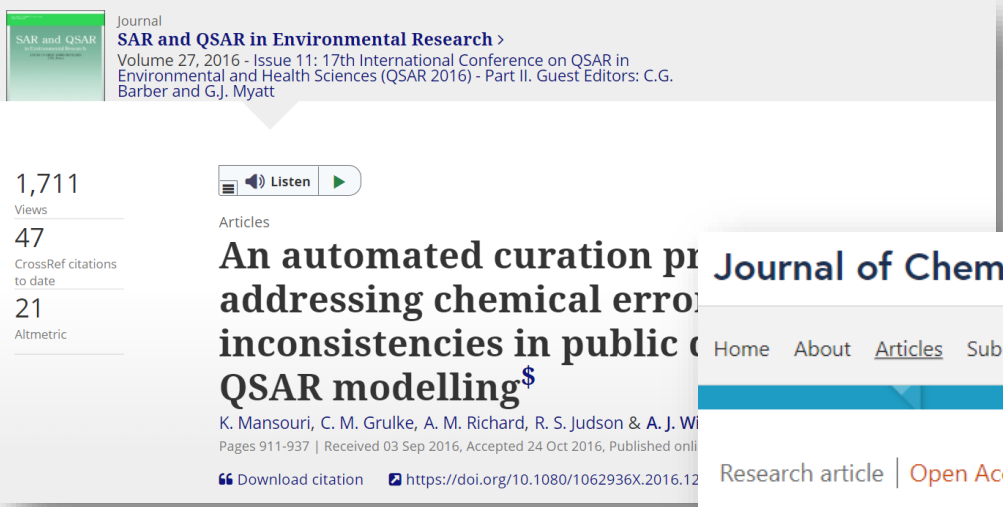
Download Experimental Data

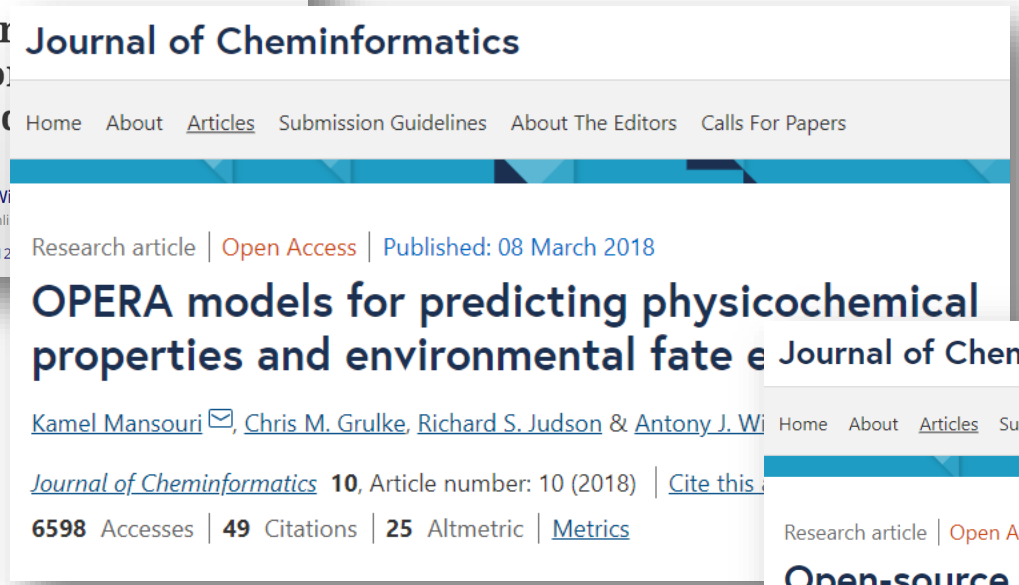
Source	Result
PhysPropNCCT	5.26e-4
Tetko et al. J. Chem. Inf. and Comp. Sci. 41.6 (2001): 1488-1493	1.51e-3
Kovdienko, et. al. Molecular informatics 29.5 (2010): 394-406.	5.25e-4

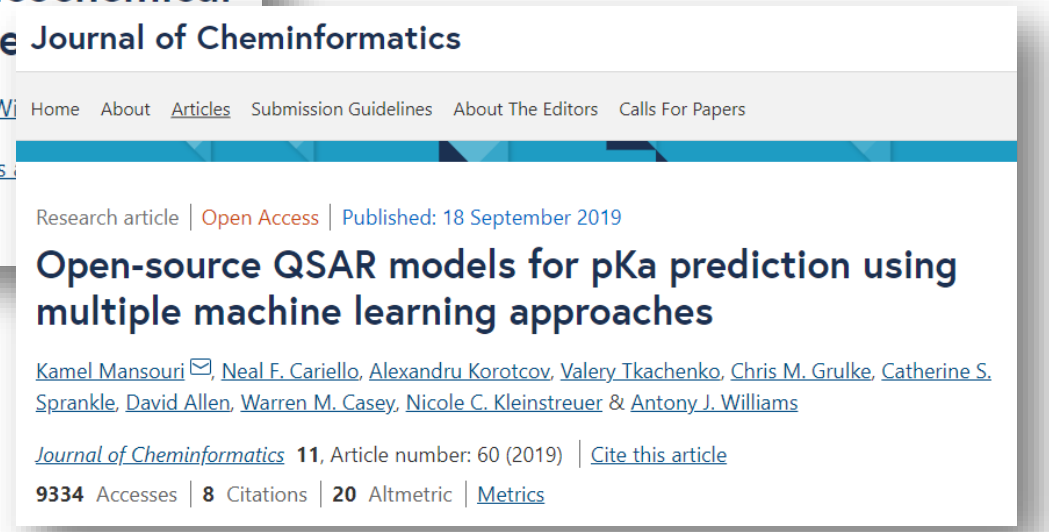
Source	Result	Calculation Details
EPISUITE	7.56e-4	Not Available
NICEATM	1.31e-3	Not Available
TEST	1.24e-3	TEST Report
OPERA	5.44e-4	OPERA Model Report [Inside AD]
OPERA2	5.35e-4	Not Available

OPERA Models

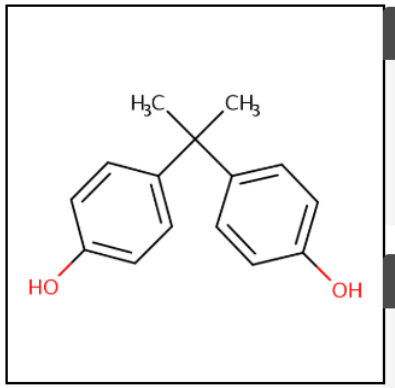
EPA United States Environmental Protection Agency







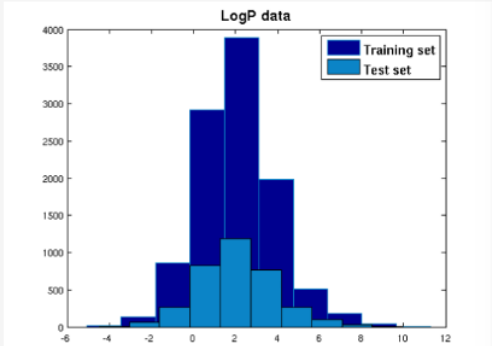
Properties, Fate and Transport
e.g. logP



Model Results

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

Model Performance

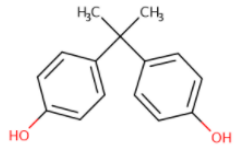


QMRF

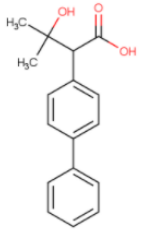
5-fold CV (75%)	
Q2	RMSE
0.850	0.690

od.epa.gov/dashboard/advanced_search/index

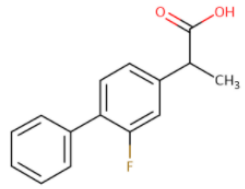
Nearest Neighbors from the Training Set



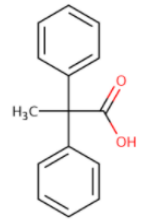
Bisphenol A
Measured:3.32
Predicted: 3.32



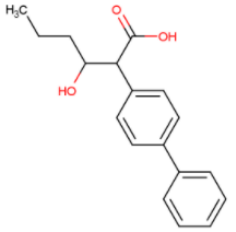
BUTANOIC ACID,2-(4-BIPHENYLYL)-3-HYDROXY-3-METHY
Measured:3.25
Predicted: 3.25



Flurbiprofen
Measured:4.16
Predicted: 4.16



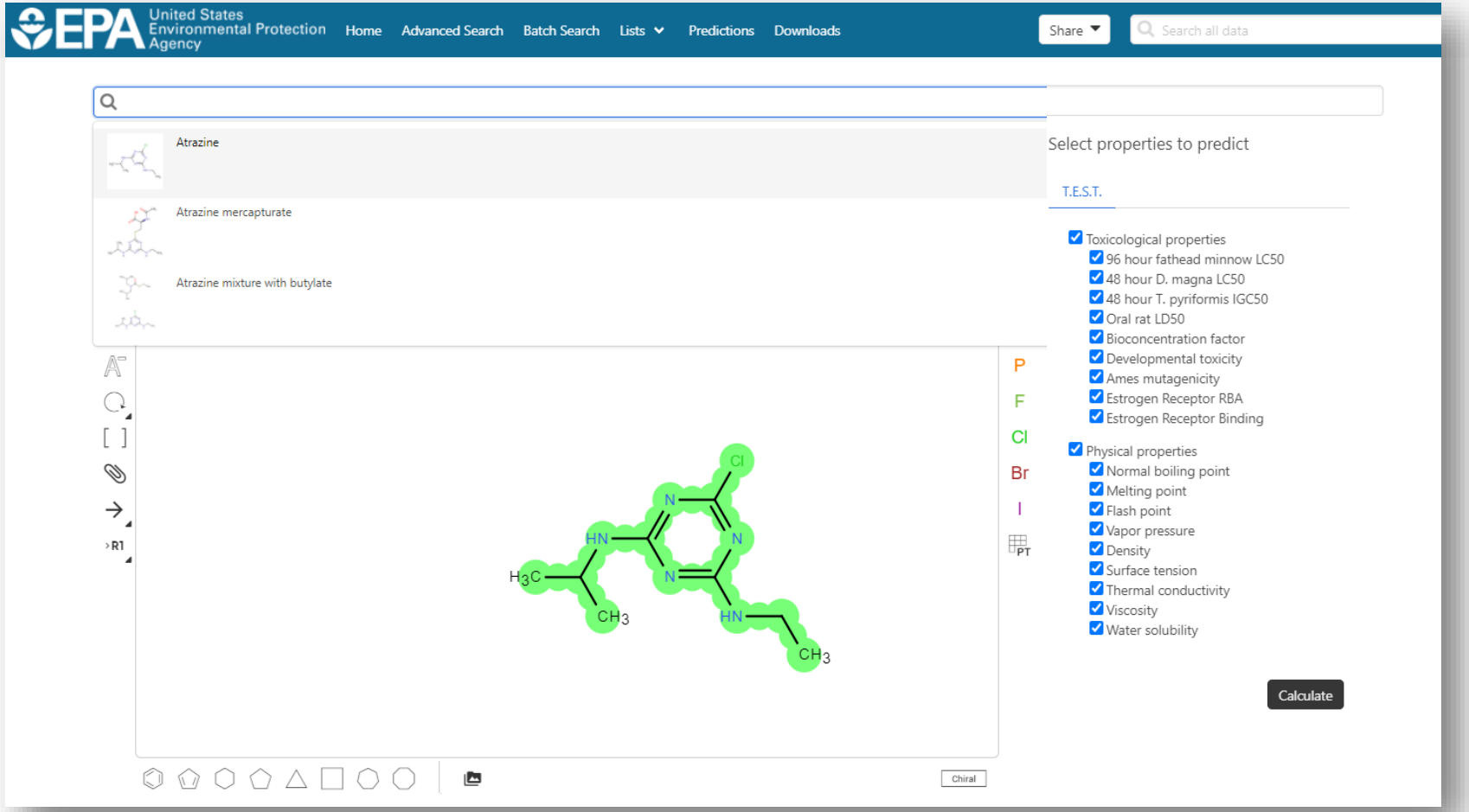
2,2-Diphenylpropionic acid
Measured:2.69
Predicted: 2.69



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

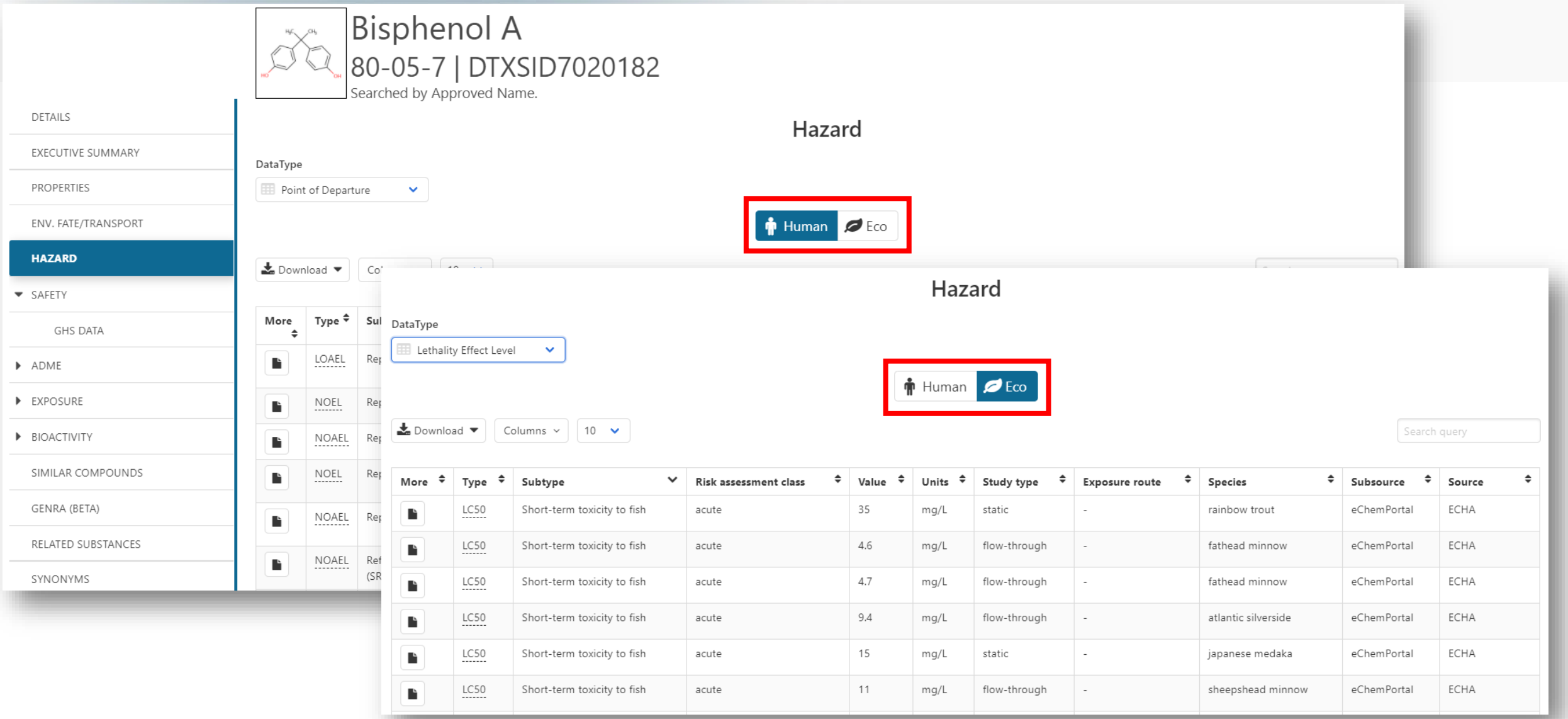
EPA United States Environmental Protection Agency

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

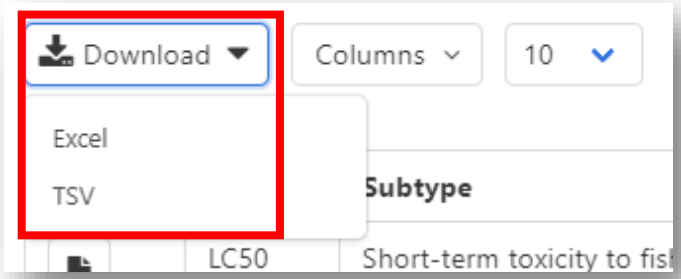
Hazard Data (Human and Eco)



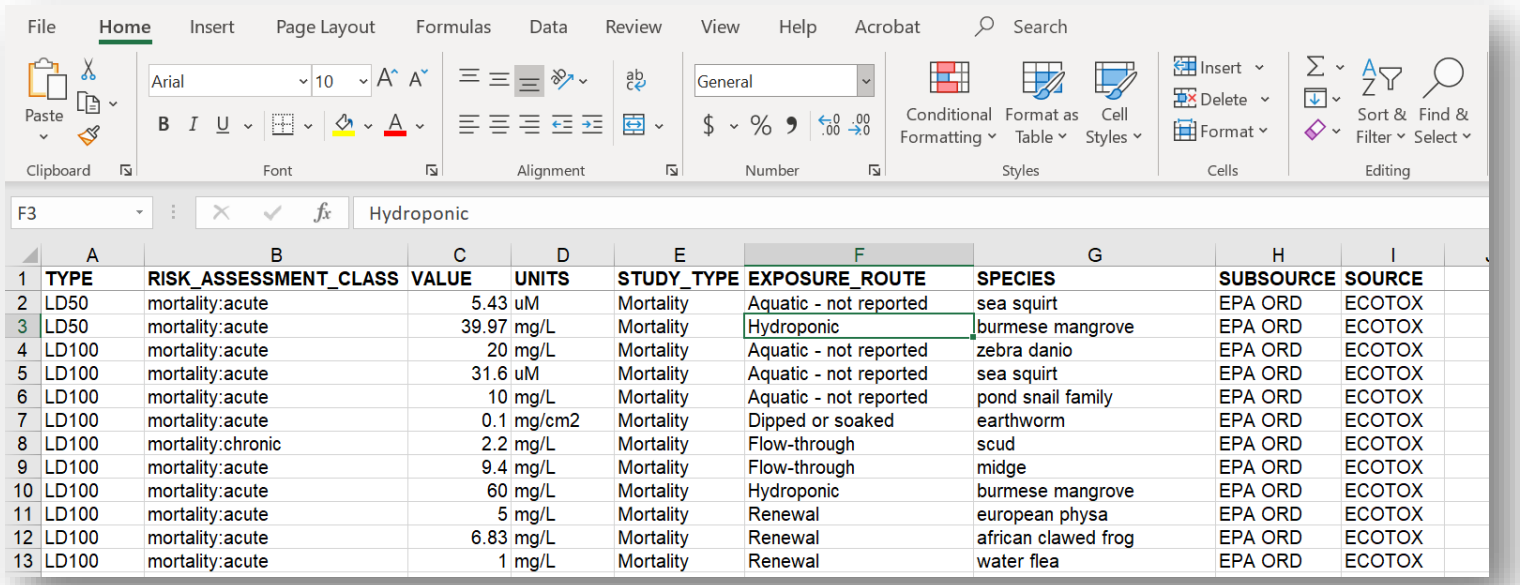
More	Type	Subtype	Risk assessment class	Value	Units	Study type	Exposure route	Species	Subsource	Source
	LC50	Short-term toxicity to fish	acute	35	mg/L	static	-	rainbow trout	eChemPortal	ECHA
	LC50	Short-term toxicity to fish	acute	4.6	mg/L	flow-through	-	fathead minnow	eChemPortal	ECHA
	LC50	Short-term toxicity to fish	acute	4.7	mg/L	flow-through	-	fathead minnow	eChemPortal	ECHA
	LC50	Short-term toxicity to fish	acute	9.4	mg/L	flow-through	-	atlantic silverside	eChemPortal	ECHA
	LC50	Short-term toxicity to fish	acute	15	mg/L	static	-	japanese medaka	eChemPortal	ECHA
	LC50	Short-term toxicity to fish	acute	11	mg/L	flow-through	-	sheepshead minnow	eChemPortal	ECHA

Hazard Data

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



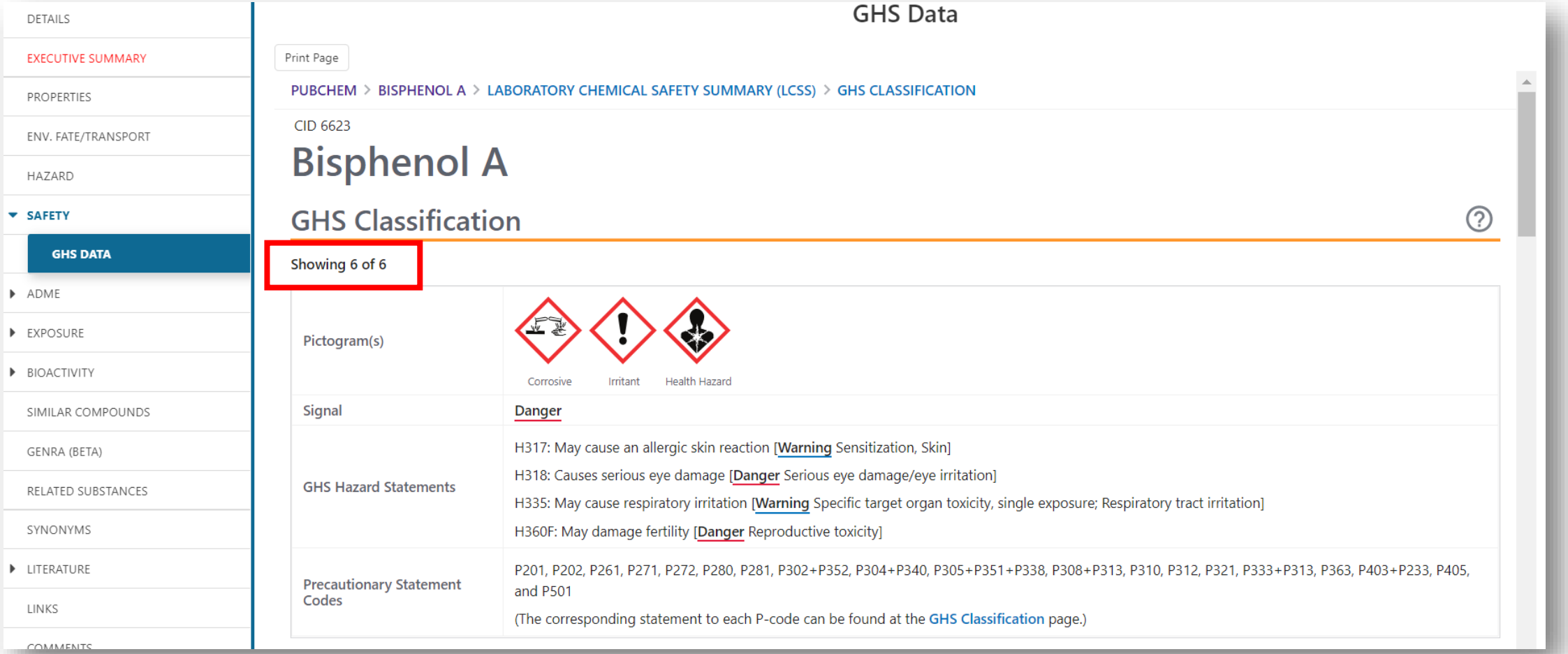
- ***General Feature*** – anywhere you see a table you can download the data…



	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

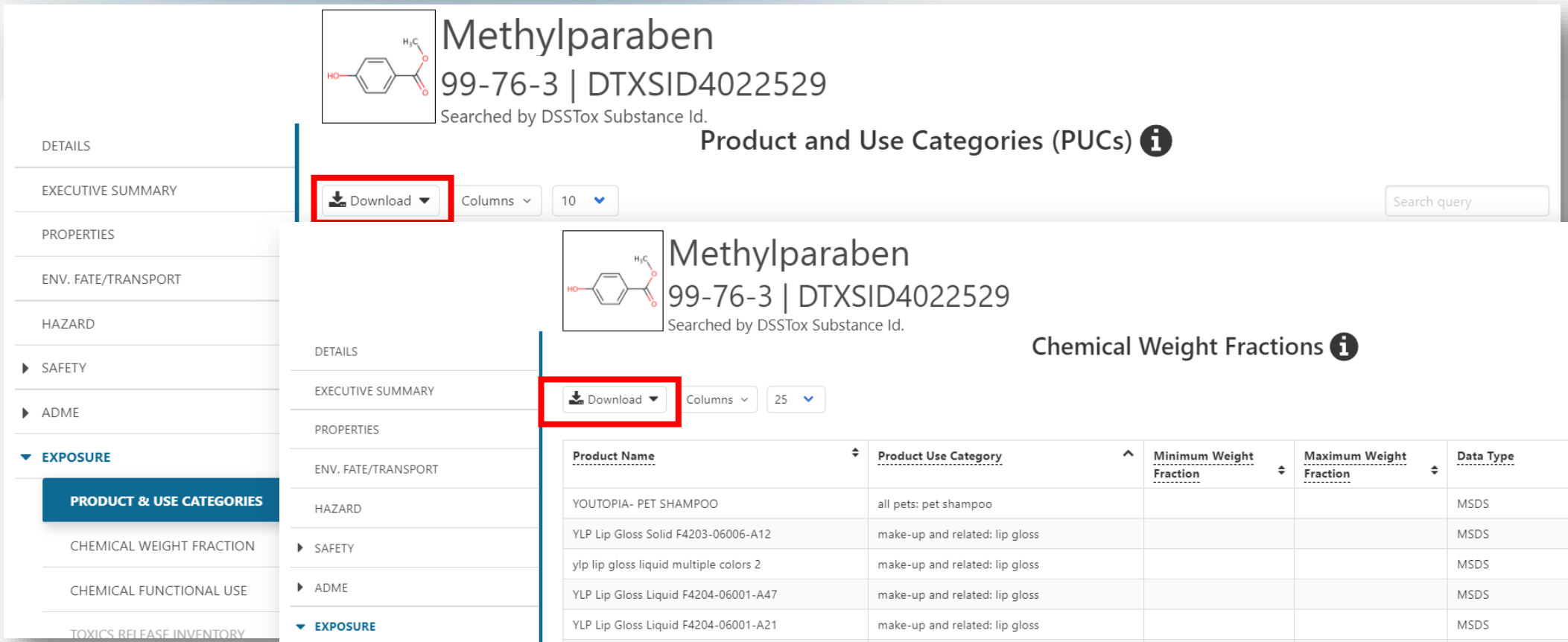
Safety Data

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



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

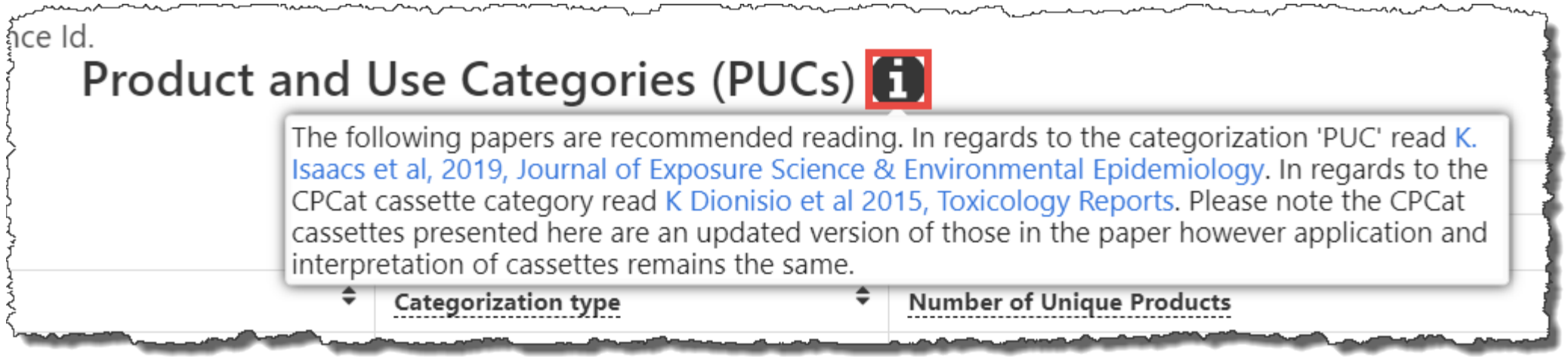
Chemical Weight Fractions

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

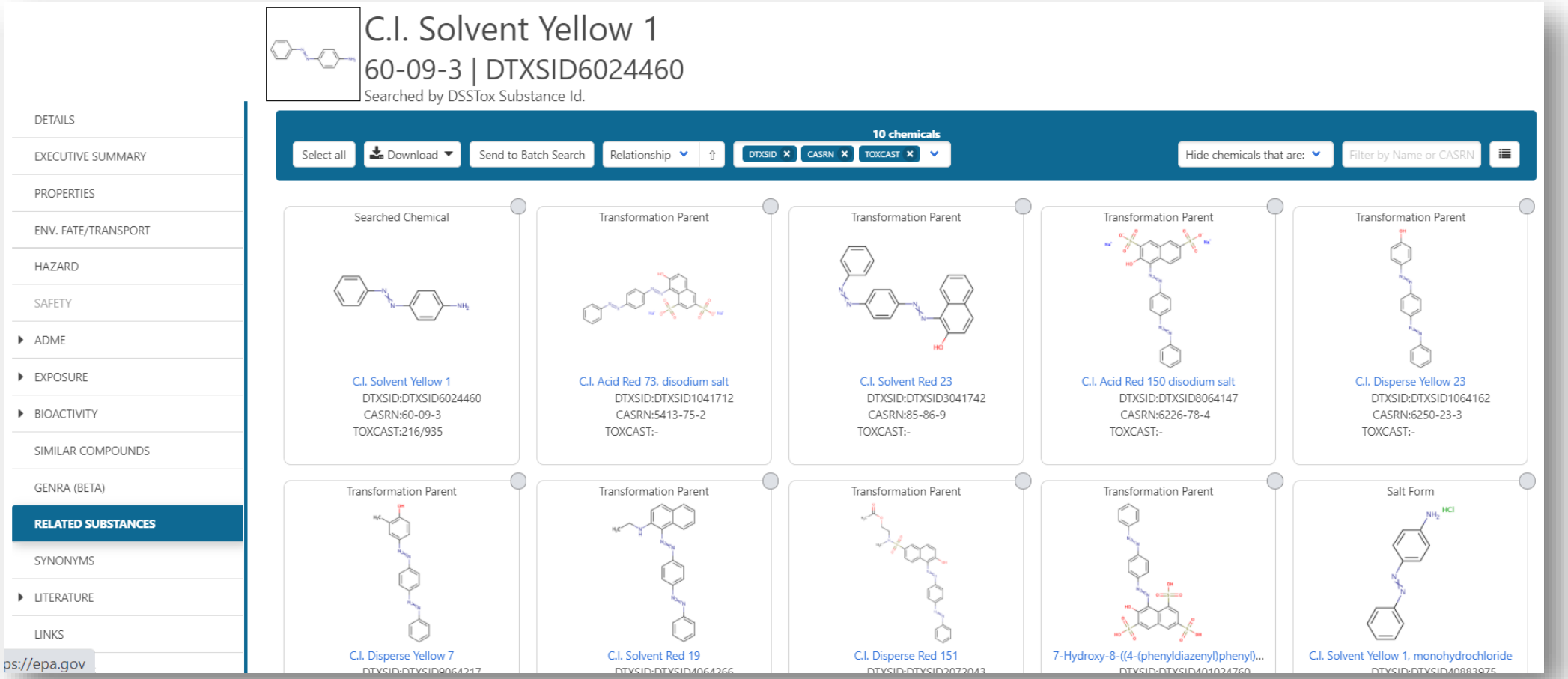
- Watch out for the on-hover informational icons to gather info



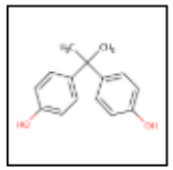
- Descriptive text or video about the data, associated publications etc.

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

EPA United States Environmental Protection Agency

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

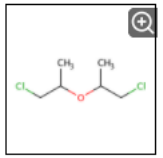
Synonym	Quality
beta,beta'-Bis(p-hydroxyphenyl)propane	Other
beta,beta-Di-(p-hydroxyphenyl)propane	Other
beta-Di-(p-hydroxyphenyl)propane	Other
beta-Di-p-hydroxyphenylpropane	Other
137885-53-1 Deleted CAS-RN	Deleted
146479-75-6 Deleted CAS-RN	Deleted
27360-89-0 Deleted CAS-RN	Deleted
28106-82-3 Deleted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

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

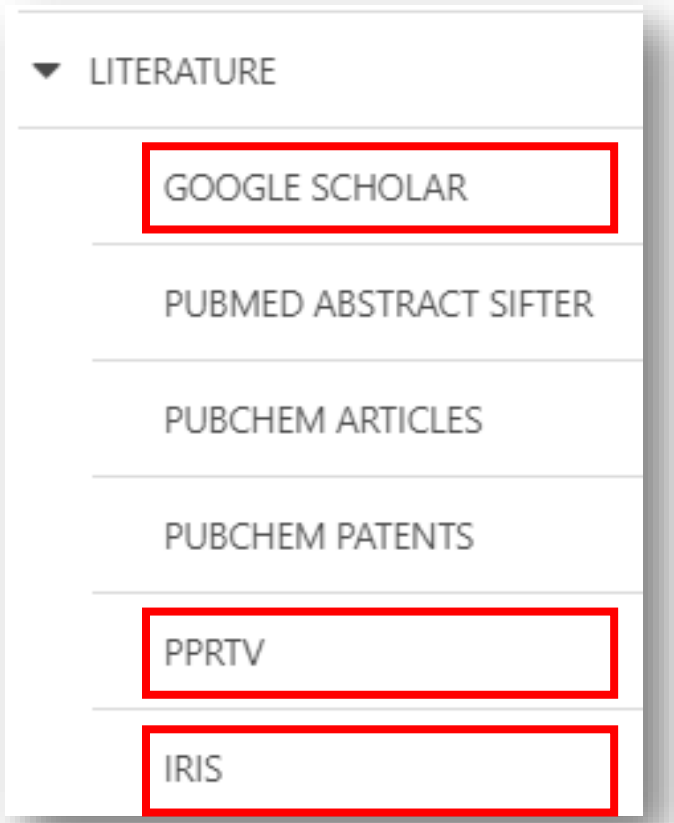
Showing 126 to 134 of 134 records

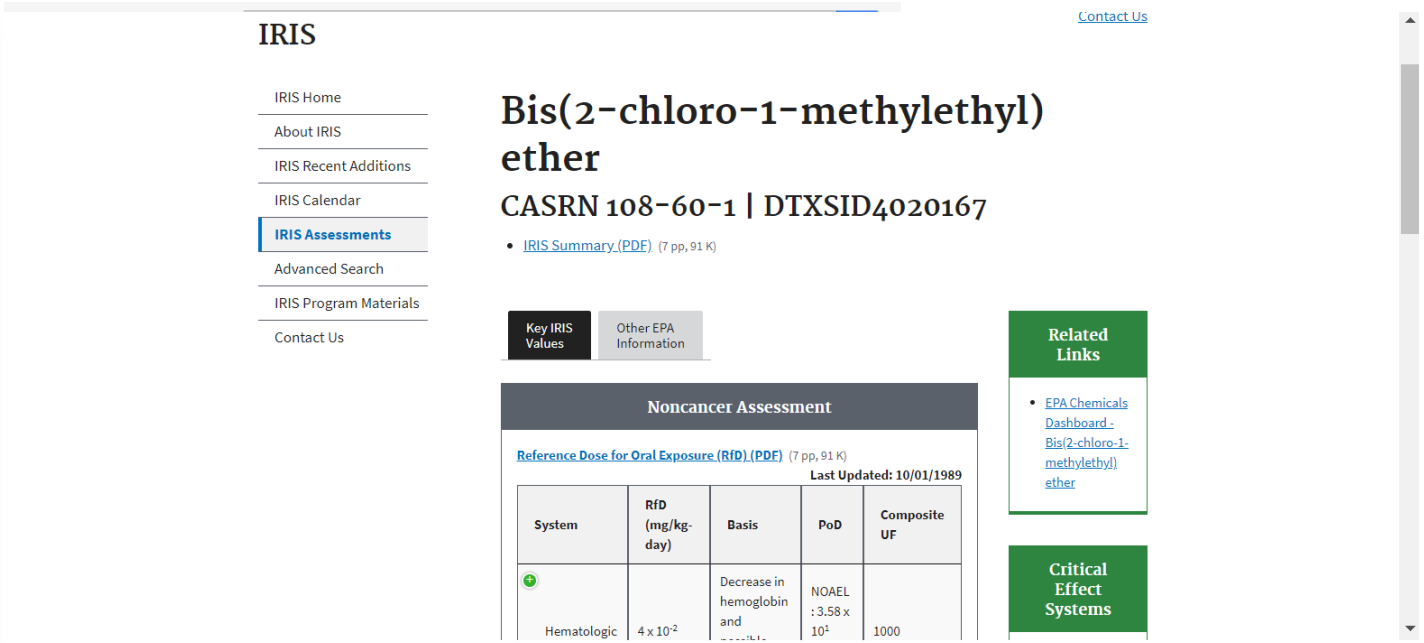
Identifiers are used in the app

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

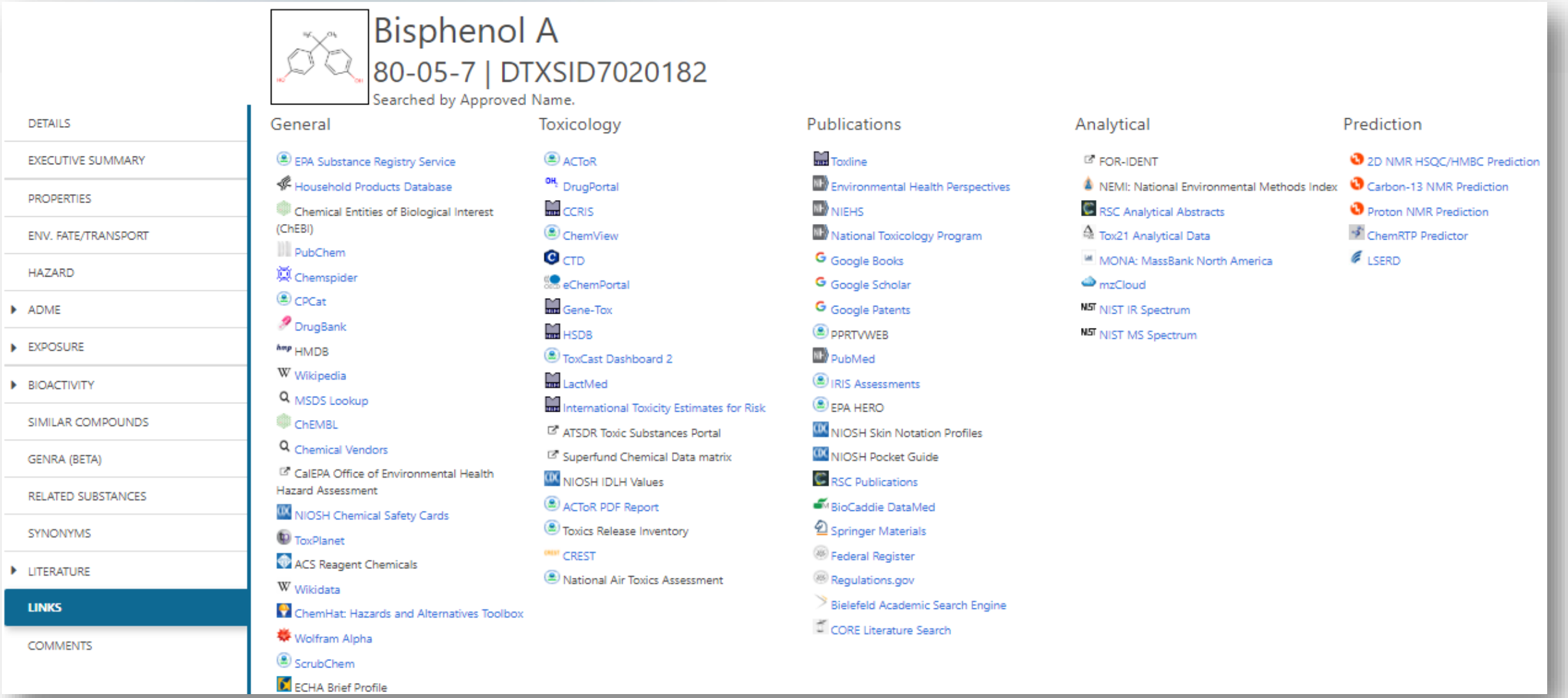


bis(2-Chloro-1-methylethyl) ether
108-60-1 | DTXSID4020167

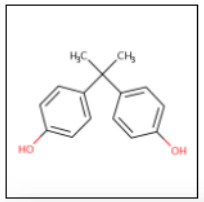




External Links – Also use Identifiers Names, CASRN, PubChem IDs…



External Links



Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

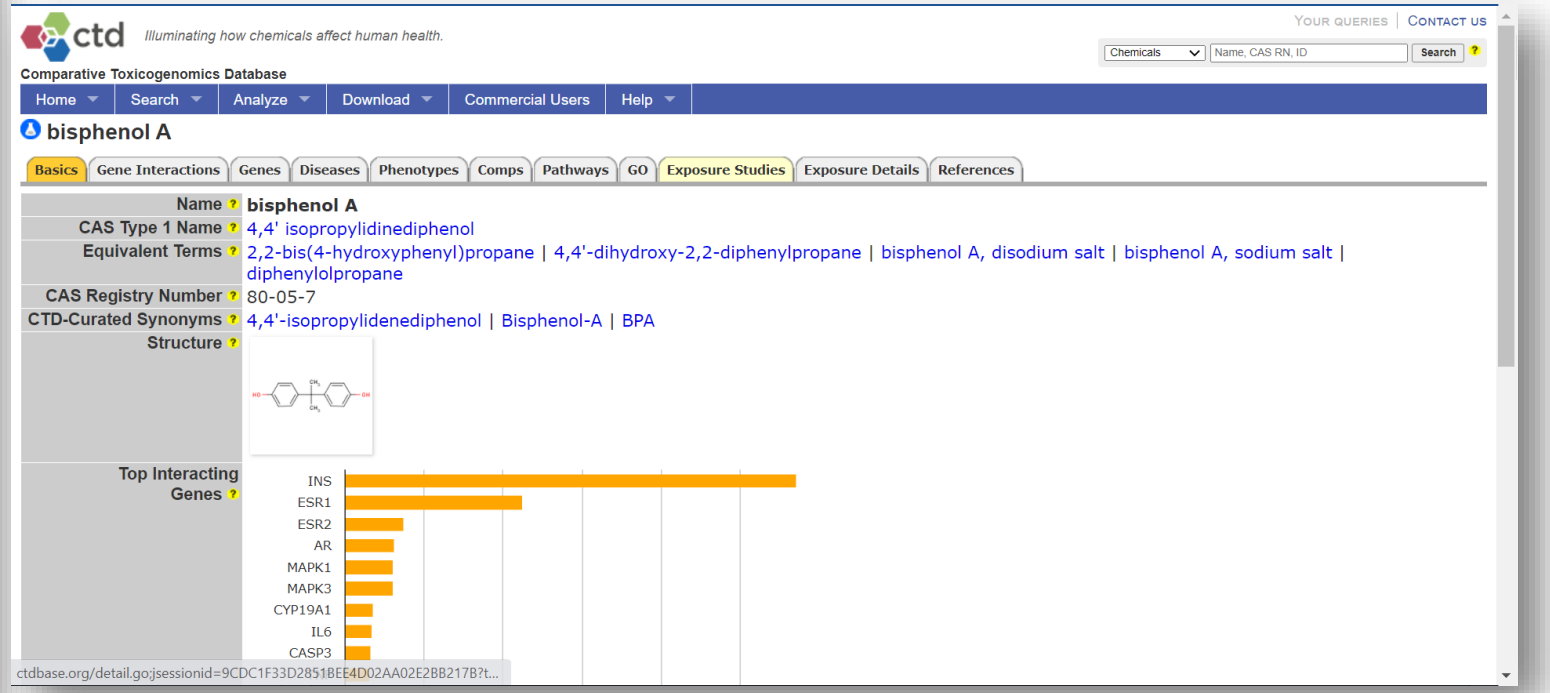
General

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

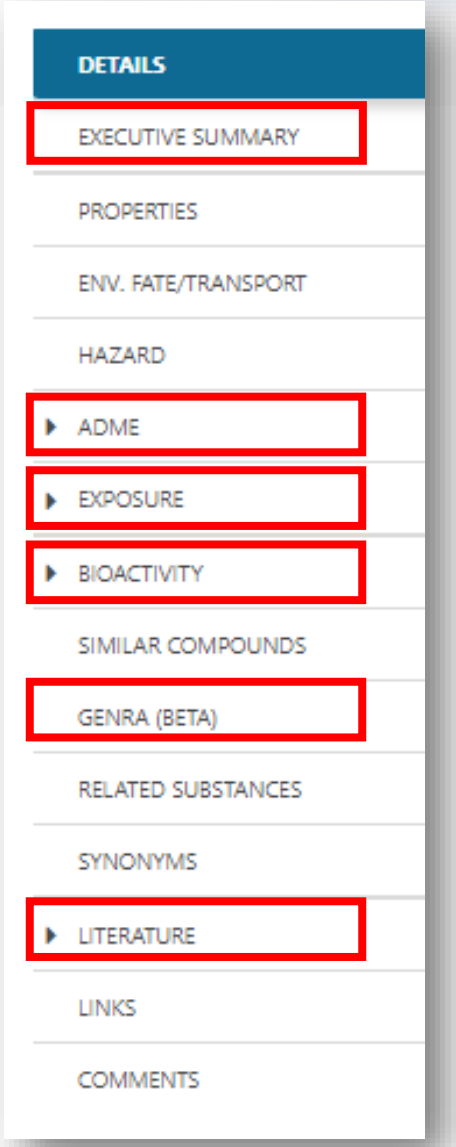
Toxicology

- 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

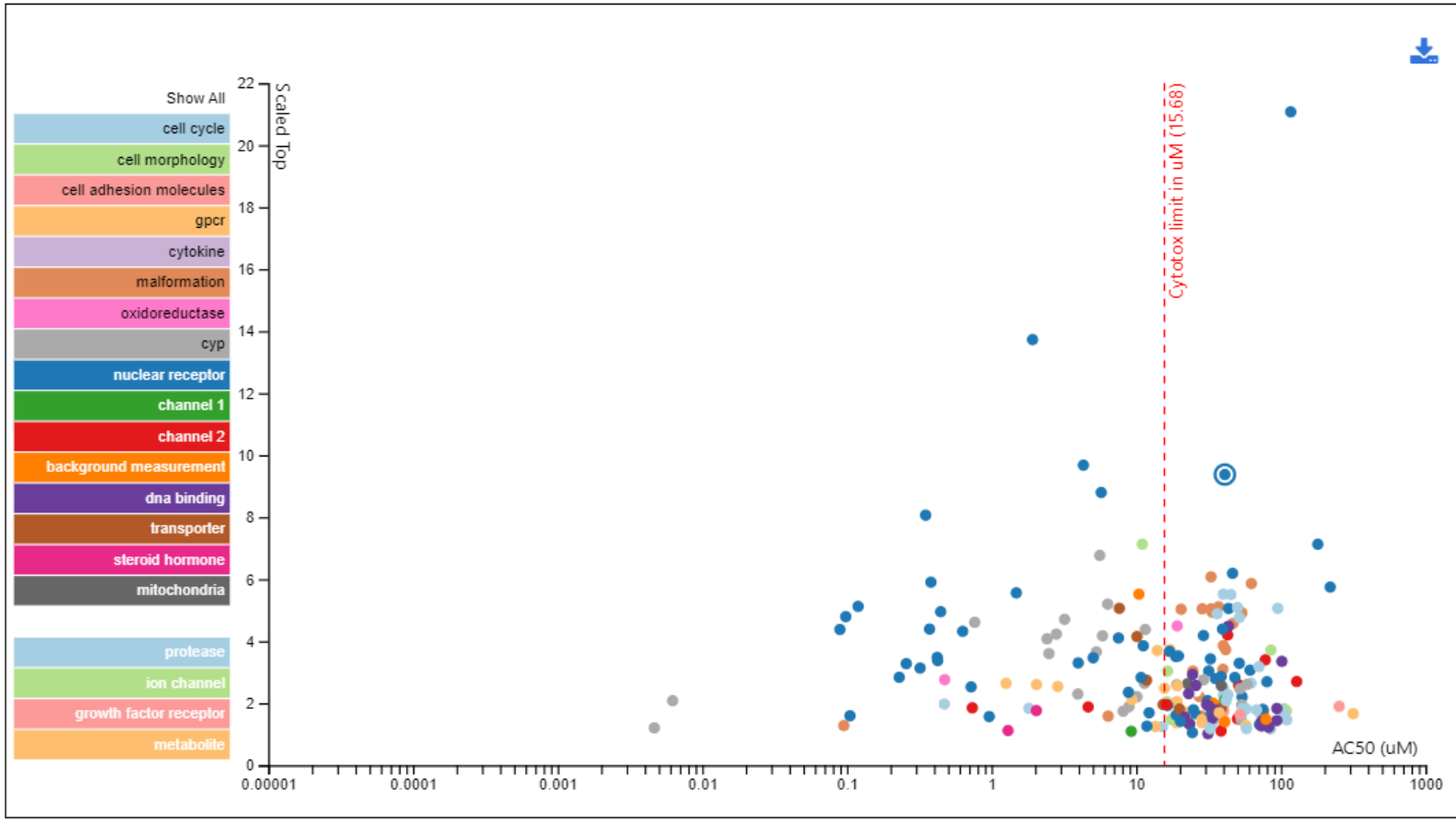
Quantitative Risk Assessment Values

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

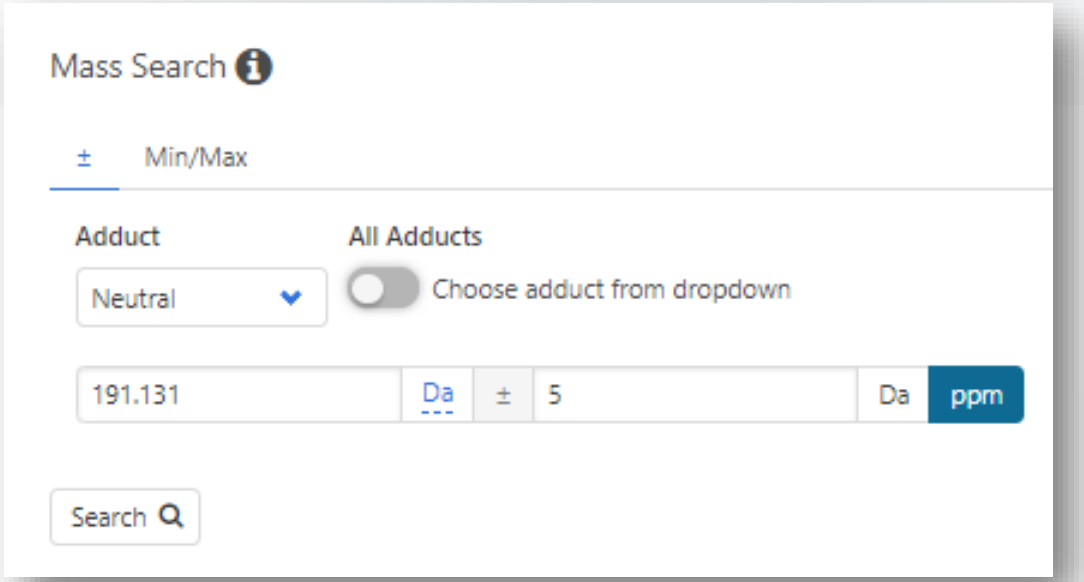
Developmental toxicity PODs available

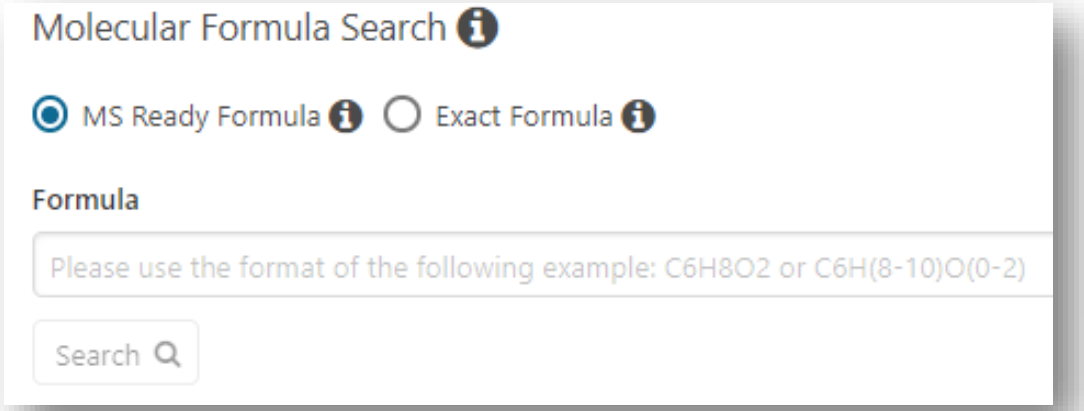
logP log(BCF) log(VP)

Advanced Searching: Mass and Formula

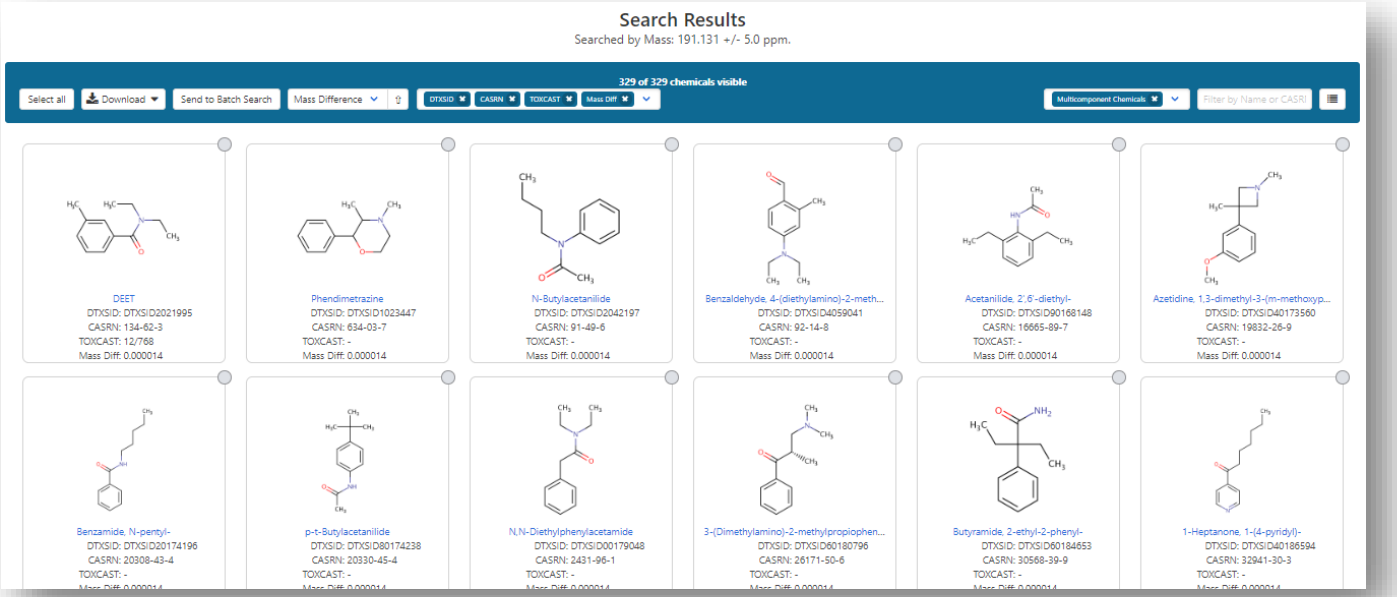
Advanced Searches
Mass and **Formula** Searches

EPA United States Environmental Protection Agency





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

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

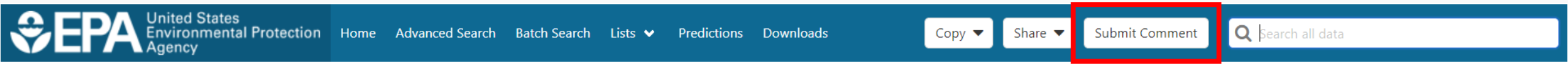
	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	INPUT	FOUND_BY	DTXSID	PREFERRE	CASRN	INCHIKEY	IUPAC_NAI	MOLECULA	TOXVAL_D	TOXCAST_	TOXCAST_	MS_READY	NUMBER_C	IRIS_LINK	PPRTV_LIN	ATMOSPHE	BIOCONCE
2	534-52-1	CAS-RN	DTXSID10	2-Methyl-4,6	534-52-1	ZXVONLUN	2-Methyl-4,6	C7H6N2O5	Y	27.56	261/947	CC1=C(O)C	179	-	Y	1.571E-12	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-Chlorop	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) s	7446-18-6	YTQVHRVI	Dithallium(1+	O4STl2	Y	-	-	-	34	Y	Y	-	-
11	62207-76-5	CAS-RN	DTXSID40	Bis(3-fluoros	62207-76-	YRZXYIHD	-	C16H14CoF	Y	-	-	-	-	-	-	-	-
12	66-81-9	CAS-RN	DTXSID60	Cycloheximi	66-81-9	YPHMISFO	4-{(2R)-2-[(1	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	YORCIIVHU	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	C12H18N2O	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	YLQBMQCU	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	YGYAWVDI	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	(Methylcyclc	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	XOOGZRUI	Tetramethyl	C4H12Pb	Y	-	-	C[Pb](C)(C)	24	-	-	-	-

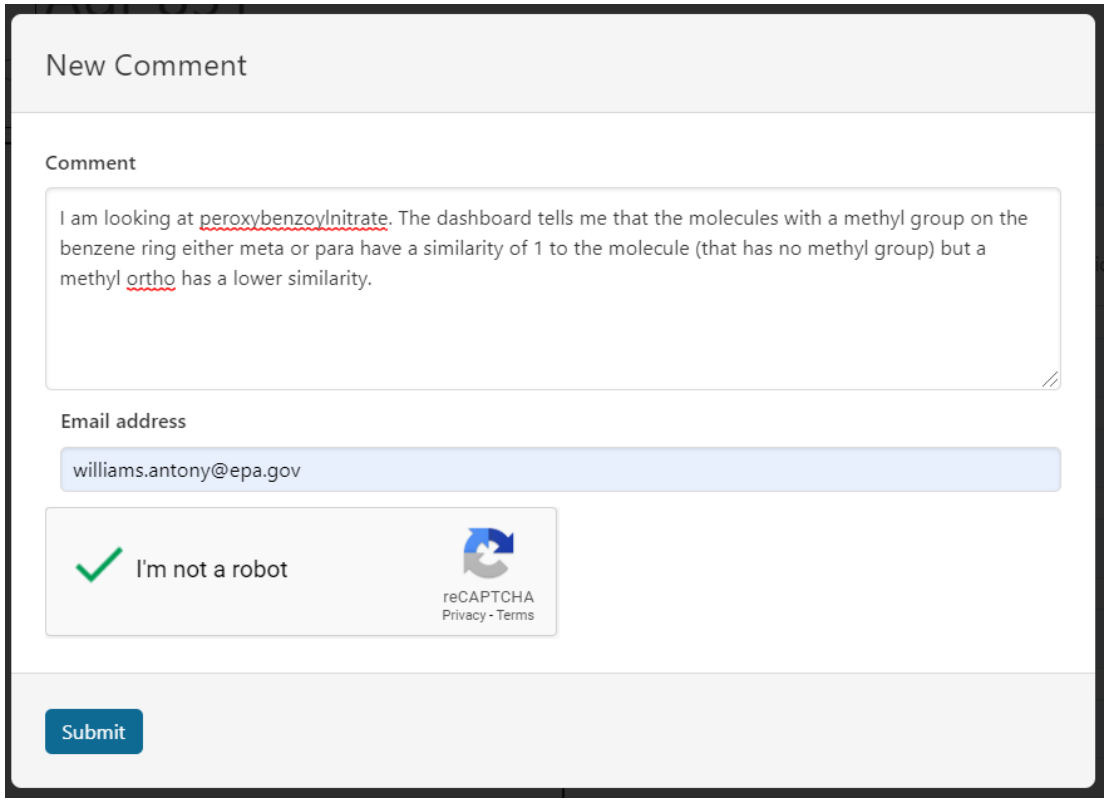
Worksheet1

How Can You Help?

How can you help?

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





Prototypes in Progress

PROTOTYPE Structure/Substructure/Similarity Search available

EPA United States Environmental Protection Agency

PROTOTYPE Hazard Comparison Dashboard

EPA 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

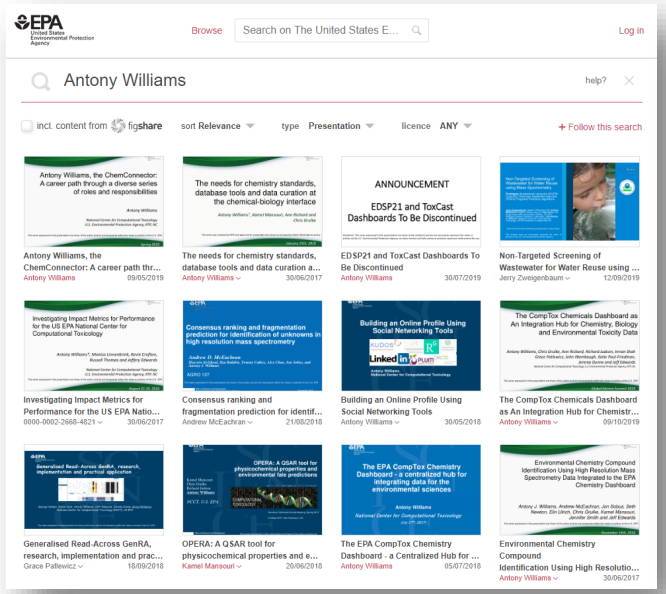
Clean Technologies and Environmental Policy **22**, 441–458(2020) | Cite this article

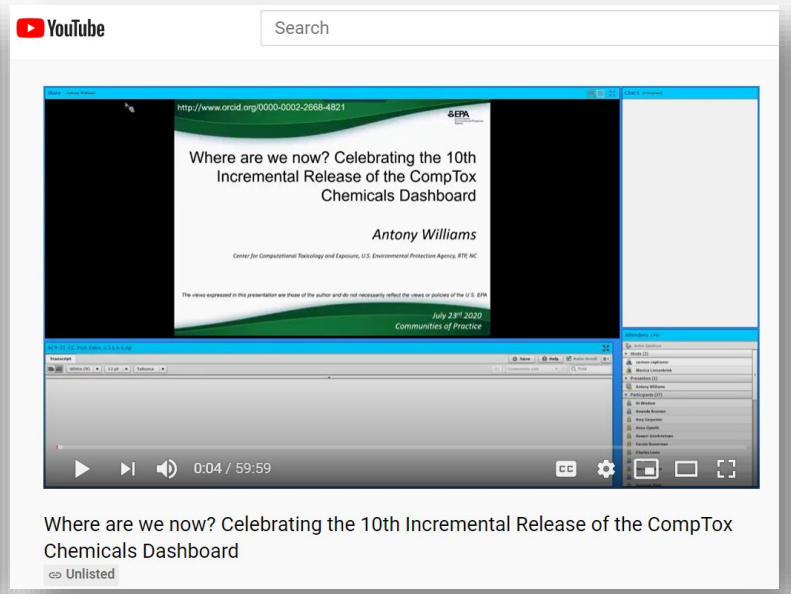
163 Accesses | Metrics

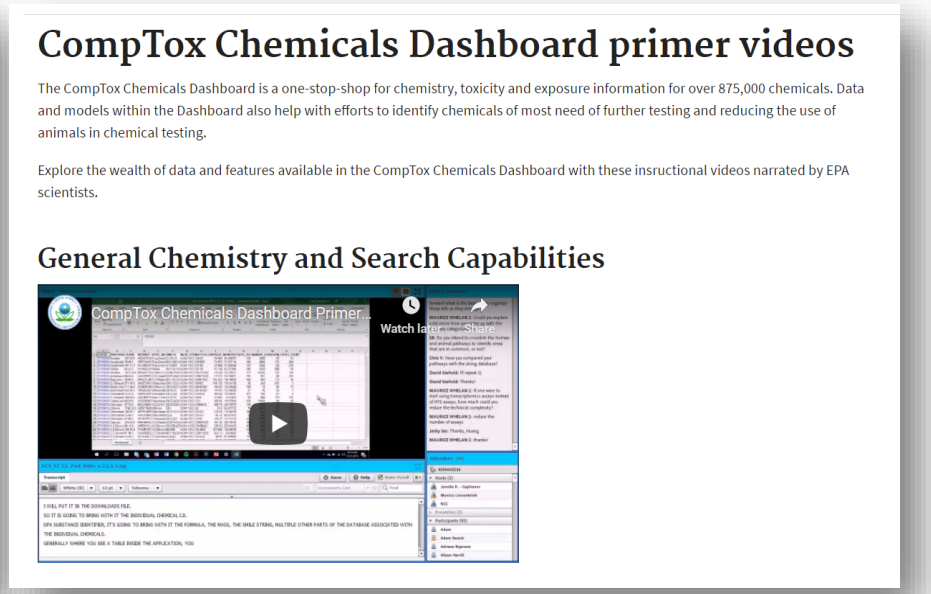
Online Materials

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

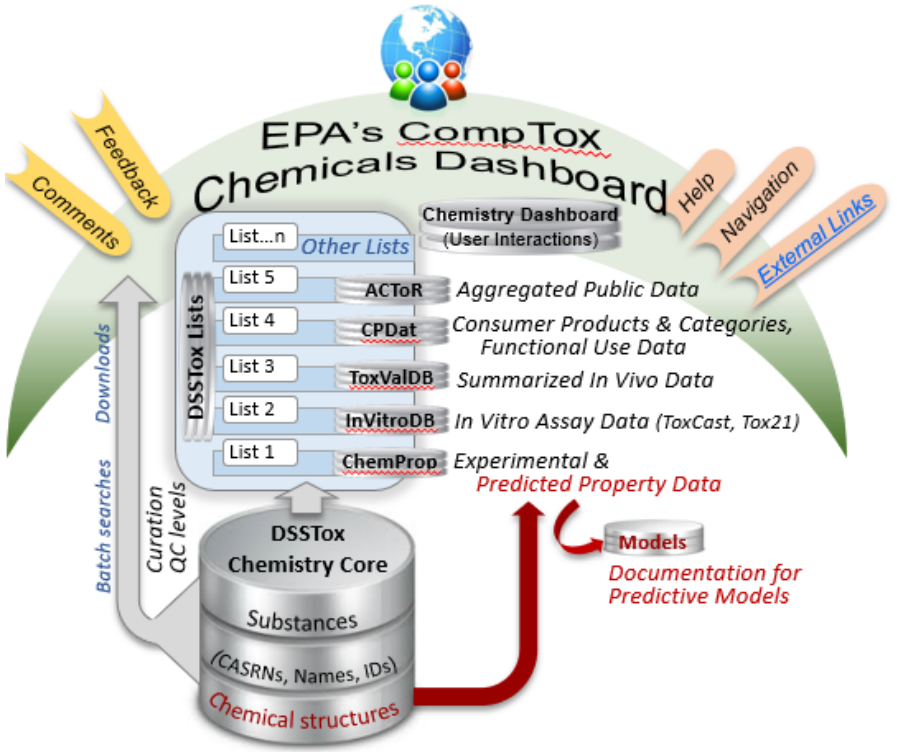






Conclusion

- 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