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The EPA CompTox Dashboard as a Data Integration Hub for Environmental Chemistry Data

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3) *Leidos, RTP, NC*
4) *Integrated Laboratory Systems, Inc., RTP, NC*

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

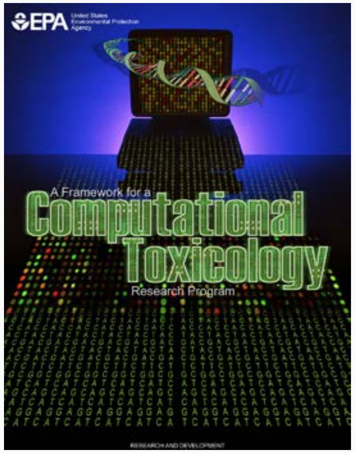
August 2018

ACS Fall Meeting, Boston

Abstract

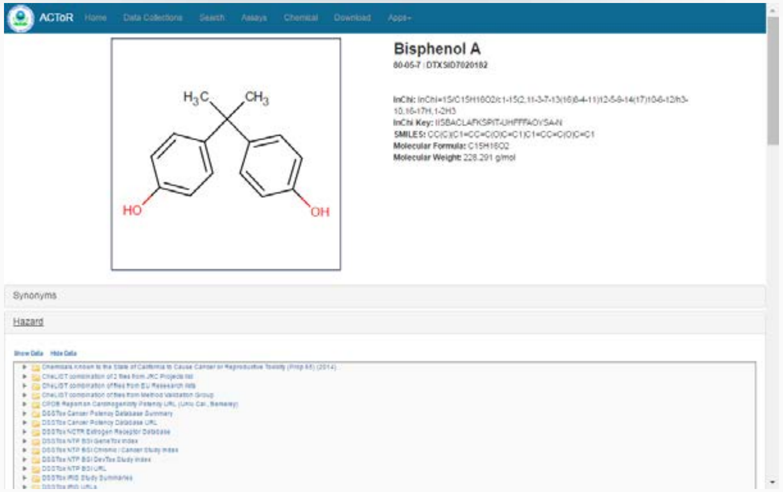
- The US EPA's CompTox Chemistry Dashboard provides access to various types of data associated with ~760,000 chemical substances. These data include experimental and predicted property data, high-throughput screening assay data and hazard and environmental exposure data. With millions of individual data points and annotations associated with hundreds of thousands of chemicals, data quality is a priority. With tens of thousands of individual users per month browsing the data on the dashboard, the ability of users to provide feedback has allowed us to identify, confirm and address issues in the data. This has required the implementation of novel approaches for data feedback via the user interface that include general feedback on the dashboard and down to individual data points contained in a table. We are presently investigating ways to garner feedback on our ToxCast bioassay data to facilitate the curation of tens of thousands of data points. This presentation will provide an overview of our existing capabilities in the CompTox Chemistry Dashboard for gathering crowdsourced data from the user base and its impact on assisting in the curation of data.

National Center for Computational Toxicology



- National Center for Computational Toxicology established in 2005 to integrate:
  - High-throughput and high-content technologies
  - Modern molecular biology
  - Data mining and statistical modeling
  - Computational biology and chemistry
- Researching computational approaches to quickly evaluate the safety of chemicals for potential risk.
- Outputs: a lot of data, models, algorithms and software applications

Early Dashboard Applications

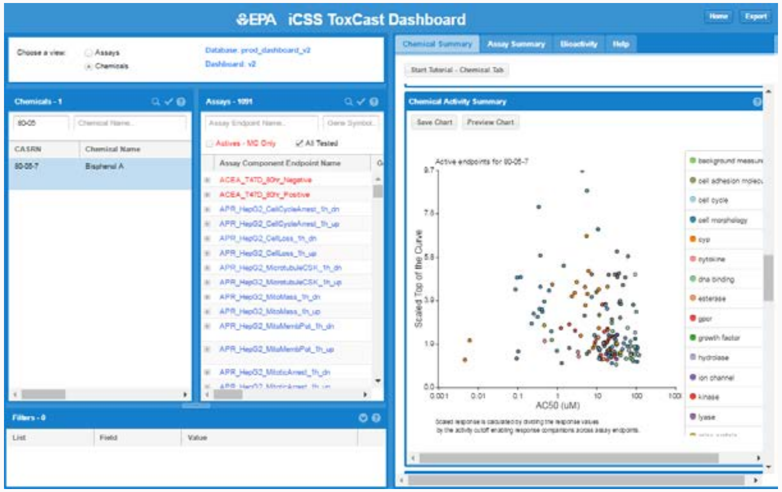


Bisphenol A

80-05-7 | DTXSID7020182

InChI: InChI=1S/C15H16O2/c1-15(2,11-3-7-13(16)8-4-11)12-5-9-14(17)10-6-12/h3-10,16-17H,1-2H3
InChI Key: IISBACLAFKSPIT-UHFFFAOYSA-N
SMILES: CC(C)(C1=CC=C(O)C=C1)C1=CC=C(O)C=C1
Molecular Formula: C15H16O2
Molecular Weight: 228.291 g/mol

- Chemicals Known to the State of California to Cause Cancer or Reproductive Toxicity (Prop 65) (2014)
- ChemIDT combination of 2 files from JRC Projects list
- ChemIDT combination of files from EU Research lists
- ChemIDT combination of files from Method Validation Group
- CPDB Report on Carcinogenicity Potency URL (Univ Cal., Berkeley)
- DSSTox Cancer Potency Database Summary
- DSSTox Cancer Potency Database URL
- DSSTox NCTR Estrogen Receptor Database
- DSSTox NTP BSI GeneTox Index
- DSSTox NTP BSI Chronic / Cancer Study Index
- DSSTox NTP BSI DevTox Study Index
- DSSTox NTP BSI URL
- DSSTox IRIS Study Summaries
- DSSTox IRIS URLs

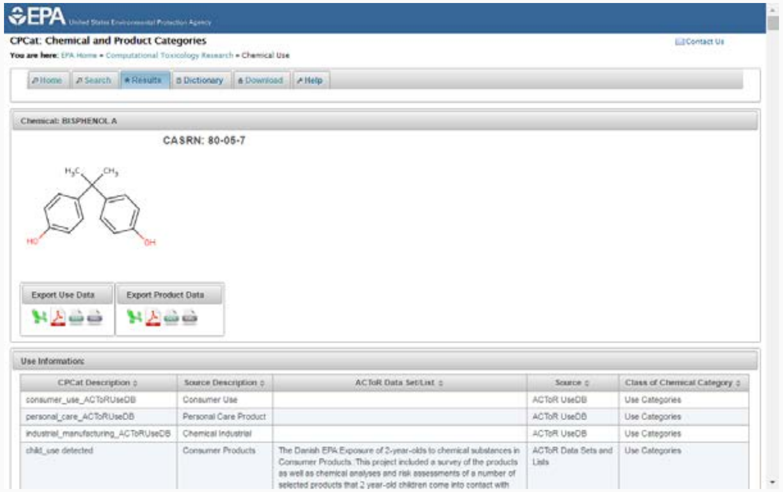


Database: prod_dashboard_v2
Dashboard: v2

CASRN	Chemical Name
80-05-7	Bisphenol A

- ACEA_T47D_80hr_Negative
- ACEA_T47D_80hr_Positive
- APR_HepG2_CellCycleArrest_1h_dn
- APR_HepG2_CellCycleArrest_1h_up
- APR_HepG2_CellLoss_1h_dn
- APR_HepG2_CellLoss_1h_up
- APR_HepG2_MicrotubuleCSK_1h_dn
- APR_HepG2_MicrotubuleCSK_1h_up
- APR_HepG2_MitoMass_1h_dn
- APR_HepG2_MitoMass_1h_up
- APR_HepG2_MitoMembPot_1h_dn
- APR_HepG2_MitoMembPot_1h_up
- APR_HepG2_MitoticArrest_1h_dn
- APR_HepG2_MitoticArrest_1h_up

Scaled response is calculated by dividing the response values by the activity cutoff enabling response comparisons across assay endpoints.



CPCat: Chemical and Product Categories

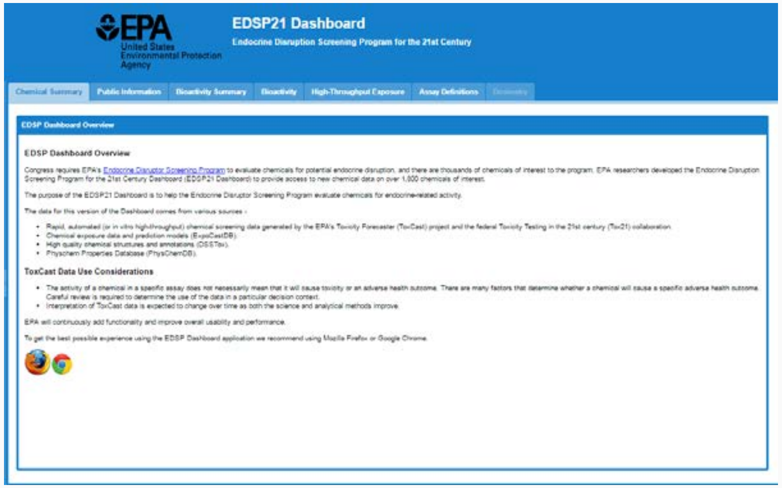
You are here: EPA Home » Computational Toxicology Research » Chemical Use

Chemical: BISPHENOL A

CASRN: 80-05-7

Use Information:

CPCat Description	Source Description	ACToR Data Set/List	Source	Class of Chemical Category
consumer_use_ACToRUseDB	Consumer Use		ACToR UseDB	Use Categories
personal_care_ACToRUseDB	Personal Care Product		ACToR UseDB	Use Categories
industrial_manufacturing_ACToRUseDB	Chemical Industrial		ACToR UseDB	Use Categories
child_use detected	Consumer Products	The Danish EPA Exposure of 2-year-olds to chemical substances in Consumer Products. This project included a survey of the products as well as chemical analyses and risk assessments of a number of selected products that 2 year-old children come into contact with	ACToR Data Sets and Lists	Use Categories



EDSP21 Dashboard

Endocrine Disruption Screening Program for the 21st Century

EDSP Dashboard Overview

Congress requires EPA's Endocrine Disruptor Screening Program to evaluate chemicals for potential endocrine disruption, and there are thousands of chemicals of interest to the program. EPA researchers developed the Endocrine Disruption Screening Program for the 21st Century Dashboard (EDSP21 Dashboard) to provide access to new chemical data on over 1,800 chemicals of interest.

The purpose of the EDSP21 Dashboard is to help the Endocrine Disruptor Screening Program evaluate chemicals for endocrine-related activity.

The data for this version of the Dashboard comes from various sources :

- Rapid, automated (or in vitro high-throughput) chemical screening data generated by the EPA's Toxicity Forecaster (ToxCast) project and the federal Toxicity Testing in the 21st century (Tox21) collaboration.
- Chemical exposure data and prediction models (ExpoCastDB).
- High quality chemical structures and annotations (DSSTox).
- Physchem Properties Database (PhysChemDB).

ToxCast Data Use Considerations

- The activity of a chemical in a specific assay does not necessarily mean that it will cause toxicity or an adverse health outcome. There are many factors that determine whether a chemical will cause a specific adverse health outcome. Careful review is required to determine the use of the data in a particular decision context.
- Interpretation of ToxCast data is expected to change over time as both the science and analytical methods improve.

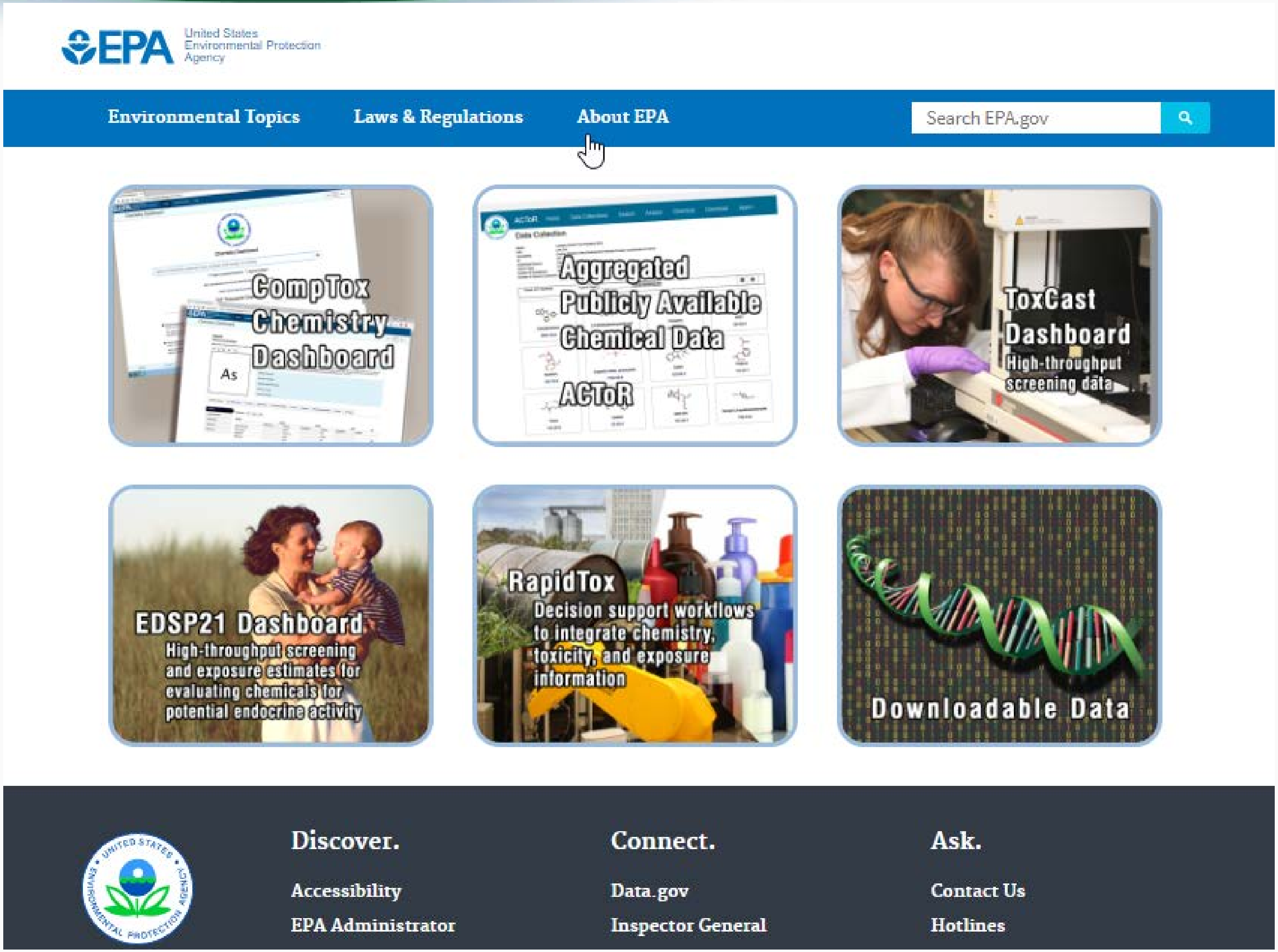
EPA will continuously add functionality and improve overall usability and performance.

To get the best possible experience using the EDSP Dashboard application we recommend using Mozilla Firefox or Google Chrome.

The CompTox ~~Chemistry~~ Dashboard

- A publicly accessible website delivering access:
  - New entry portal for all NCCT dashboards
  - ~**762,000** chemicals with related property data
  - **Searchable by chemical, product use, gene and assay (ToxCast)**
  - Experimental and predicted physicochemical property data
  - **"Bioactivity data" for the ToxCast/Tox21 project**
  - **Generalized Read-Across (GenRA) module**
  - Links to other agency websites and public data resources
  - "Literature" searches for chemicals using public resources
  - "Batch searching" for thousands of chemicals
  - DOWNLOADABLE Open Data for reuse and repurposing

CompTox Portal



CompTox Chemistry Dashboard

Aggregated Publicly Available Chemical Data
ACToR

ToxCast Dashboard
High-throughput screening data

EDSP21 Dashboard
High-throughput screening and exposure estimates for evaluating chemicals for potential endocrine activity

RapidTox
Decision support workflows to integrate chemistry, toxicity, and exposure information

Downloadable Data

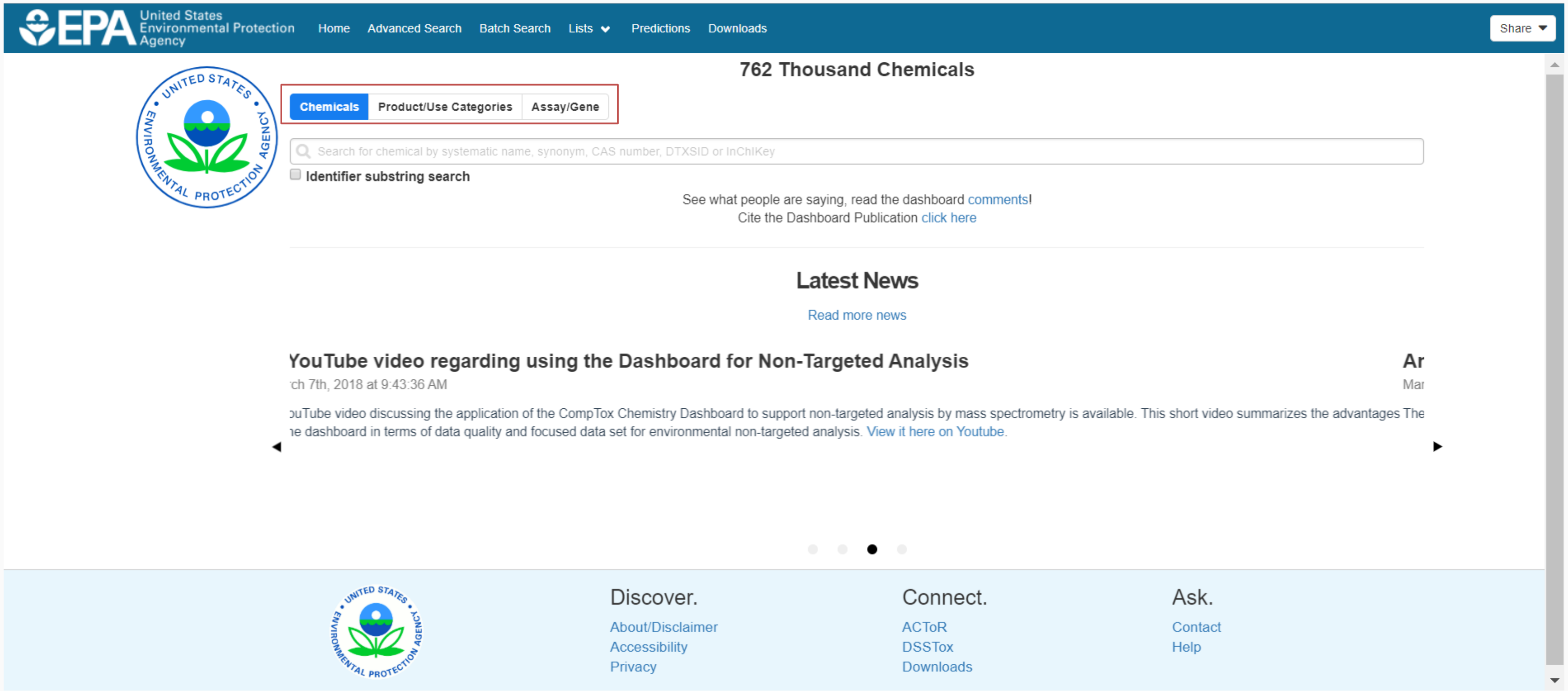
Discover.
Accessibility
EPA Administrator

Connect.
Data.gov
Inspector General

Ask.
Contact Us
Hotlines

CompTox Dashboard

https://comptox.epa.gov/dashboard



EPA United States Environmental Protection Agency
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Advanced Search
Batch Search
Lists
Predictions
Downloads
Share
Chemicals
Product/Use Categories
Assay/Gene
Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey

762 Thousand Chemicals

□ Identifier substring search

See what people are saying, read the dashboard comments!
Cite the Dashboard Publication click here

Latest News

Read more news

YouTube video regarding using the Dashboard for Non-Targeted Analysis

ch 7th, 2018 at 9:43:36 AM

ouTube video discussing the application of the CompTox Chemistry Dashboard to support non-targeted analysis by mass spectrometry is available. This short video summarizes the advantages The ne dashboard in terms of data quality and focused data set for environmental non-targeted analysis. View it here on Youtube.

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Mar

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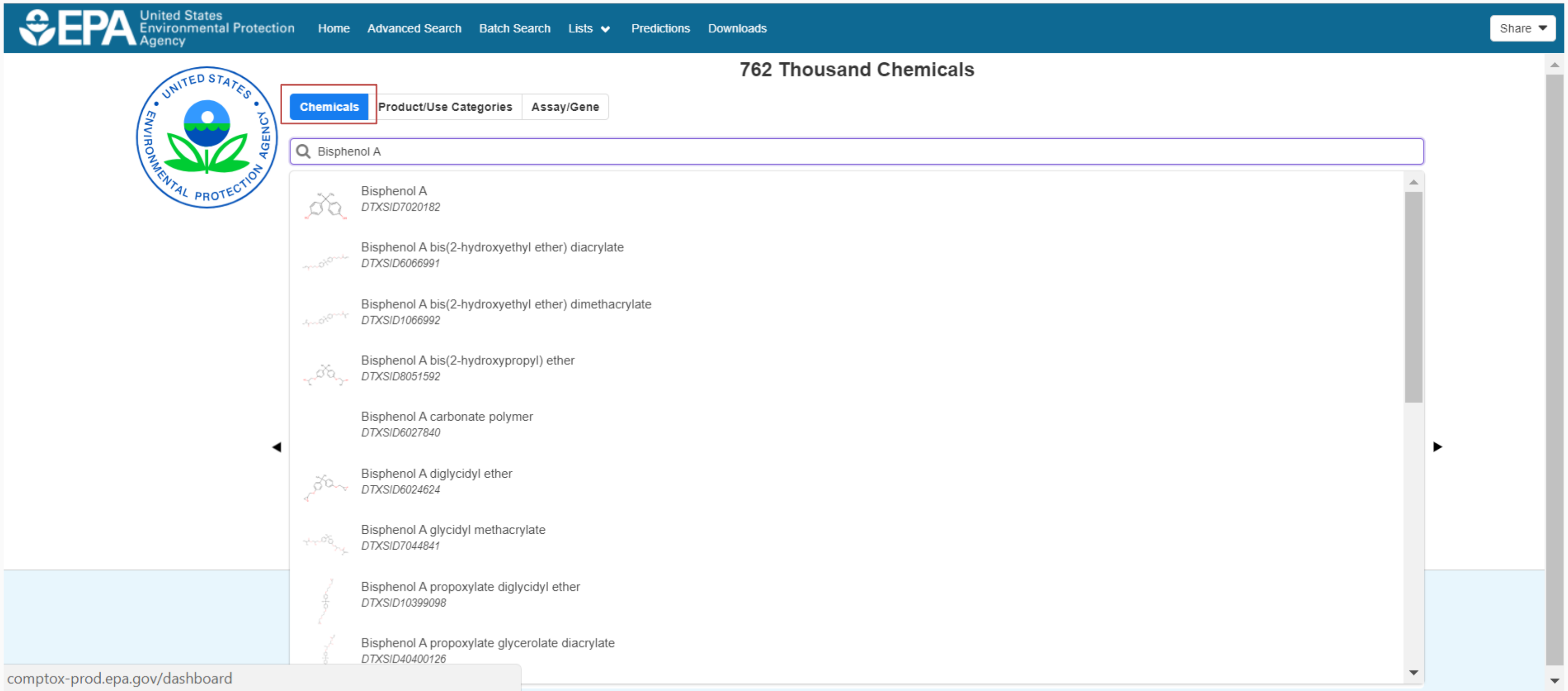
CompTox Dashboard Chemicals



762 Thousand Chemicals

Bisphenol A

Bisphenol A
DTXSID7020182

Bisphenol A bis(2-hydroxyethyl ether) diacrylate
DTXSID6066991

Bisphenol A bis(2-hydroxyethyl ether) dimethacrylate
DTXSID1066992

Bisphenol A bis(2-hydroxypropyl) ether
DTXSID8051592

Bisphenol A carbonate polymer
DTXSID6027840

Bisphenol A diglycidyl ether
DTXSID6024624

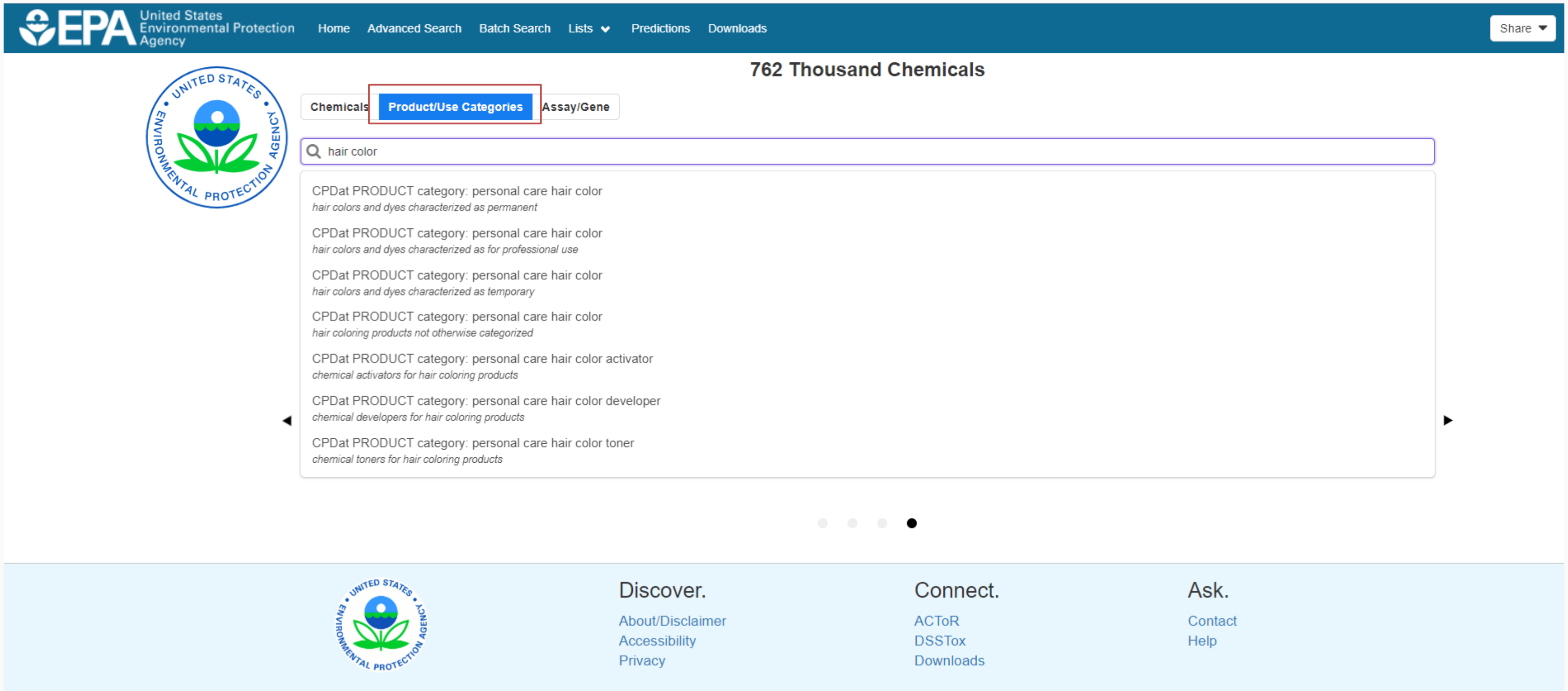
Bisphenol A glycidyl methacrylate
DTXSID7044841

Bisphenol A propoxylate diglycidyl ether
DTXSID10399098

Bisphenol A propoxylate glycerolate diacrylate
DTXSID40400126

comptox-prod.epa.gov/dashboard

CompTox Dashboard
Products and Use Categories



762 Thousand Chemicals

hair color

CPDat PRODUCT category: personal care hair color
hair colors and dyes characterized as permanent

CPDat PRODUCT category: personal care hair color
hair colors and dyes characterized as for professional use

CPDat PRODUCT category: personal care hair color
hair colors and dyes characterized as temporary

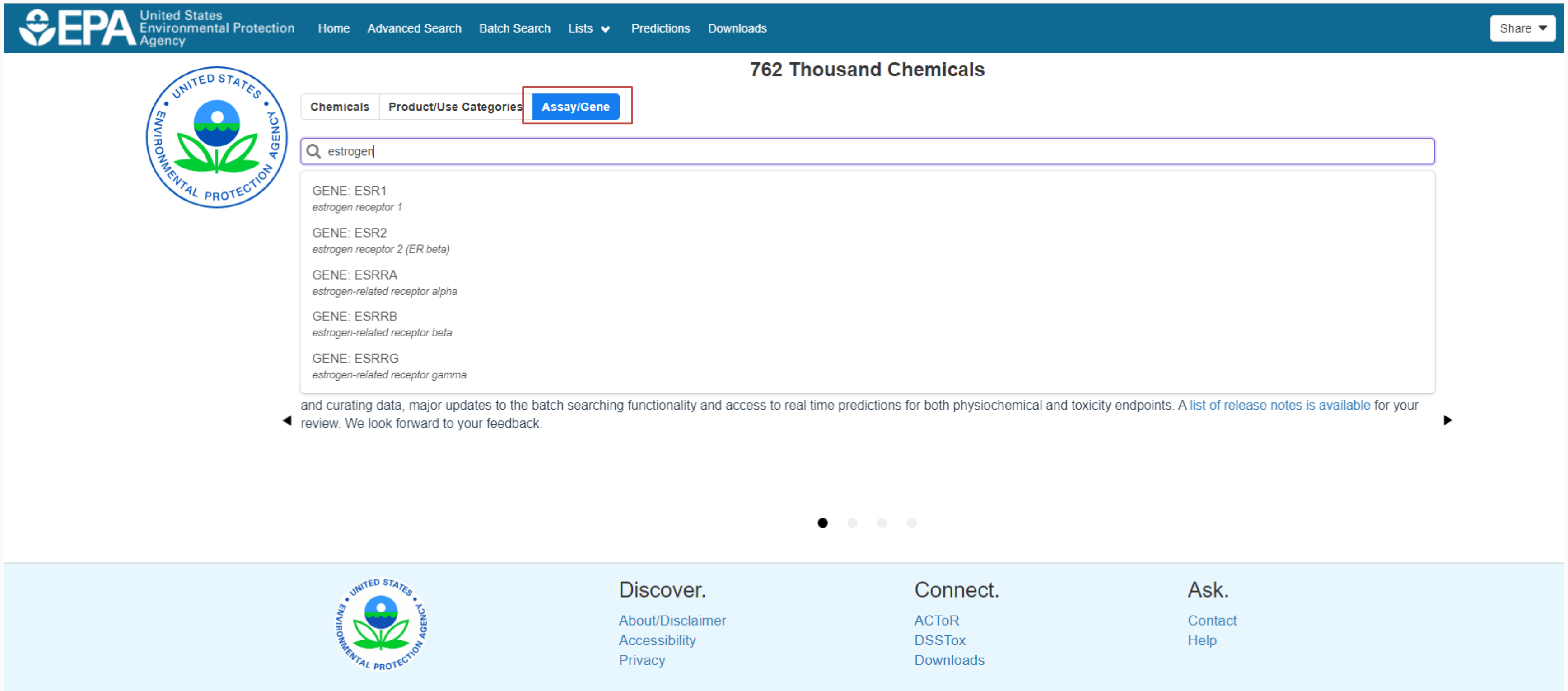
CPDat PRODUCT category: personal care hair color
hair coloring products not otherwise categorized

CPDat PRODUCT category: personal care hair color activator
chemical activators for hair coloring products

CPDat PRODUCT category: personal care hair color developer
chemical developers for hair coloring products

CPDat PRODUCT category: personal care hair color toner
chemical toners for hair coloring products

CompTox Dashboard
Assays and Genes



762 Thousand Chemicals

estrogen

GENE: ESR1
estrogen receptor 1

GENE: ESR2
estrogen receptor 2 (ER beta)

GENE: ESRRA
estrogen-related receptor alpha

GENE: ESRRB
estrogen-related receptor beta

GENE: ESRRG
estrogen-related receptor gamma

and curating data, major updates to the batch searching functionality and access to real time predictions for both physiochemical and toxicity endpoints. A list of release notes is available for your review. We look forward to your feedback.

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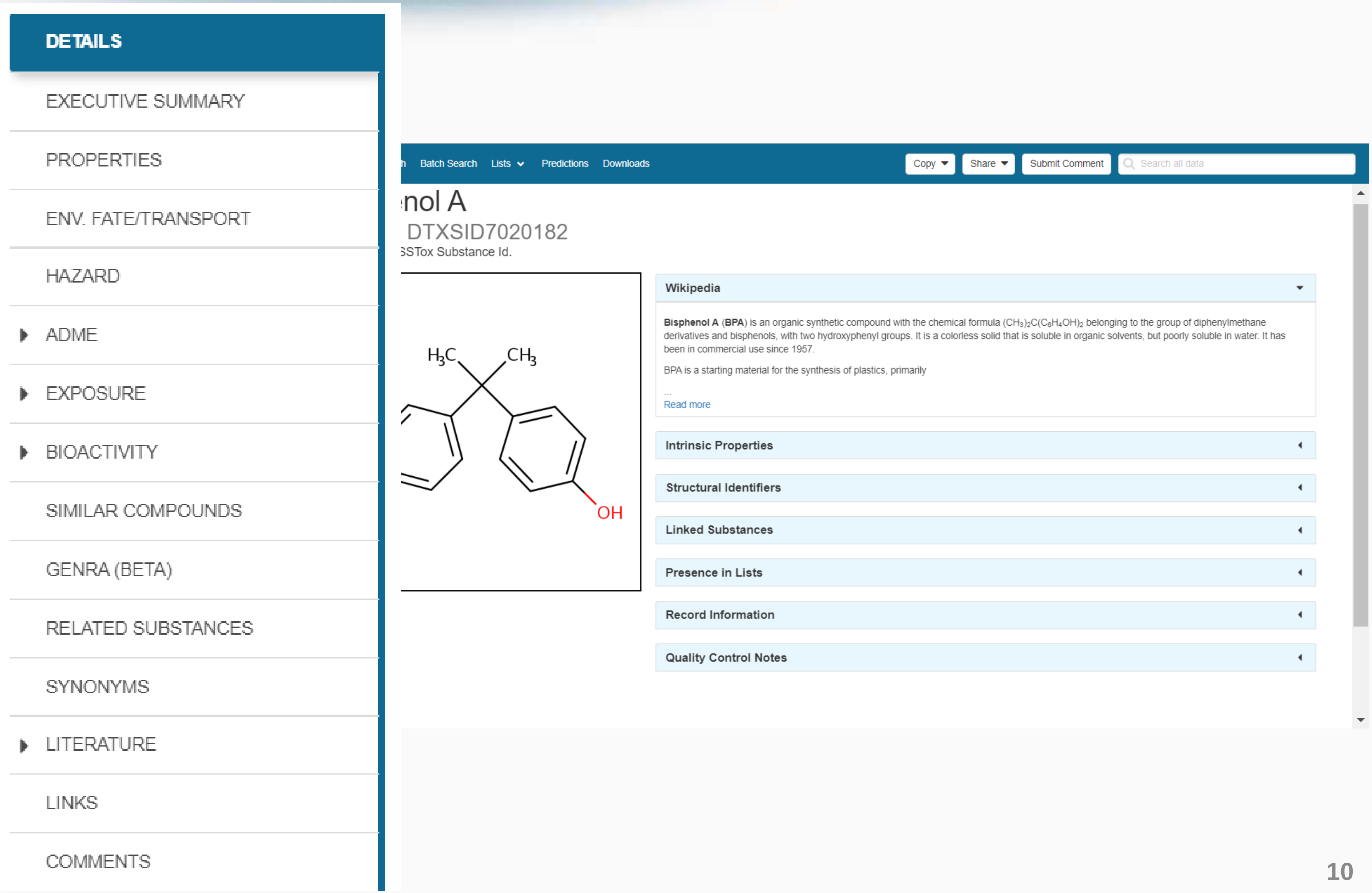
Ask.
Contact
Help

Detailed Chemical Pages



DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

EXPOSURE

BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

LITERATURE

LINKS

COMMENTS

nol A

DTXSID7020182

SSTox Substance Id.

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. It has been in commercial use since 1957.

BPA is a starting material for the synthesis of plastics, primarily

...

Read more

Intrinsic Properties

Structural Identifiers

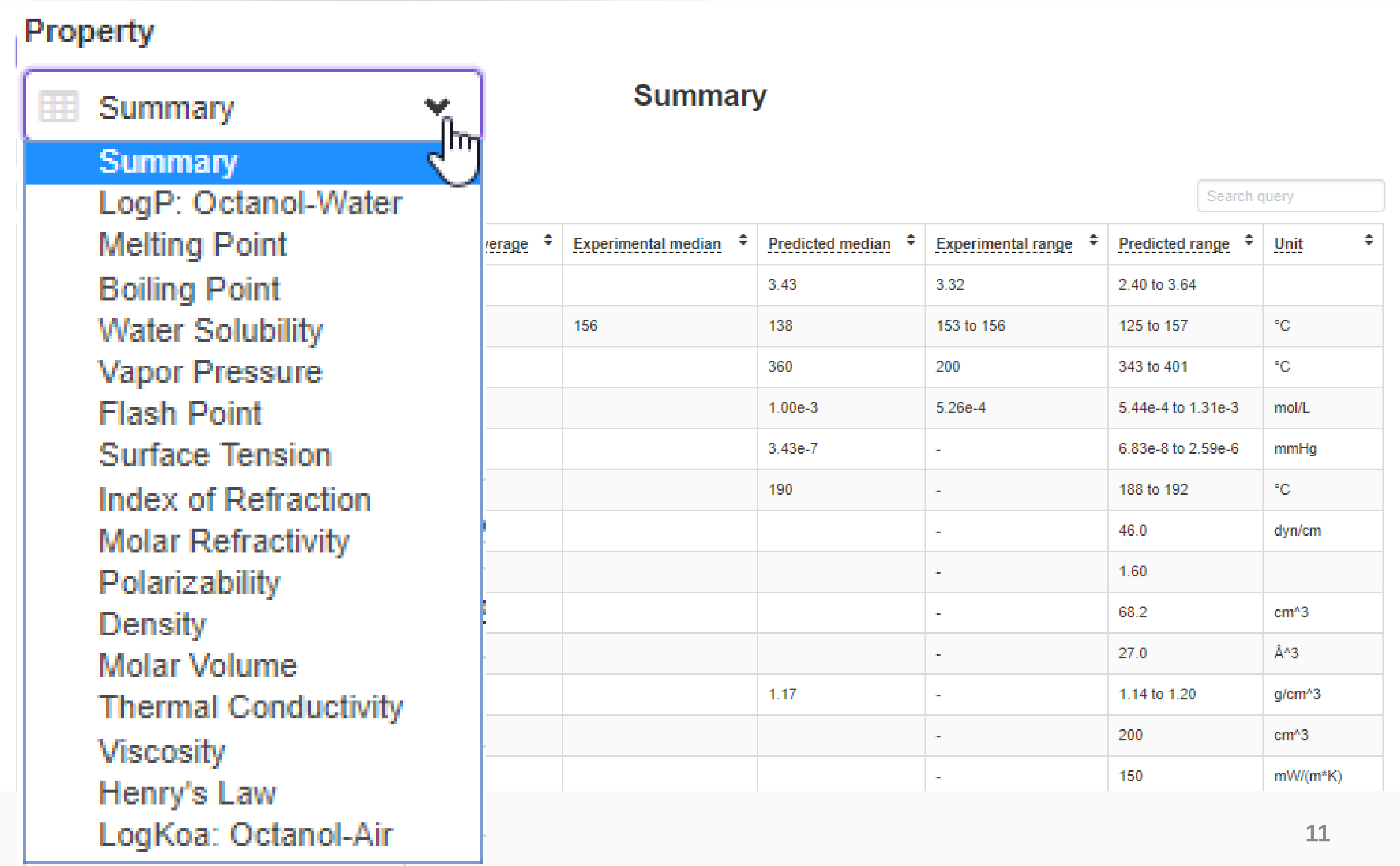
Linked Substances

Presence in Lists

Record Information

Quality Control Notes

Physicochemical properties



Property

Summary

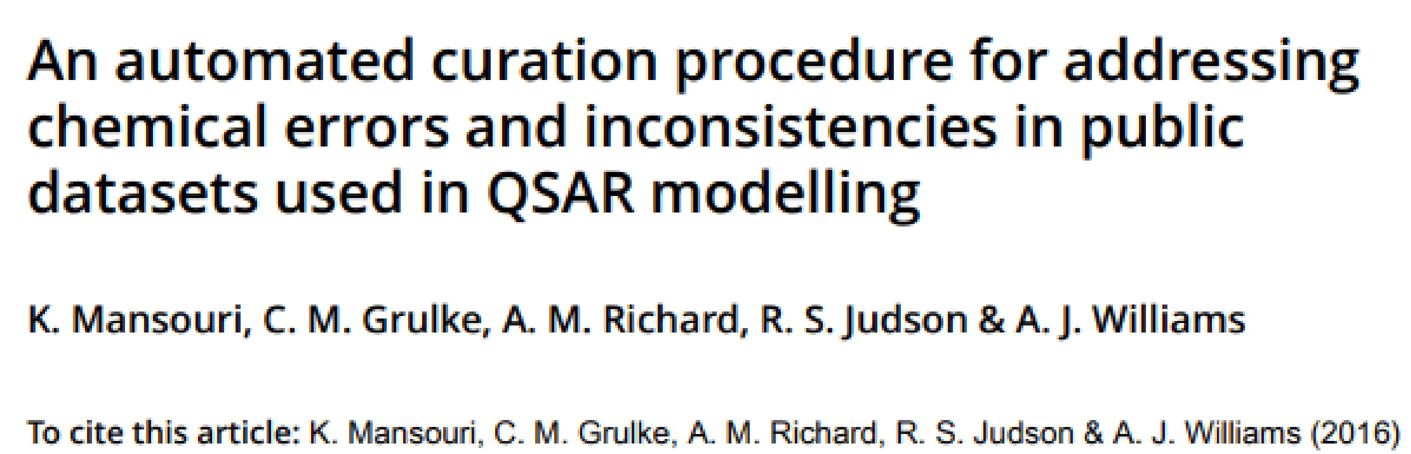
Summary
LogP: Octanol-Water
Melting Point
Boiling Point
Water Solubility
Vapor Pressure
Flash Point
Surface Tension
Index of Refraction
Molar Refractivity
Polarizability
Density
Molar Volume
Thermal Conductivity
Viscosity
Henry's Law
LogKoa: Octanol-Air

Summary

Search query

erage	Experimental median	Predicted median	Experimental range	Predicted range	Unit
		3.43	3.32	2.40 to 3.64	
	156	138	153 to 156	125 to 157	°C
		360	200	343 to 401	°C
		1.00e-3	5.26e-4	5.44e-4 to 1.31e-3	mol/L
		3.43e-7	-	6.83e-8 to 2.59e-6	mmHg
		190	-	188 to 192	°C
			-	46.0	dyn/cm
			-	1.60	
			-	68.2	cm^3
			-	27.0	Å^3
		1.17	-	1.14 to 1.20	g/cm^3
			-	200	cm^3
			-	150	mW/(m*K)

OPERA Predicted Properties

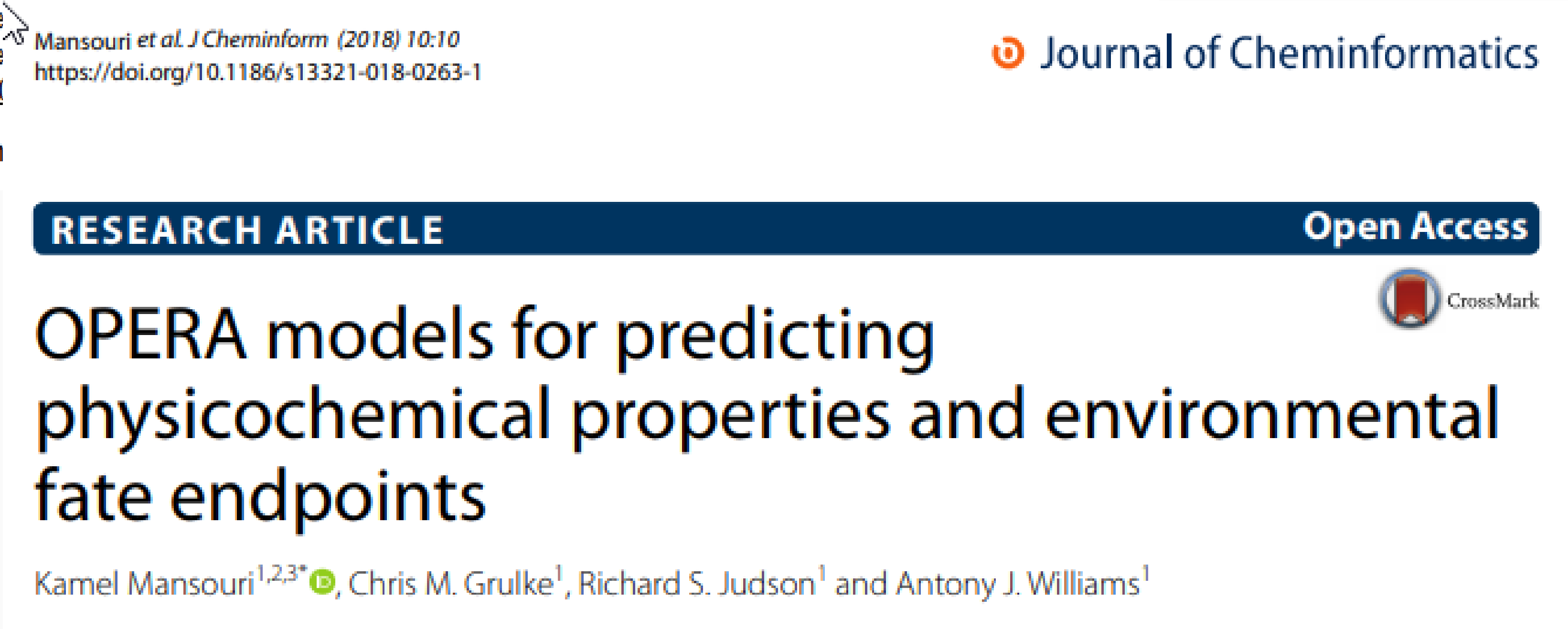


An automated curation procedure for addressing chemical errors and inconsistencies in public datasets used in QSAR modelling

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

To cite this article: K. Mansouri, C. M. Grulke, A. M. Richard, R. S. Judson & A. J. Williams (2016) An automate datasets use DOI: 10.108(

To link to th



Mansouri *et al. J Cheminform (2018) 10:10*
https://doi.org/10.1186/s13321-018-0263-1

Journal of Cheminformatics

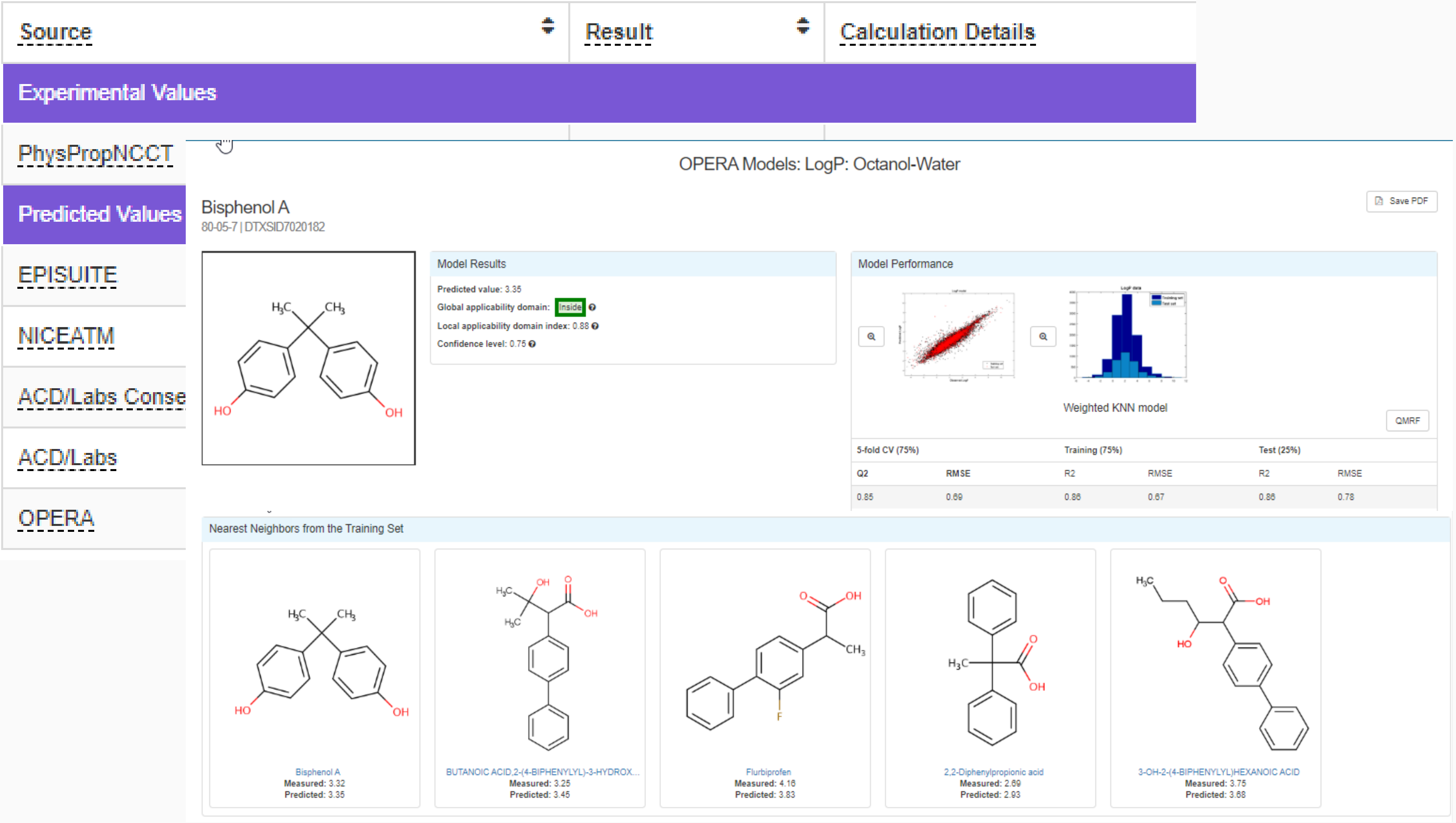
RESEARCH ARTICLE Open Access

CrossMark

OPERA models for predicting physicochemical properties and environmental fate endpoints

Kamel Mansouri[1,2,3*], Chris M. Grulke[1], Richard S. Judson[1] and Antony J. Williams[1]

Detailed OPERA Prediction Reports



Source	Result	Calculation Details
Experimental Values		
PhysPropNCCT		
Predicted Values		
EPISUITE		
NICEATM		
ACD/Labs Conse		
ACD/Labs		
OPERA		

OPERA Models: LogP: Octanol-Water

Bisphenol A
80-05-7 | DTXSID7020182

Model Results

Predicted value: 3.35
Global applicability domain: Inside
Local applicability domain index: 0.88
Confidence level: 0.75

Model Performance

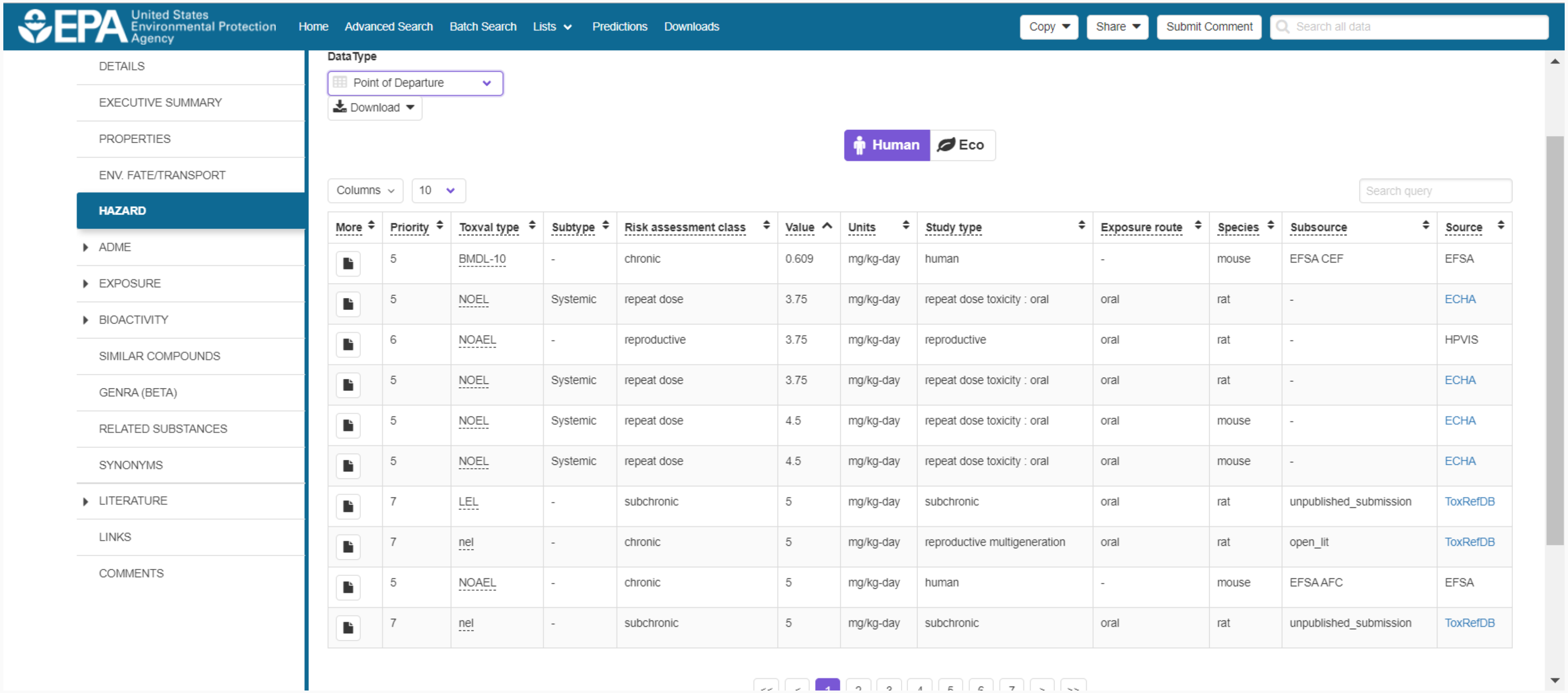
Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Nearest Neighbors from the Training Set

Bisphenol A	BUTANOIC ACID,2-(4-BIPHENYLYL)-3-HYDROX...	Flurbiprofen	2,2-Diphenylpropionic acid	3-OH-2-(4-BIPHENYLYL)HEXANOIC ACID
Measured: 3.32	Measured: 3.25	Measured: 4.16	Measured: 2.69	Measured: 3.75
Predicted: 3.35	Predicted: 3.45	Predicted: 3.83	Predicted: 2.93	Predicted: 3.68

Access to Chemical Hazard Data

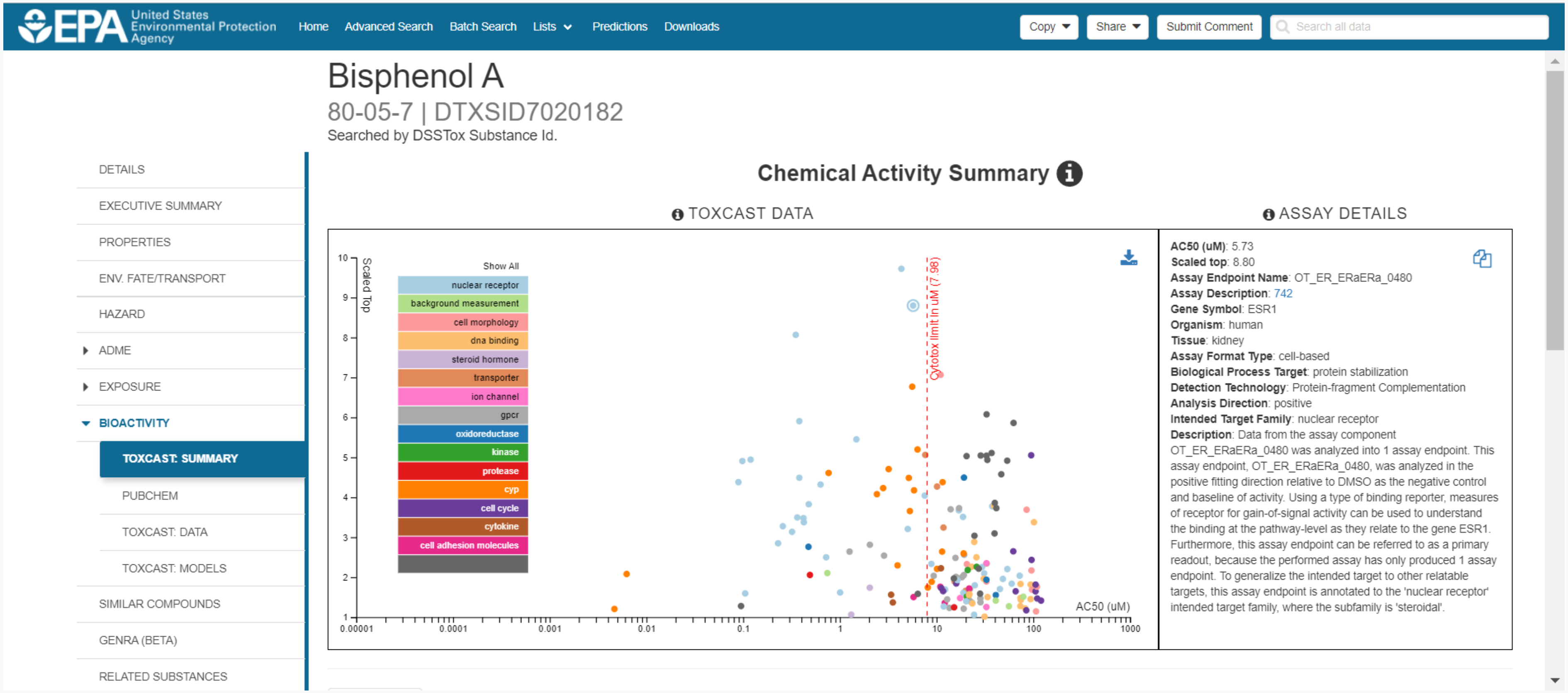


Data Type: Point of Departure

More	Priority	Toxval type	Subtype	Risk assessment class	Value	Units	Study type	Exposure route	Species	Subsource	Source
	5	BMDL-10	-	chronic	0.609	mg/kg-day	human	-	mouse	EFSA CEF	EFSA
	5	NOEL	Systemic	repeat dose	3.75	mg/kg-day	repeat dose toxicity : oral	oral	rat	-	ECHA
	6	NOAEL	-	reproductive	3.75	mg/kg-day	reproductive	oral	rat	-	HPVIS
	5	NOEL	Systemic	repeat dose	3.75	mg/kg-day	repeat dose toxicity : oral	oral	rat	-	ECHA
	5	NOEL	Systemic	repeat dose	4.5	mg/kg-day	repeat dose toxicity : oral	oral	mouse	-	ECHA
	5	NOEL	Systemic	repeat dose	4.5	mg/kg-day	repeat dose toxicity : oral	oral	mouse	-	ECHA
	7	LEL	-	subchronic	5	mg/kg-day	subchronic	oral	rat	unpublished_submission	ToxRefDB
	7	nel	-	chronic	5	mg/kg-day	reproductive multigeneration	oral	rat	open_lit	ToxRefDB
	5	NOAEL	-	chronic	5	mg/kg-day	human	-	mouse	EFSA AFC	EFSA
	7	nel	-	subchronic	5	mg/kg-day	subchronic	oral	rat	unpublished_submission	ToxRefDB

In Vitro Bioassay Screening

ToxCast and Tox21



Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

Chemical Activity Summary

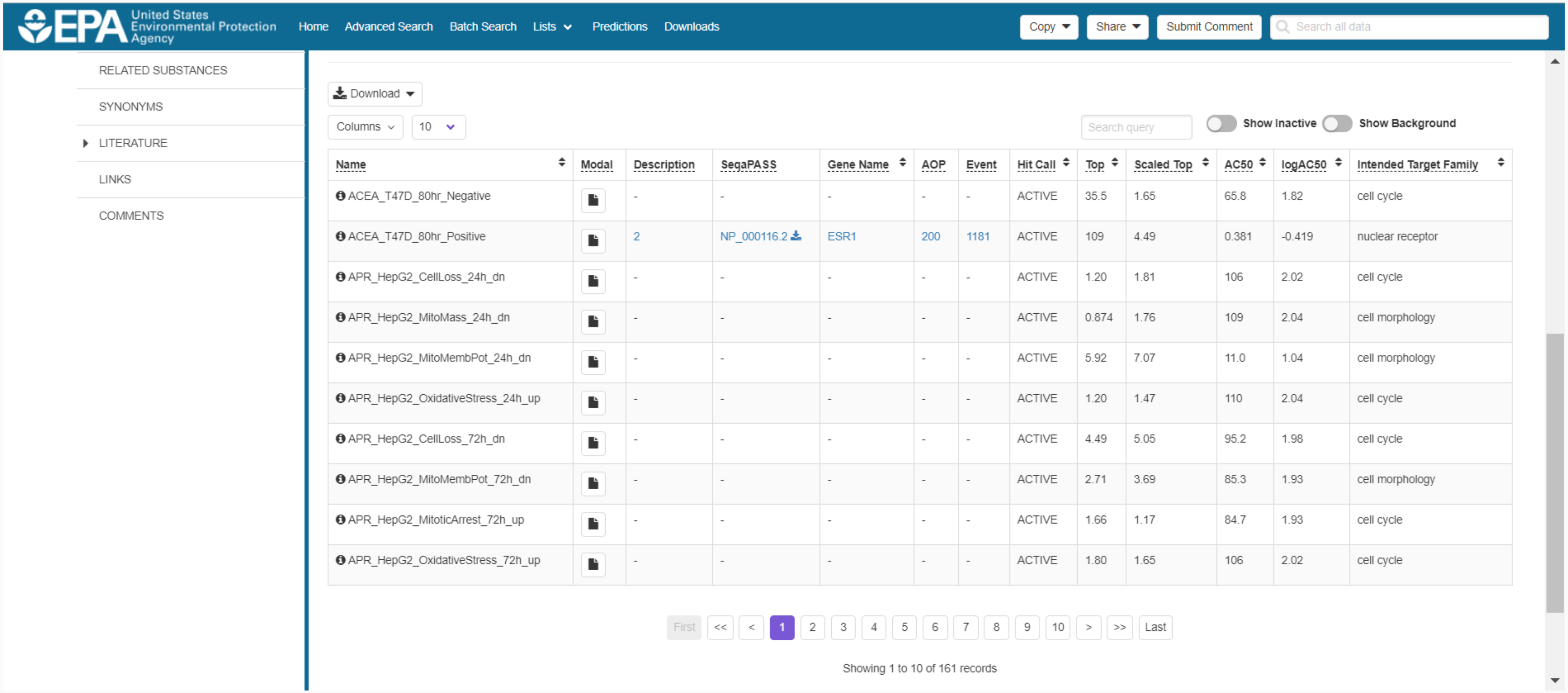
TOXCAST DATA

ASSAY DETAILS

AC50 (uM): 5.73
Scaled top: 8.80
Assay Endpoint Name: OT_ER_ERaERa_0480
Assay Description: 742
Gene Symbol: ESR1
Organism: human
Tissue: kidney
Assay Format Type: cell-based
Biological Process Target: protein stabilization
Detection Technology: Protein-fragment Complementation
Analysis Direction: positive
Intended Target Family: nuclear receptor
Description: Data from the assay component OT_ER_ERaERa_0480 was analyzed into 1 assay endpoint. This assay endpoint, OT_ER_ERaERa_0480, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of binding reporter, measures of receptor for gain-of-signal activity can be used to understand the binding at the pathway-level as they relate to the gene ESR1. Furthermore, this assay endpoint can be referred to as a primary readout, because the performed assay has only produced 1 assay endpoint. 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'.

In Vitro Bioassay Screening

ToxCast and Tox21

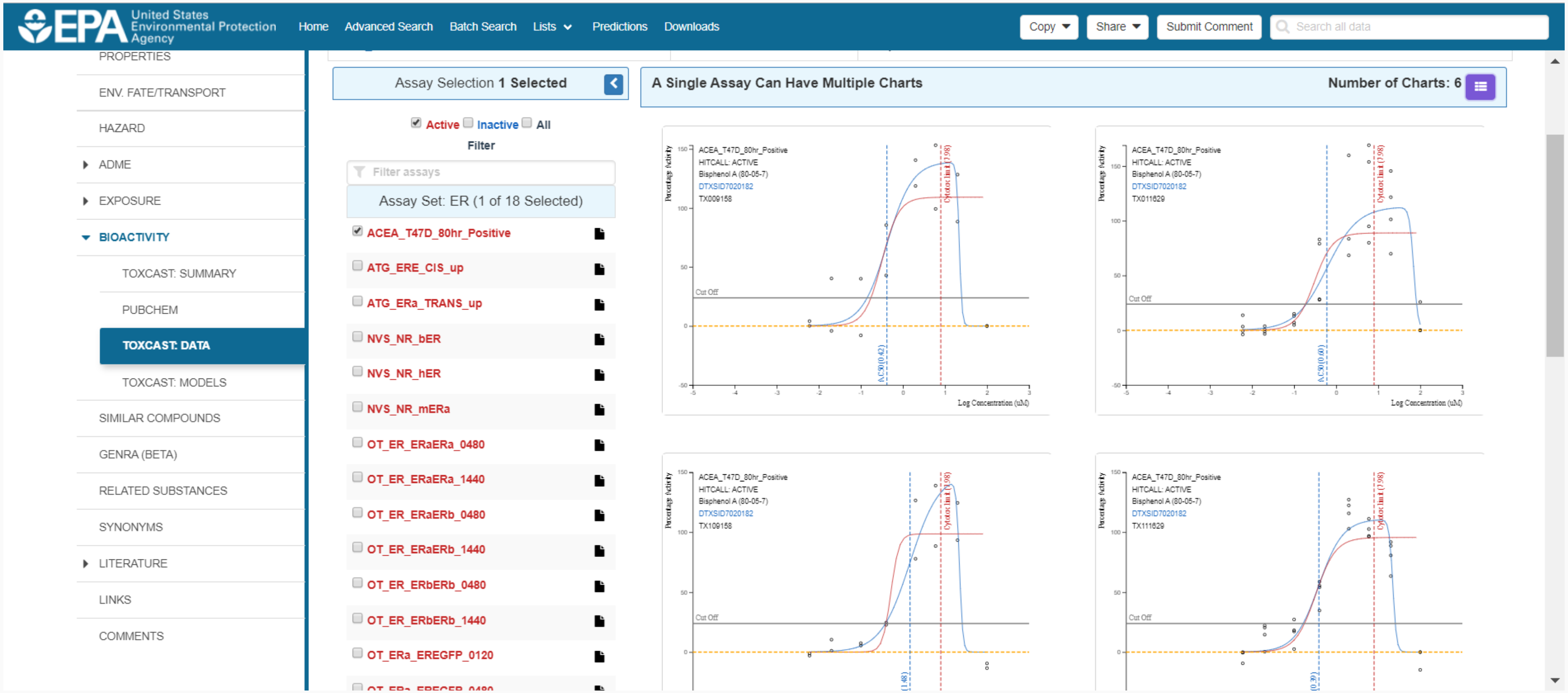


Name	Modal	Description	SeqaPASS	Gene Name	AOP	Event	Hit Call	Top	Scaled Top	AC50	logAC50	Intended Target Family
ACEA_T47D_80hr_Negative		-	-	-	-	-	ACTIVE	35.5	1.65	65.8	1.82	cell cycle
ACEA_T47D_80hr_Positive		2	NP_000116.2	ESR1	200	1181	ACTIVE	109	4.49	0.381	-0.419	nuclear receptor
APR_HepG2_CellLoss_24h_dn		-	-	-	-	-	ACTIVE	1.20	1.81	106	2.02	cell cycle
APR_HepG2_MitoMass_24h_dn		-	-	-	-	-	ACTIVE	0.874	1.76	109	2.04	cell morphology
APR_HepG2_MitoMembPot_24h_dn		-	-	-	-	-	ACTIVE	5.92	7.07	11.0	1.04	cell morphology
APR_HepG2_OxidativeStress_24h_up		-	-	-	-	-	ACTIVE	1.20	1.47	110	2.04	cell cycle
APR_HepG2_CellLoss_72h_dn		-	-	-	-	-	ACTIVE	4.49	5.05	95.2	1.98	cell cycle
APR_HepG2_MitoMembPot_72h_dn		-	-	-	-	-	ACTIVE	2.71	3.69	85.3	1.93	cell morphology
APR_HepG2_MitoticArrest_72h_up		-	-	-	-	-	ACTIVE	1.66	1.17	84.7	1.93	cell cycle
APR_HepG2_OxidativeStress_72h_up		-	-	-	-	-	ACTIVE	1.80	1.65	106	2.02	cell cycle

Showing 1 to 10 of 161 records

In Vitro Bioassay Screening

ToxCast and Tox21



Assay Selection **1 Selected**

☑ Active □ Inactive □ All

Filter

Filter assays

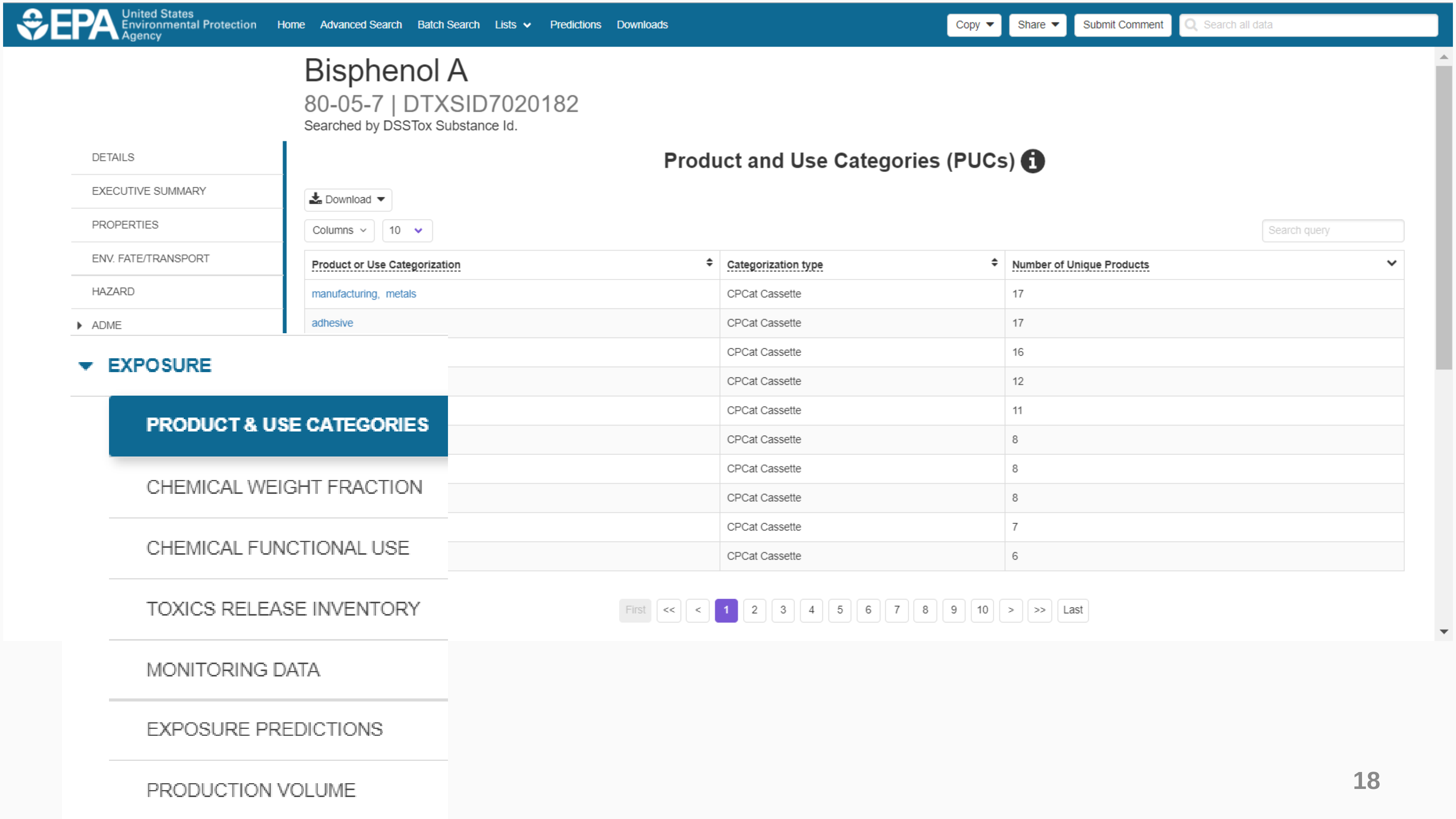
Assay Set: ER (1 of 18 Selected)

- ☑ ACEA_T47D_80hr_Positive
- □ ATG_ERE_CIS_up
- □ ATG_ERa_TRANS_up
- □ NVS_NR_bER
- □ NVS_NR_hER
- □ NVS_NR_mERa
- □ OT_ER_ERaERa_0480
- □ OT_ER_ERaERa_1440
- □ OT_ER_ERaERb_0480
- □ OT_ER_ERaERb_1440
- □ OT_ER_ERbERb_0480
- □ OT_ER_ERbERb_1440
- □ OT_ERa_EREGFP_0120
- □ OT_ERa_EREGFP_0480

A Single Assay Can Have Multiple Charts

Number of Charts: 6

Sources of Exposure to Chemicals



Bisphenol A

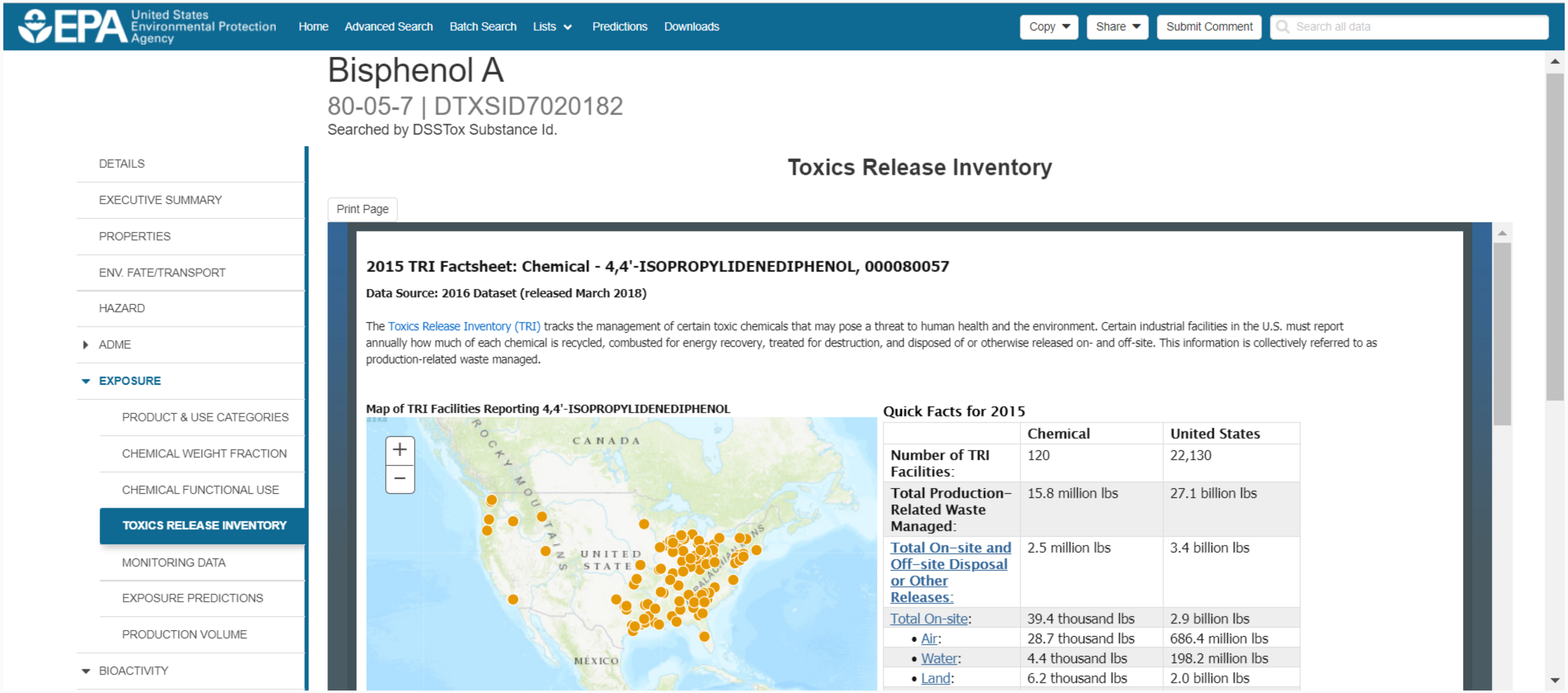
80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

Product and Use Categories (PUCs)

Product or Use Categorization	Categorization type	Number of Unique Products
manufacturing, metals	CPCat Cassette	17
adhesive	CPCat Cassette	17
	CPCat Cassette	16
	CPCat Cassette	12
	CPCat Cassette	11
	CPCat Cassette	8
	CPCat Cassette	8
	CPCat Cassette	8
	CPCat Cassette	7
	CPCat Cassette	6

Sources of Exposure to Chemicals



Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

Toxics Release Inventory

2015 TRI Factsheet: Chemical - 4,4'-ISOPROPYLIDENEDIPHENOL, 000080057

Data Source: 2016 Dataset (released March 2018)

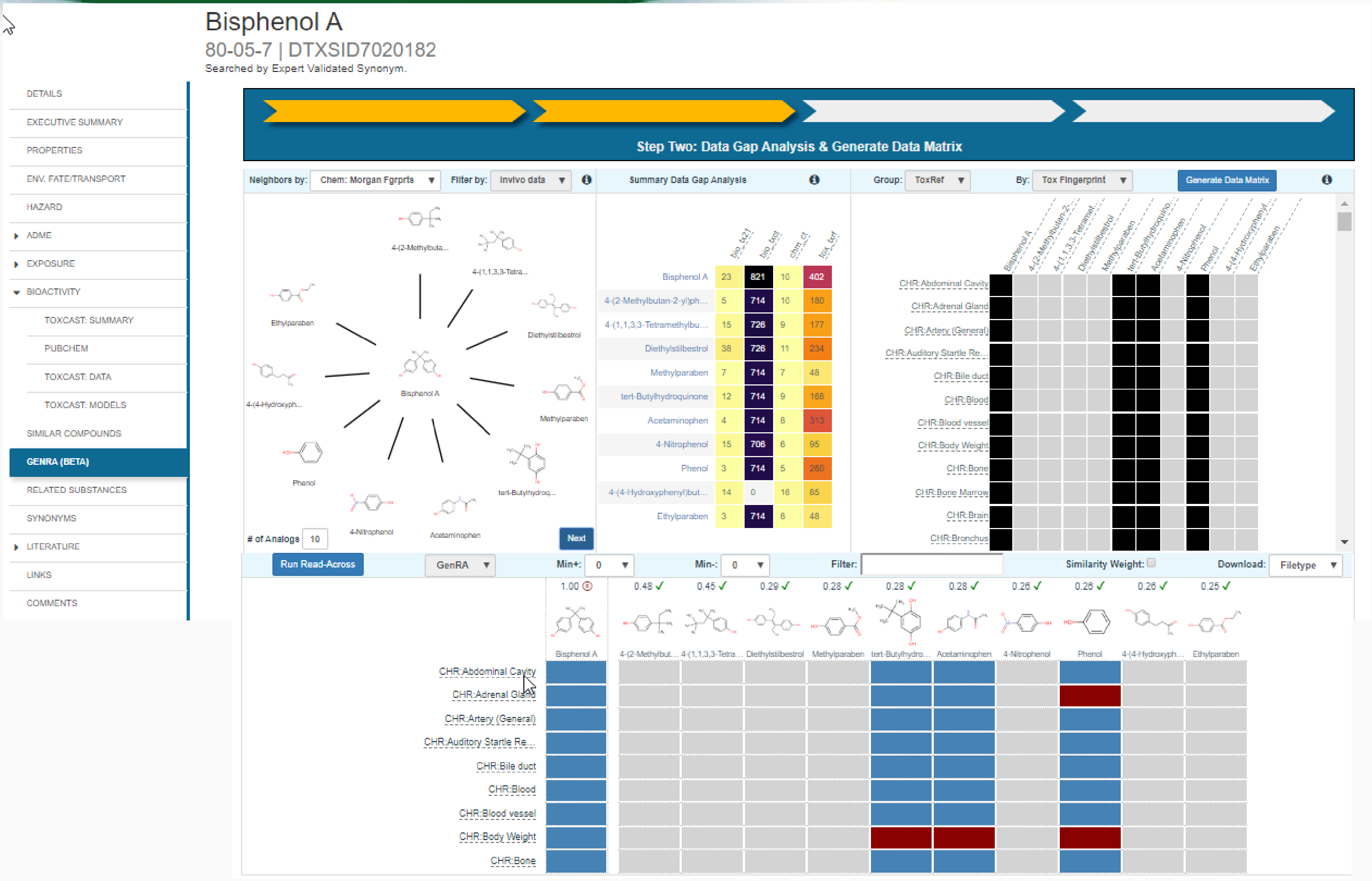
The Toxics Release Inventory (TRI) tracks the management of certain toxic chemicals that may pose a threat to human health and the environment. Certain industrial facilities in the U.S. must report annually how much of each chemical is recycled, combusted for energy recovery, treated for destruction, and disposed of or otherwise released on- and off-site. This information is collectively referred to as production-related waste managed.

Map of TRI Facilities Reporting 4,4'-ISOPROPYLIDENEDIPHENOL

Quick Facts for 2015

	Chemical	United States
Number of TRI Facilities:	120	22,130
Total Production–Related Waste Managed:	15.8 million lbs	27.1 billion lbs
Total On–site and Off–site Disposal or Other Releases:	2.5 million lbs	3.4 billion lbs
Total On-site:	39.4 thousand lbs	2.9 billion lbs
• Air:	28.7 thousand lbs	686.4 million lbs
• Water:	4.4 thousand lbs	198.2 million lbs
• Land:	6.2 thousand lbs	2.0 billion lbs

Generalized Read-Across (GenRA)



Bisphenol A

80-05-7 | DTXSID7020182

Searched by Expert Validated Synonym.

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

Step Two: Data Gap Analysis & Generate Data Matrix

Neighbors by: Chem: Morgan Fgrprts ▼ Filter by: Invivo data ▼

Summary Data Gap Analysis

Group: ToxRef ▼ By: Tox Fingerprint ▼ Generate Data Matrix

# of Analogs 10 Next

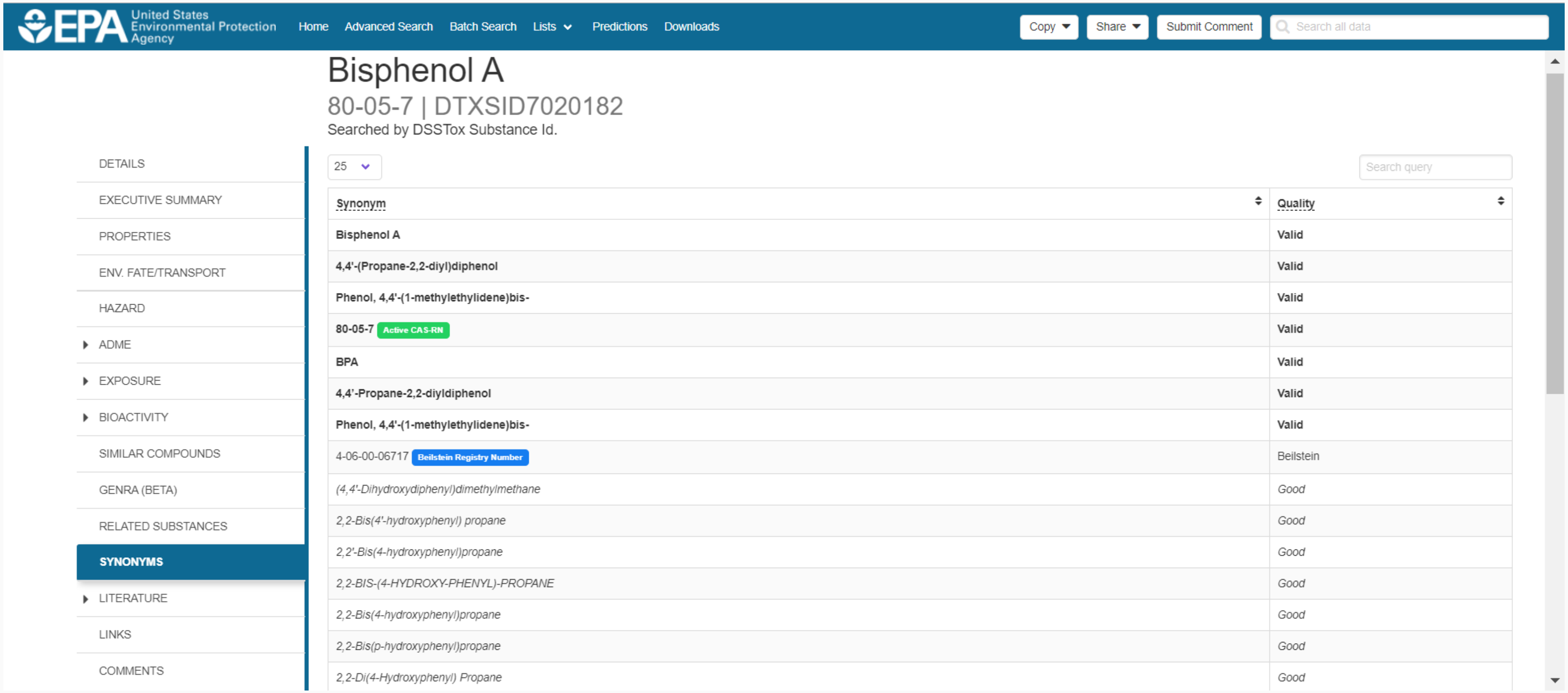
	bio_tx21	bio_txct	chm_ct	tox_txrf
Bisphenol A	23	821	10	402
4-(2-Methylbutan-2-yl)ph...	5	714	10	180
4-(1,1,3,3-Tetramethylbu...	15	726	9	177
Diethylstilbestrol	38	726	11	234
Methylparaben	7	714	7	48
tert-Butylhydroquinone	12	714	9	168
Acetaminophen	4	714	8	313
4-Nitrophenol	15	706	6	95
Phenol	3	714	5	280
4-(4-Hydroxyphenyl)but...	14	0	16	65
Ethylparaben	3	714	8	48

	Bisphenol A	4-(2-Methylbutan-2-...	4-(1,1,3,3-Tetramet...	Diethylstilbestrol	Methylparaben	tert-Butylhydroquino...	Acetaminophen	4-Nitrophenol	Phenol	4-(4-Hydroxyphenyl)...	Ethylparaben
CHR:Abdominal Cavity	■	□	□	□	□	■	■	□	■	□	□
CHR:Adrenal Gland	■	□	□	□	□	■	■	□	■	□	□
CHR:Artery (General)	■	□	□	□	□	■	■	□	■	□	□
CHR:Auditory Startle Re...	■	□	□	□	□	■	■	□	■	□	□
CHR:Bile duct	■	□	□	□	□	■	■	□	■	□	□
CHR:Blood	■	□	□	□	□	■	■	□	■	□	□
CHR:Blood vessel	■	□	□	□	□	■	■	□	■	□	□
CHR:Body Weight	■	□	□	□	□	■	■	□	■	□	□
CHR:Bone	■	□	□	□	□	■	■	□	■	□	□
CHR:Bone Marrow	■	□	□	□	□	■	■	□	■	□	□
CHR:Brain	■	□	□	□	□	■	■	□	■	□	□
CHR:Bronchus	■	□	□	□	□	■	■	□	■	□	□

Run Read-Across GenRA ▼ Min+: 0 ▼ Min-: 0 ▼ Filter: Similarity Weight: □ Download: Filetype ▼

	1.00	0.48 ✓	0.45 ✓	0.29 ✓	0.28 ✓	0.28 ✓	0.28 ✓	0.26 ✓	0.26 ✓	0.26 ✓	0.25 ✓
	Bisphenol A	4-(2-Methylbut...	4-(1,1,3,3-Tetra...	Diethylstilbestrol	Methylparaben	tert-Butylhydro...	Acetaminophen	4-Nitrophenol	Phenol	4-(4-Hydroxyph...	Ethylparaben
CHR:Abdominal Cavity	🟦	⬜	⬜	⬜	⬜	🟦	🟦	⬜	🟦	⬜	⬜
CHR:Adrenal Gland	🟦	⬜	⬜	⬜	⬜	🟦	🟦	⬜	🟥	⬜	⬜
CHR:Artery (General)	🟦	⬜	⬜	⬜	⬜	🟦	🟦	⬜	🟦	⬜	⬜
CHR:Auditory Startle Re...	🟦	⬜	⬜	⬜	⬜	🟦	🟦	⬜	🟦	⬜	⬜
CHR:Bile duct	🟦	⬜	⬜	⬜	⬜	🟦	🟦	⬜	🟦	⬜	⬜
CHR:Blood	🟦	⬜	⬜	⬜	⬜	🟦	🟦	⬜	🟦	⬜	⬜
CHR:Blood vessel	🟦	⬜	⬜	⬜	⬜	🟦	🟦	⬜	🟦	⬜	⬜
CHR:Body Weight	🟦	⬜	⬜	⬜	⬜	🟥	🟥	⬜	🟥	⬜	⬜
CHR:Bone	🟦	⬜	⬜	⬜	⬜	🟦	🟦	⬜	🟦	⬜	⬜

Identifiers to Support Searches



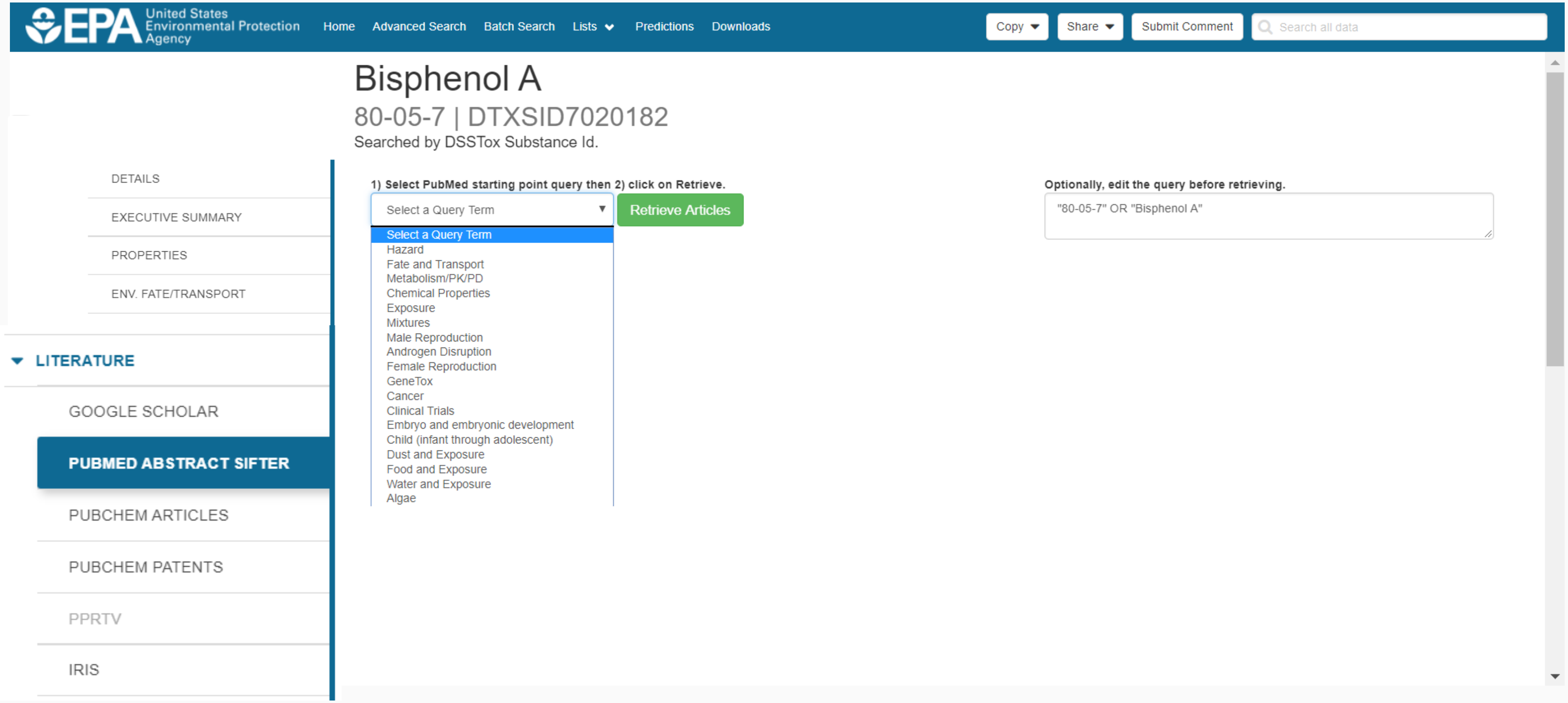
Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

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*

Literature Searches and Links



Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

1) Select PubMed starting point query then 2) click on Retrieve.

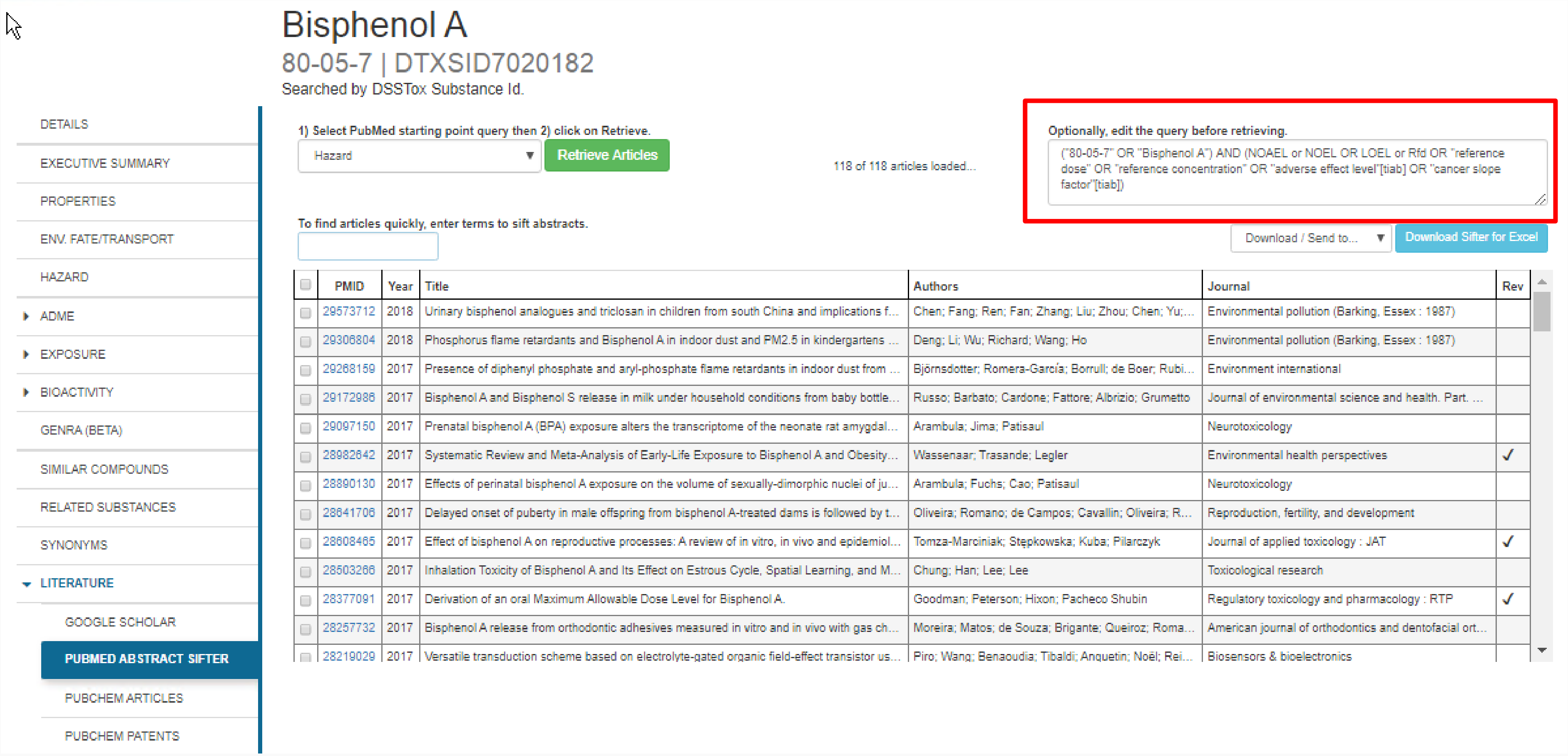
Select a Query Term

Select a Query Term
Hazard
Fate and Transport
Metabolism/PK/PD
Chemical Properties
Exposure
Mixtures
Male Reproduction
Androgen Disruption
Female Reproduction
GeneTox
Cancer
Clinical Trials
Embryo and embryonic development
Child (infant through adolescent)
Dust and Exposure
Food and Exposure
Water and Exposure
Algae

Optionally, edit the query before retrieving.

"80-05-7" OR "Bisphenol A"

Abstract Sifter – PubMed Integration



Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

1) Select PubMed starting point query then 2) click on Retrieve.

Hazard

118 of 118 articles loaded...

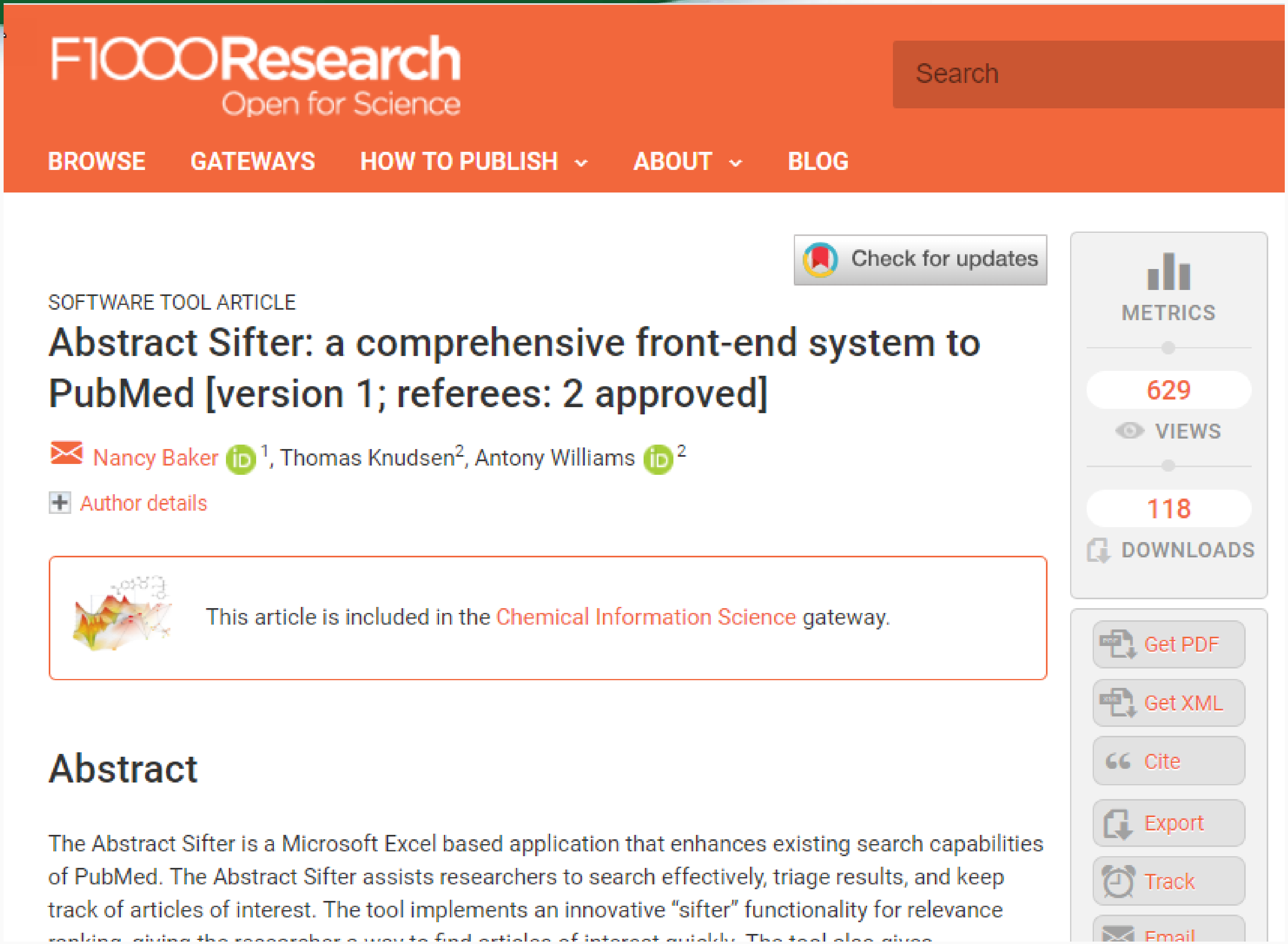
Optionally, edit the query before retrieving.

("80-05-7" OR "Bisphenol A") AND (NOAEL or NOEL OR LOEL or Rfd OR "reference dose" OR "reference concentration" OR "adverse effect level"[tiab] OR "cancer slope factor"[tiab])

To find articles quickly, enter terms to sift abstracts.

□	PMID	Year	Title	Authors	Journal	Rev
□	29573712	2018	Urinary bisphenol analogues and triclosan in children from south China and implications f...	Chen; Fang; Ren; Fan; Zhang; Liu; Zhou; Chen; Yu;...	Environmental pollution (Barking, Essex : 1987)	
□	29306804	2018	Phosphorus flame retardants and Bisphenol A in indoor dust and PM2.5 in kindergartens ...	Deng; Li; Wu; Richard; Wang; Ho	Environmental pollution (Barking, Essex : 1987)	
□	29268159	2017	Presence of diphenyl phosphate and aryl-phosphate flame retardants in indoor dust from ...	Björnsdotter; Romera-García; Borrull; de Boer; Rubi...	Environment international	
□	29172986	2017	Bisphenol A and Bisphenol S release in milk under household conditions from baby bottle...	Russo; Barbato; Cardone; Fattore; Albrizio; Grumetto	Journal of environmental science and health. Part. ...	
□	29097150	2017	Prenatal bisphenol A (BPA) exposure alters the transcriptome of the neonate rat amygdal...	Arambula; Jima; Patisaul	Neurotoxicology	
□	28982642	2017	Systematic Review and Meta-Analysis of Early-Life Exposure to Bisphenol A and Obesity...	Wassenaar; Trasande; Legler	Environmental health perspectives	✓
□	28890130	2017	Effects of perinatal bisphenol A exposure on the volume of sexually-dimorphic nuclei of ju...	Arambula; Fuchs; Cao; Patisaul	Neurotoxicology	
□	28641706	2017	Delayed onset of puberty in male offspring from bisphenol A-treated dams is followed by t...	Oliveira; Romano; de Campos; Cavallin; Oliveira; R...	Reproduction, fertility, and development	
□	28608465	2017	Effect of bisphenol A on reproductive processes: A review of in vitro, in vivo and epidemiol...	Tomza-Marciniak; Stępkowska; Kuba; Pilarczyk	Journal of applied toxicology : JAT	✓
□	28503266	2017	Inhalation Toxicity of Bisphenol A and Its Effect on Estrous Cycle, Spatial Learning, and M...	Chung; Han; Lee; Lee	Toxicological research	
□	28377091	2017	Derivation of an oral Maximum Allowable Dose Level for Bisphenol A.	Goodman; Peterson; Hixon; Pacheco Shubin	Regulatory toxicology and pharmacology : RTP	✓
□	28257732	2017	Bisphenol A release from orthodontic adhesives measured in vitro and in vivo with gas ch...	Moreira; Matos; de Souza; Brigante; Queiroz; Roma...	American journal of orthodontics and dentofacial ort...	
□	28219029	2017	Versatile transduction scheme based on electrolyte-gated organic field-effect transistor us...	Piro; Wang; Benaoudia; Tibaldi; Anquetin; Noël; Rei...	Biosensors & bioelectronics	

Abstract Sifter for Excel



SOFTWARE TOOL ARTICLE

Abstract Sifter: a comprehensive front-end system to PubMed [version 1; referees: 2 approved]

Nancy Baker [1], Thomas Knudsen[2], Antony Williams [2]

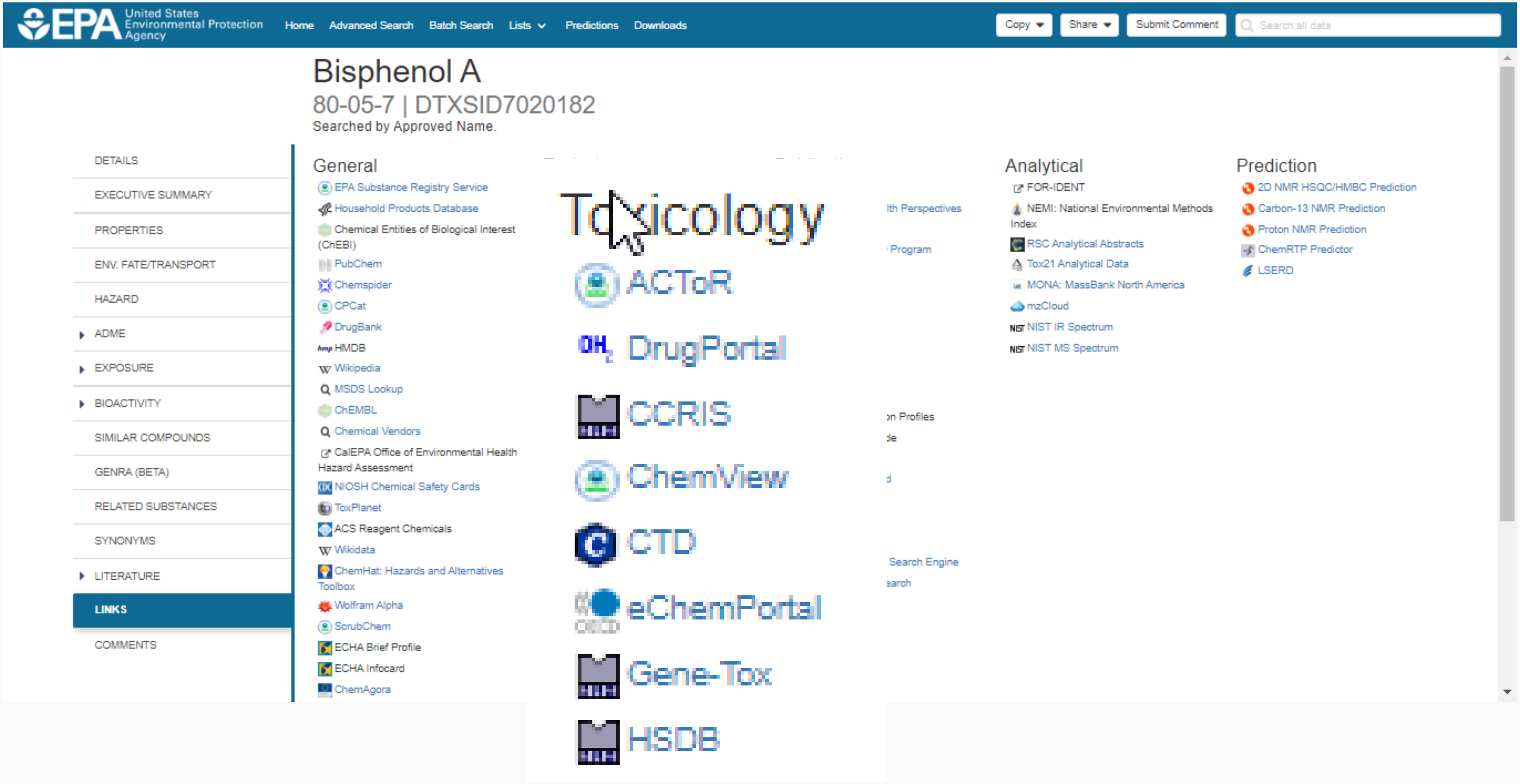
Author details

This article is included in the Chemical Information Science gateway.

Abstract

The Abstract Sifter is a Microsoft Excel based application that enhances existing search capabilities of PubMed. The Abstract Sifter assists researchers to search effectively, triage results, and keep track of articles of interest. The tool implements an innovative "sifter" functionality for relevance ranking, giving the researcher a way to find articles of interest quickly. The tool also gives

External Links to ~80 websites



Bisphenol A

80-05-7 | DTXSID7020182

Searched by Approved Name.

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
- ECHA Infocard
- ChemAgora

Toxicology

- ACToR
- DrugPortal
- CCRIS
- ChemView
- CTD
- eChemPortal
- Gene-Tox
- HSDB

lth Perspectives

Program

on Profiles

de

d

Search Engine

earch

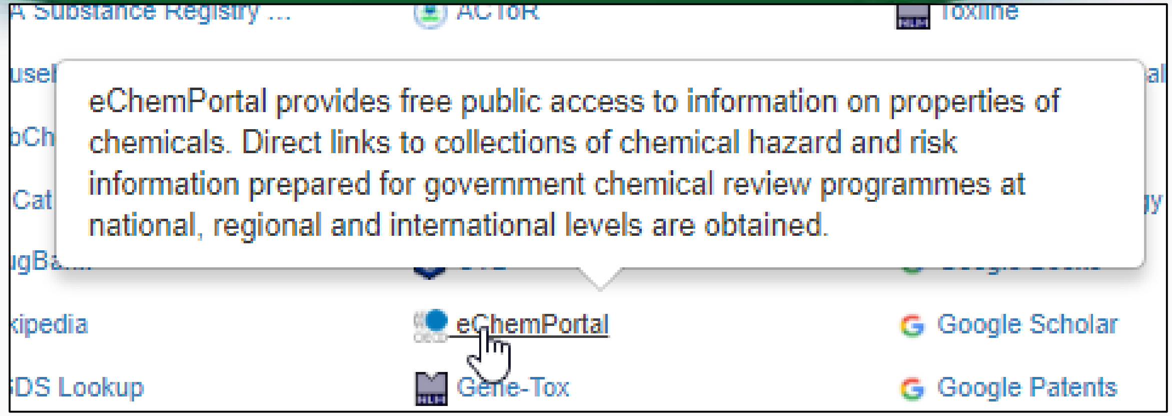
Analytical

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

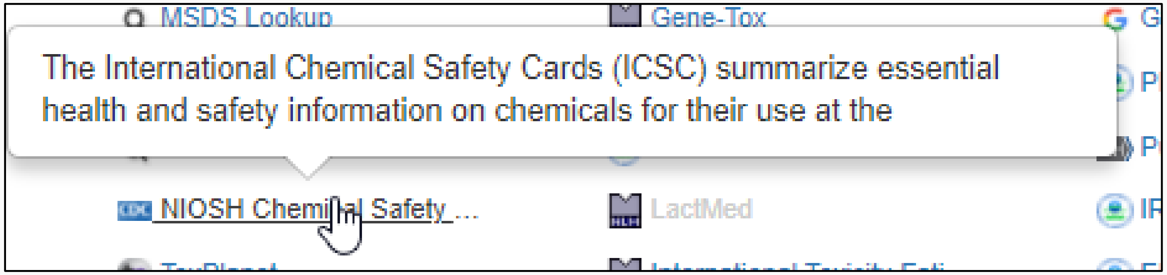
Prediction

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

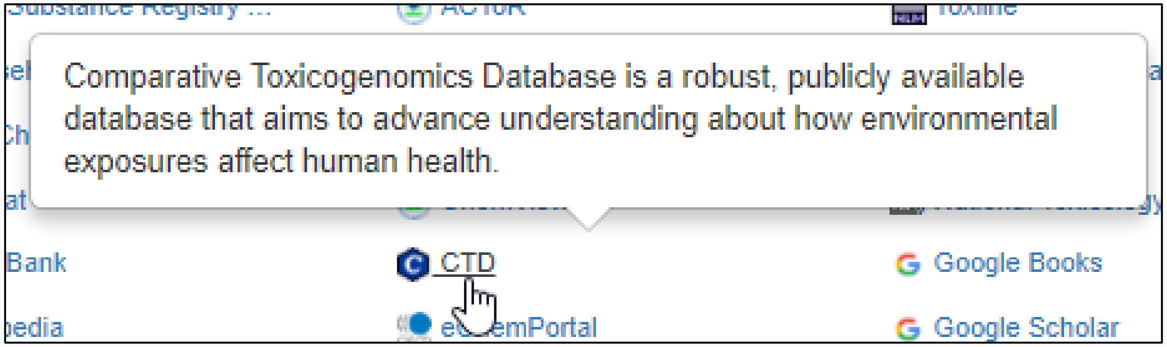
Integrated Linkouts



eChemPortal provides free public access to information on properties of chemicals. Direct links to collections of chemical hazard and risk information prepared for government chemical review programmes at national, regional and international levels are obtained.



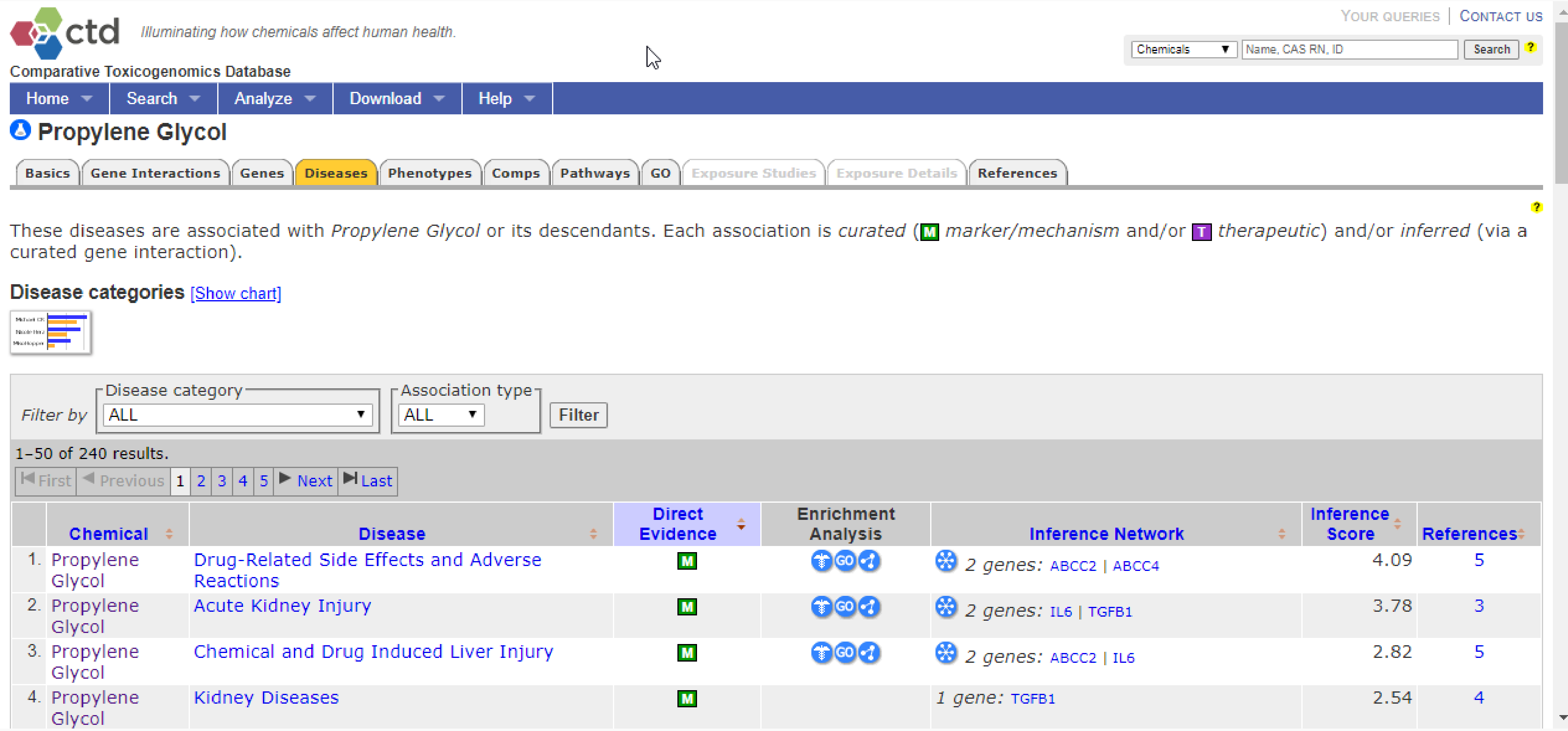
The International Chemical Safety Cards (ICSC) summarize essential health and safety information on chemicals for their use at the



Comparative Toxicogenomics Database is a robust, publicly available database that aims to advance understanding about how environmental exposures affect human health.

Integrated Linkouts

Comparative Toxicogenomics DB



ctd
Illuminating how chemicals affect human health.
Comparative Toxicogenomics Database
YOUR QUERIES | CONTACT US
Chemicals ▾ | Name, CAS RN, ID | Search
Home ▾ | Search ▾ | Analyze ▾ | Download ▾ | Help ▾
Basics | Gene Interactions | Genes | Diseases | Phenotypes | Comps | Pathways | GO | Exposure Studies | Exposure Details | References

Propylene Glycol

These diseases are associated with *Propylene Glycol* or its descendants. Each association is *curated* (M *marker/mechanism* and/or T *therapeutic*) and/or *inferred* (via a curated gene interaction).

Disease categories [Show chart]

Filter by Disease category: ALL ▾ Association type: ALL ▾ Filter

1–50 of 240 results.

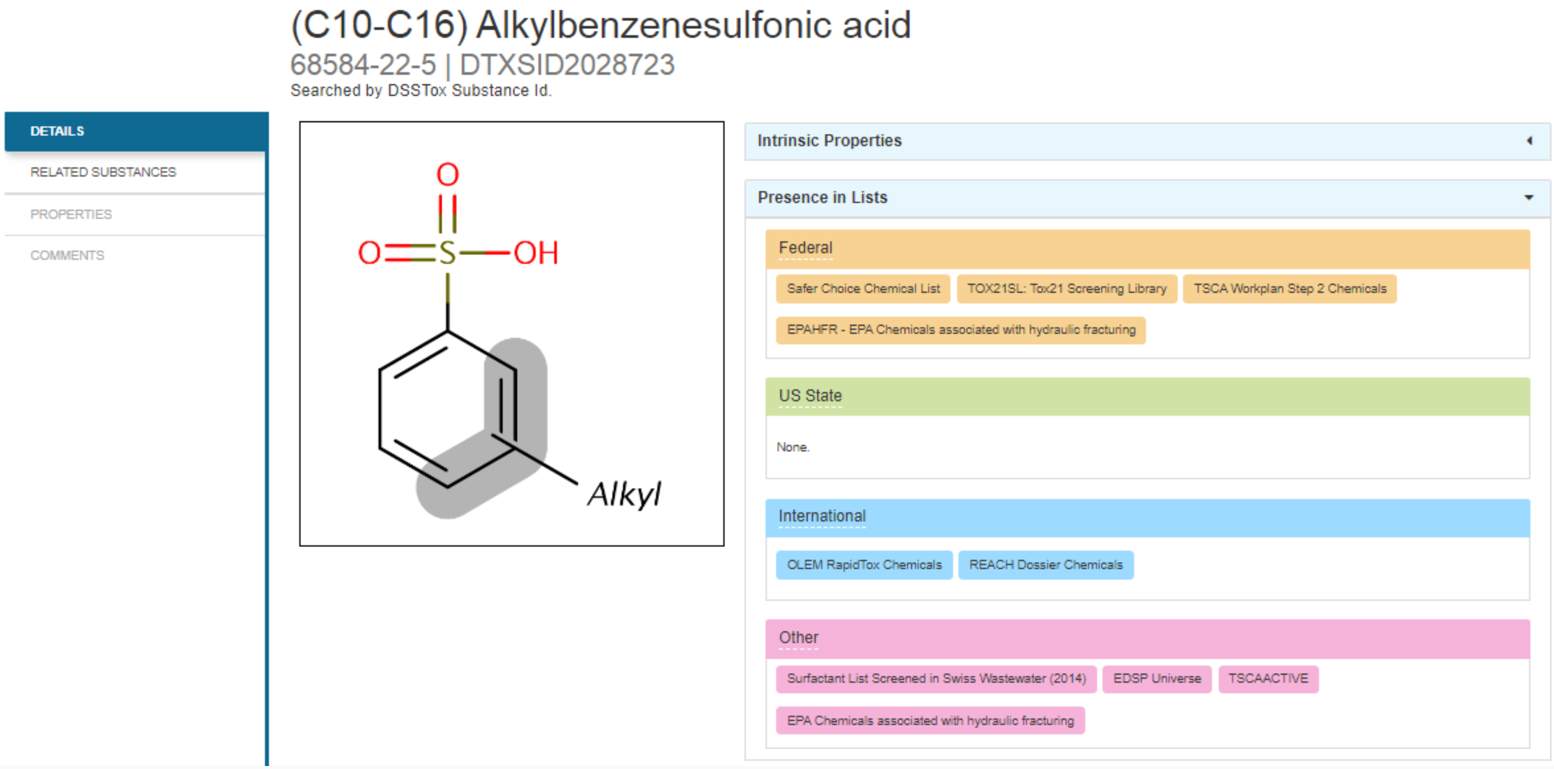
First | Previous | 1 | 2 | 3 | 4 | 5 | Next | Last

	Chemical	Disease	Direct Evidence	Enrichment Analysis	Inference Network	Inference Score	References
1.	Propylene Glycol	Drug-Related Side Effects and Adverse Reactions	M	GO	*2 genes:* ABCC2 | ABCC4	4.09	5
2.	Propylene Glycol	Acute Kidney Injury	M	GO	*2 genes:* IL6 | TGFB1	3.78	3
3.	Propylene Glycol	Chemical and Drug Induced Liver Injury	M	GO	*2 genes:* ABCC2 | IL6	2.82	5
4.	Propylene Glycol	Kidney Diseases	M		*1 gene:* TGFB1	2.54	4

Not just chemical “structures”

- Chemicals in commerce, of interest to the EPA, are not all easily represented by structures
- Different chemical substances supported
  - Chemical structures
  - “UVCB chemicals” - Unknown or Variable Composition, Complex Reaction Products and Biological Materials
  - Metabolites and transformation products
  - Homologous series as Markush Structures
  - Curated classes of chemicals

UVCB Chemicals



(C10-C16) Alkylbenzenesulfonic acid

68584-22-5 | DTXSID2028723

Searched by DSSTox Substance Id.

- DETAILS
- RELATED SUBSTANCES
- PROPERTIES
- COMMENTS

Intrinsic Properties

Presence in Lists

Federal

Safer Choice Chemical List | TOX21SL: Tox21 Screening Library | TSCA Workplan Step 2 Chemicals | EPAHFR - EPA Chemicals associated with hydraulic fracturing

US State

None.

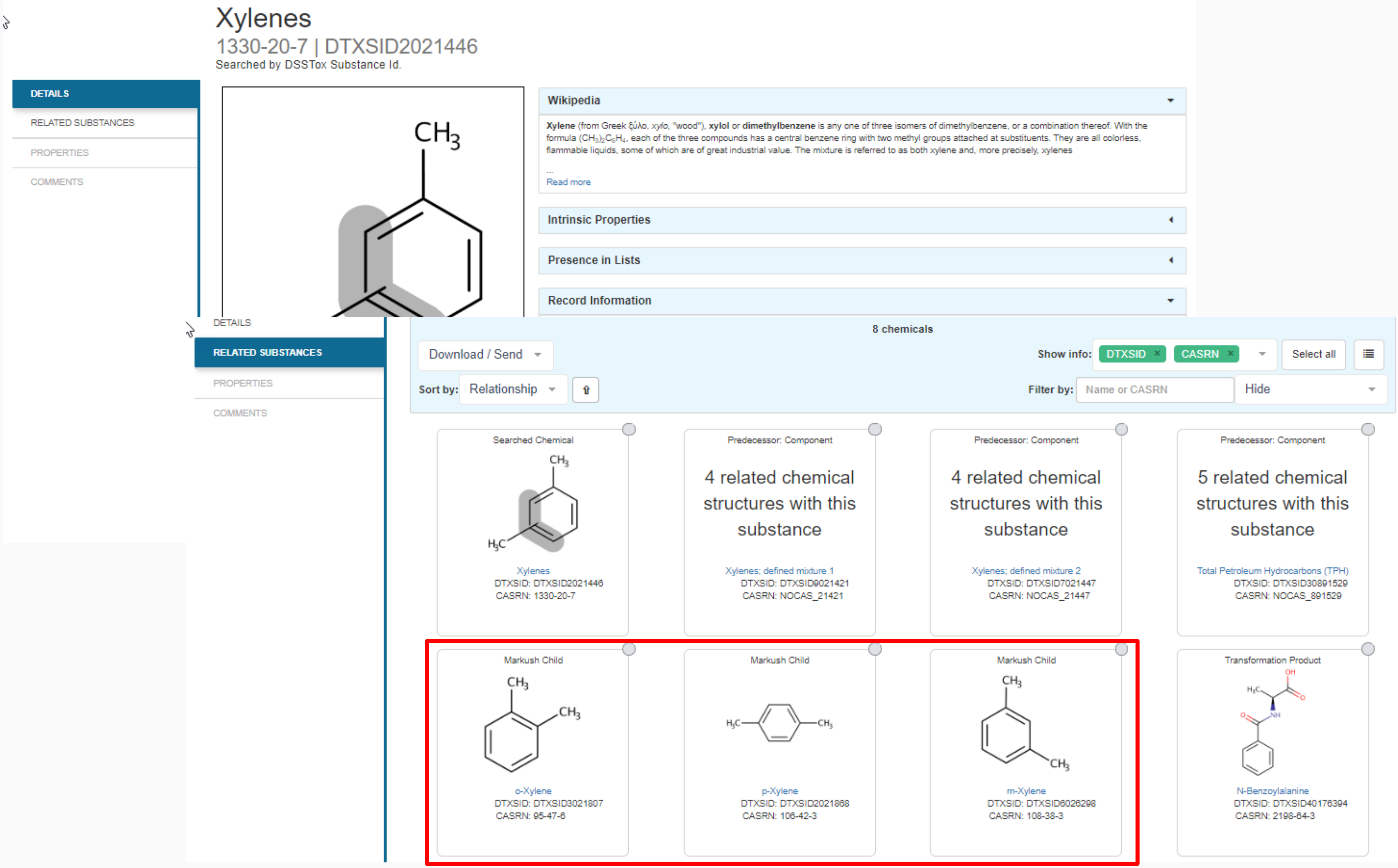
International

OLEM RapidTox Chemicals | REACH Dossier Chemicals

Other

Surfactant List Screened in Swiss Wastewater (2014) | EDSP Universe | TSCAACTIVE | EPA Chemicals associated with hydraulic fracturing

Markush Structures



Xylenes

1330-20-7 | DTXSID2021446

Searched by DSSTox Substance Id.

DETAILS
RELATED SUBSTANCES
PROPERTIES
COMMENTS

Wikipedia

Xylene (from Greek ξύλο, *xylo*, "wood"), **xylol** or **dimethylbenzene** is any one of three isomers of dimethylbenzene, or a combination thereof. With the formula $(CH_3)_2C_6H_4$, each of the three compounds has a central benzene ring with two methyl groups attached at substituents. They are all colorless, flammable liquids, some of which are of great industrial value. The mixture is referred to as both xylene and, more precisely, xylenes

...
Read more

Intrinsic Properties

Presence in Lists

Record Information

DETAILS
RELATED SUBSTANCES
PROPERTIES
COMMENTS

8 chemicals

Download / Send

Show info: DTXSID × CASRN × | Select all

Sort by: Relationship

Filter by: Name or CASRN | Hide

Searched Chemical
Xylenes
DTXSID: DTXSID2021446
CASRN: 1330-20-7

Predecessor: Component
4 related chemical structures with this substance
Xylenes; defined mixture 1
DTXSID: DTXSID9021421
CASRN: NOCAS_21421

Predecessor: Component
4 related chemical structures with this substance
Xylenes; defined mixture 2
DTXSID: DTXSID7021447
CASRN: NOCAS_21447

Predecessor: Component
5 related chemical structures with this substance
Total Petroleum Hydrocarbons (TPH)
DTXSID: DTXSID30891529
CASRN: NOCAS_891529

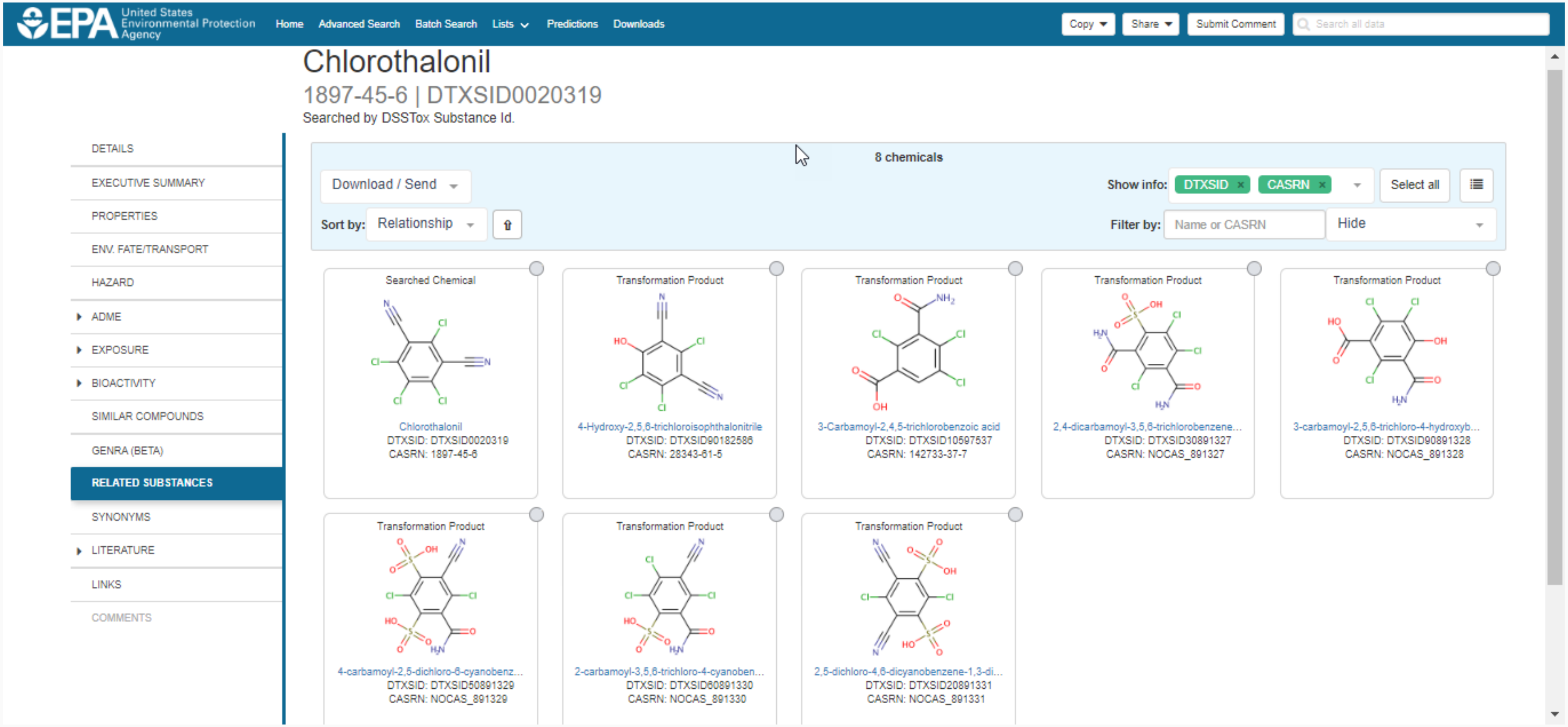
Markush Child
o-Xylene
DTXSID: DTXSID3021807
CASRN: 95-47-6

Markush Child
p-Xylene
DTXSID: DTXSID2021868
CASRN: 106-42-3

Markush Child
m-Xylene
DTXSID: DTXSID6026298
CASRN: 108-38-3

Transformation Product
N-Benzoylalanine
DTXSID: DTXSID40176394
CASRN: 2198-64-3

Transformation Products



Chlorothalonil

1897-45-6 | DTXSID0020319

Searched by DSSTox Substance Id.

8 chemicals

Sort by: Relationship

Filter by:

Searched Chemical
Chlorothalonil
DTXSID: DTXSID0020319
CASRN: 1897-45-6

Transformation Product
4-Hydroxy-2,5,6-trichloroisophthalonitrile
DTXSID: DTXSID90182586
CASRN: 28343-61-5

Transformation Product
3-Carbamoyl-2,4,5-trichlorobenzoic acid
DTXSID: DTXSID10597537
CASRN: 142733-37-7

Transformation Product
2,4-dicarbamoyl-3,5,6-trichlorobenzene...
DTXSID: DTXSID30891327
CASRN: NOCAS_891327

Transformation Product
3-carbamoyl-2,5,6-trichloro-4-hydroxyb...
DTXSID: DTXSID90891328
CASRN: NOCAS_891328

Transformation Product
4-carbamoyl-2,5-dichloro-6-cyanobenz...
DTXSID: DTXSID50891329
CASRN: NOCAS_891329

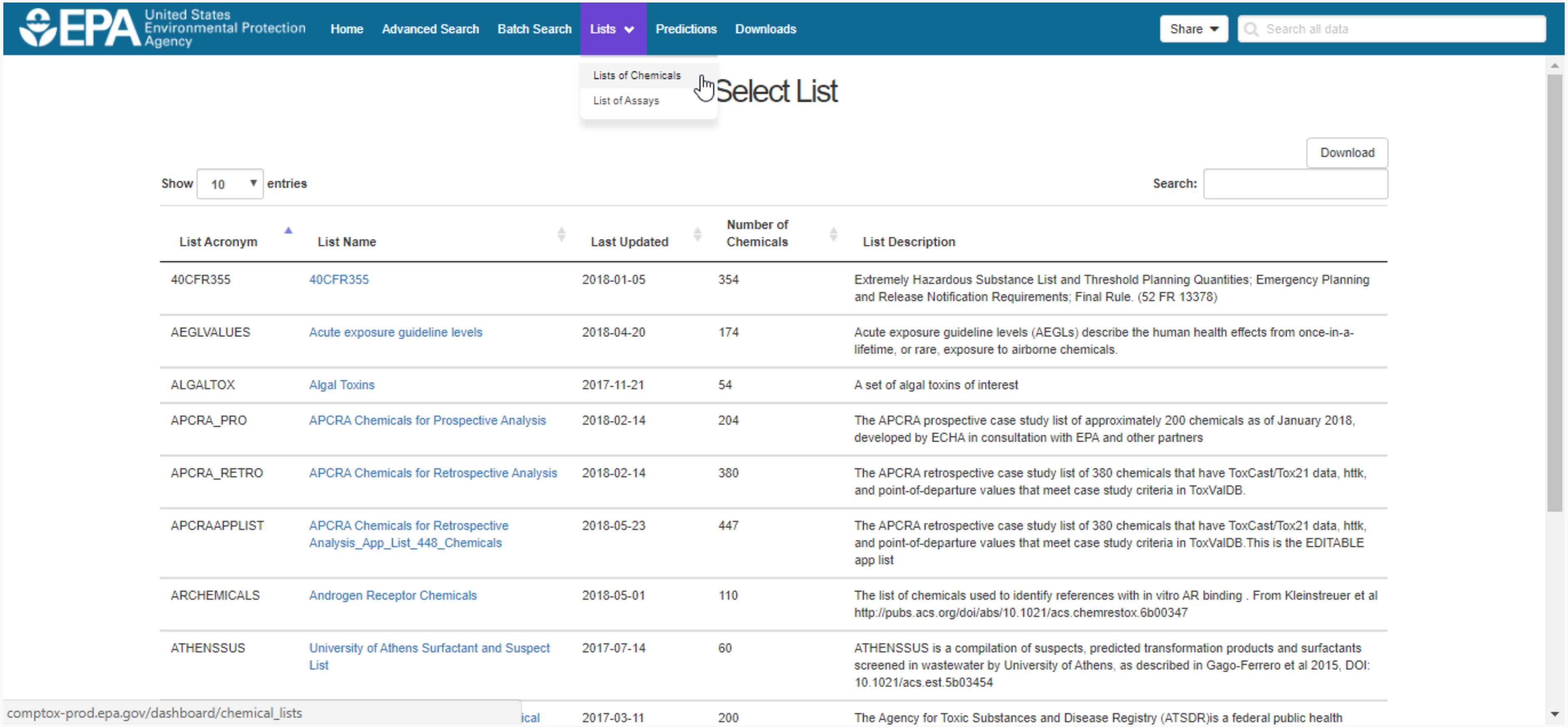
Transformation Product
2-carbamoyl-3,5,6-trichloro-4-cyanoben...
DTXSID: DTXSID60891330
CASRN: NOCAS_891330

Transformation Product
2,5-dichloro-4,6-dicyanobenzene-1,3-di...
DTXSID: DTXSID20891331
CASRN: NOCAS_891331

Not just chemical "structures"

- Different chemical substances supported
  - Chemical structures
  - "UVCB chemicals" - Unknown or Variable Composition, Complex Reaction Products and Biological Materials
  - Metabolites and transformation products
  - Homologous series as Markush Structures
  - Curated classes of chemicals
- Lists of chemicals
  - Submitted lists of chemicals – Federal, State, International and other general lists
  - Growing lists to support specific projects – e.g. ToxCast phases, algal toxins, our publication datasets

List of Chemicals



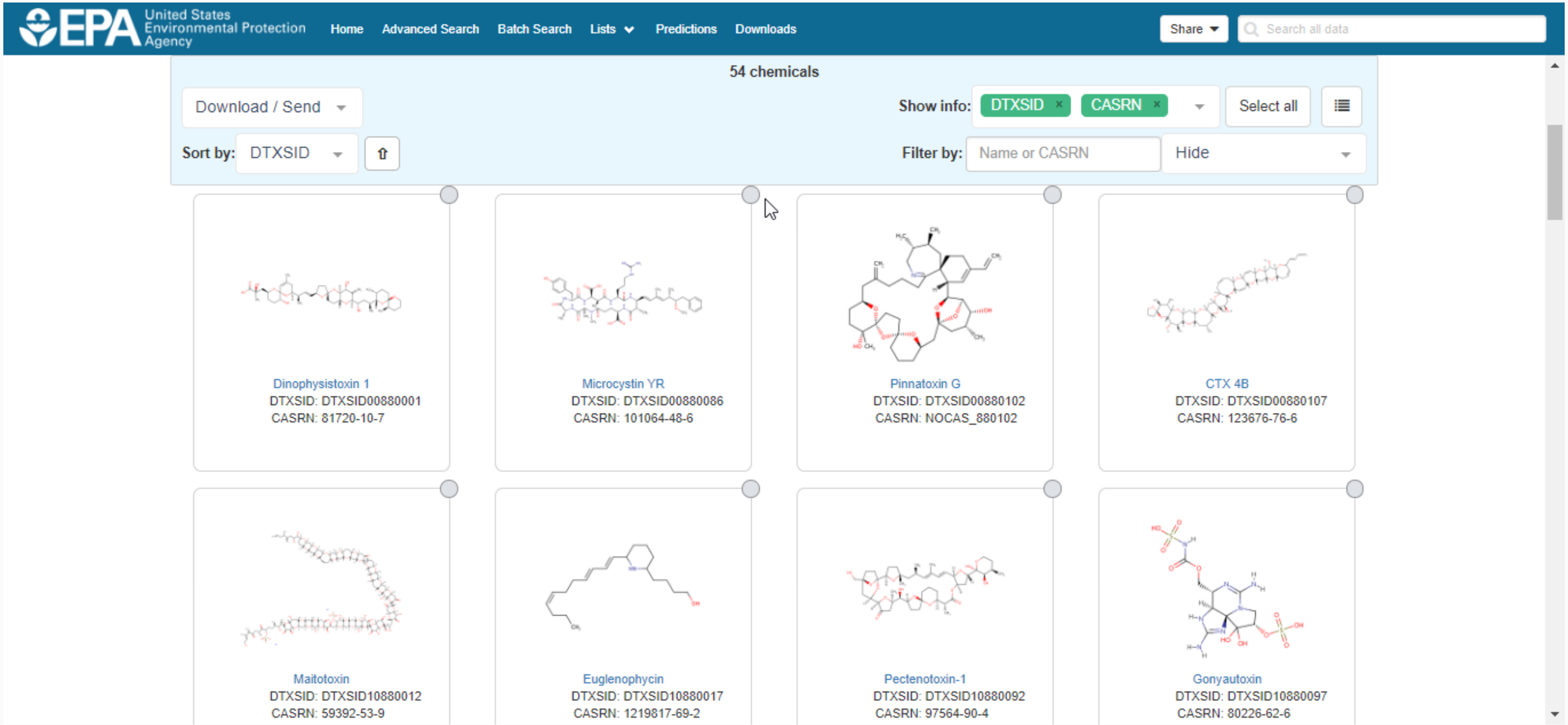
Select List

Show 10 entries

Search:

List Acronym	List Name	Last Updated	Number of Chemicals	List Description
40CFR355	40CFR355	2018-01-05	354	Extremely Hazardous Substance List and Threshold Planning Quantities; Emergency Planning and Release Notification Requirements; Final Rule. (52 FR 13378)
AEGLVALUES	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	Algal Toxins	2017-11-21	54	A set of algal toxins of interest
APCRA_PRO	APCRA Chemicals for Prospective Analysis	2018-02-14	204	The APCRA prospective case study list of approximately 200 chemicals as of January 2018, developed by ECHA in consultation with EPA and other partners
APCRA_RETRO	APCRA Chemicals for Retrospective Analysis	2018-02-14	380	The APCRA retrospective case study list of 380 chemicals that have ToxCast/Tox21 data, httk, and point-of-departure values that meet case study criteria in ToxValDB.
APCRAAPPLIST	APCRA Chemicals for Retrospective Analysis_App_List_448_Chemicals	2018-05-23	447	The APCRA retrospective case study list of 380 chemicals that have ToxCast/Tox21 data, httk, and point-of-departure values that meet case study criteria in ToxValDB.This is the EDITABLE app list
ARCHEMICALS	Androgen Receptor Chemicals	2018-05-01	110	The list of chemicals used to identify references with in vitro AR binding . From Kleinstreuer et al http://pubs.acs.org/doi/abs/10.1021/acs.chemrestox.6b00347
ATHENSSUS	University of Athens Surfactant and Suspect List	2017-07-14	60	ATHENSSUS is a compilation of suspects, predicted transformation products and surfactants screened in wastewater by University of Athens, as described in Gago-Ferrero et al 2015, DOI: 10.1021/acs.est.5b03454
	ical	2017-03-11	200	The Agency for Toxic Substances and Disease Registry (ATSDR)is a federal public health

Algal Toxins

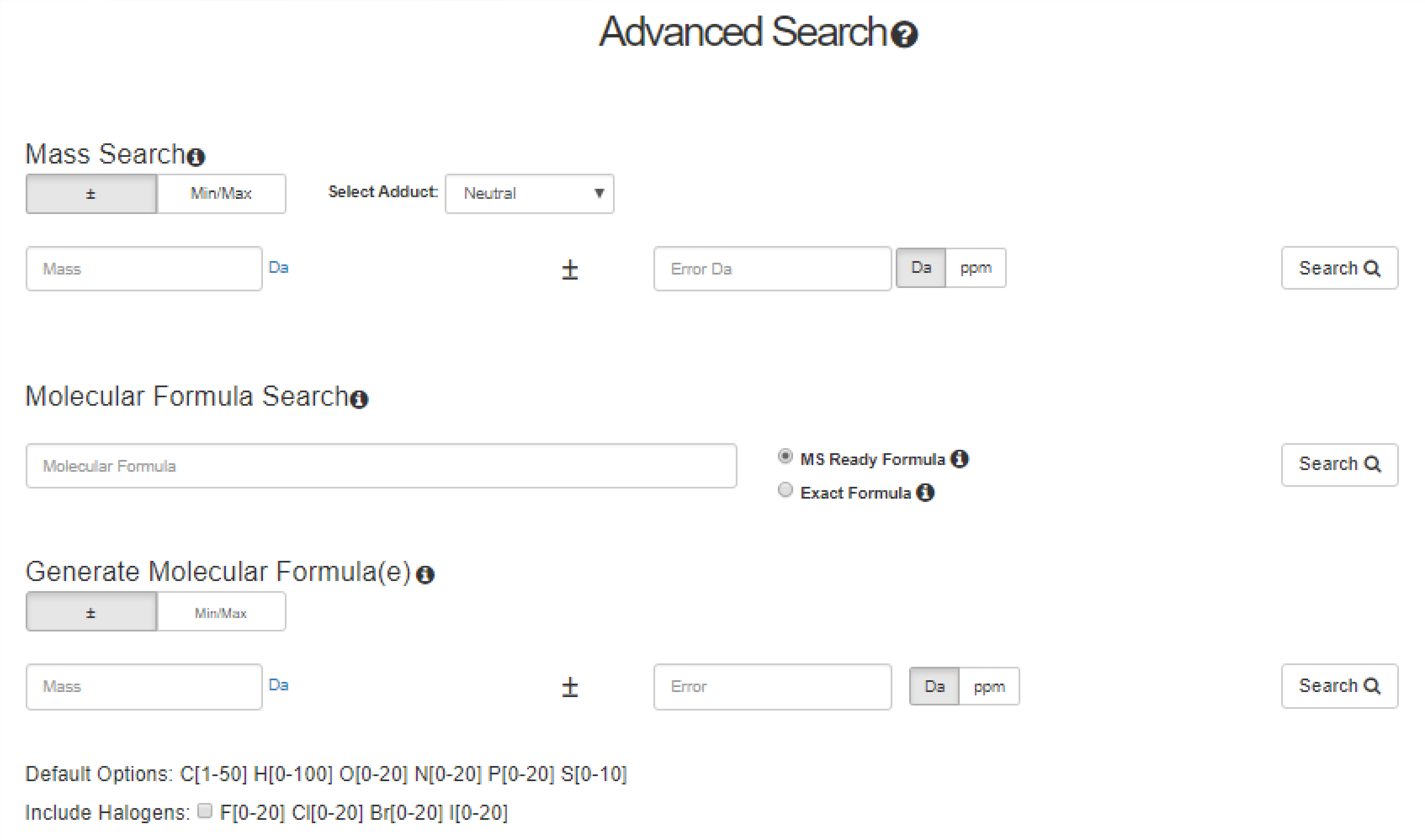


54 chemicals

Show info: DTXSID × CASRN ×

Dinophysistoxin 1 DTXSID: DTXSID00880001 CASRN: 81720-10-7	Microcystin YR DTXSID: DTXSID00880086 CASRN: 101064-48-6	Pinnatoxin G DTXSID: DTXSID00880102 CASRN: NOCAS_880102	CTX 4B DTXSID: DTXSID00880107 CASRN: 123676-76-6
Maitotoxin DTXSID: DTXSID10880012 CASRN: 59392-53-9	Euglenophycin DTXSID: DTXSID10880017 CASRN: 1219817-69-2	Pectenotoxin-1 DTXSID: DTXSID10880092 CASRN: 97564-90-4	Gonyautoxin DTXSID: DTXSID10880097 CASRN: 80226-62-6

Mass and Formula Searches Supporting Mass Spectrometry



Advanced Search

Mass Search

± | Min/Max

Select Adduct: Neutral

Molecular Formula Search

● MS Ready Formula

○ Exact Formula

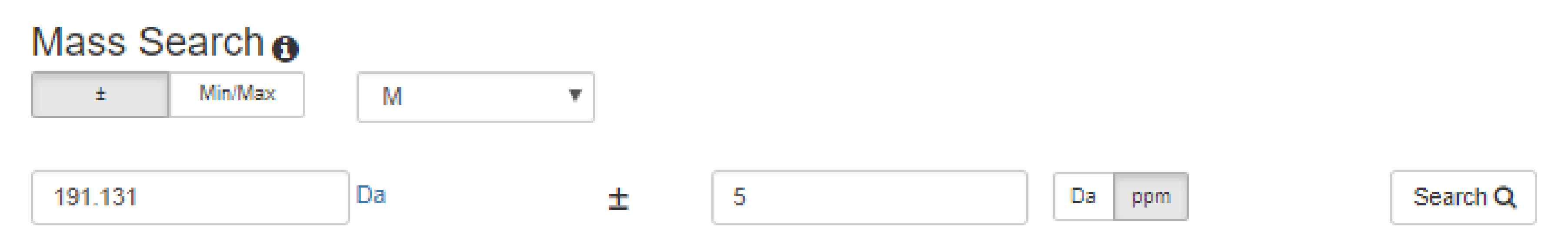
Generate Molecular Formula(e)

± | Min/Max

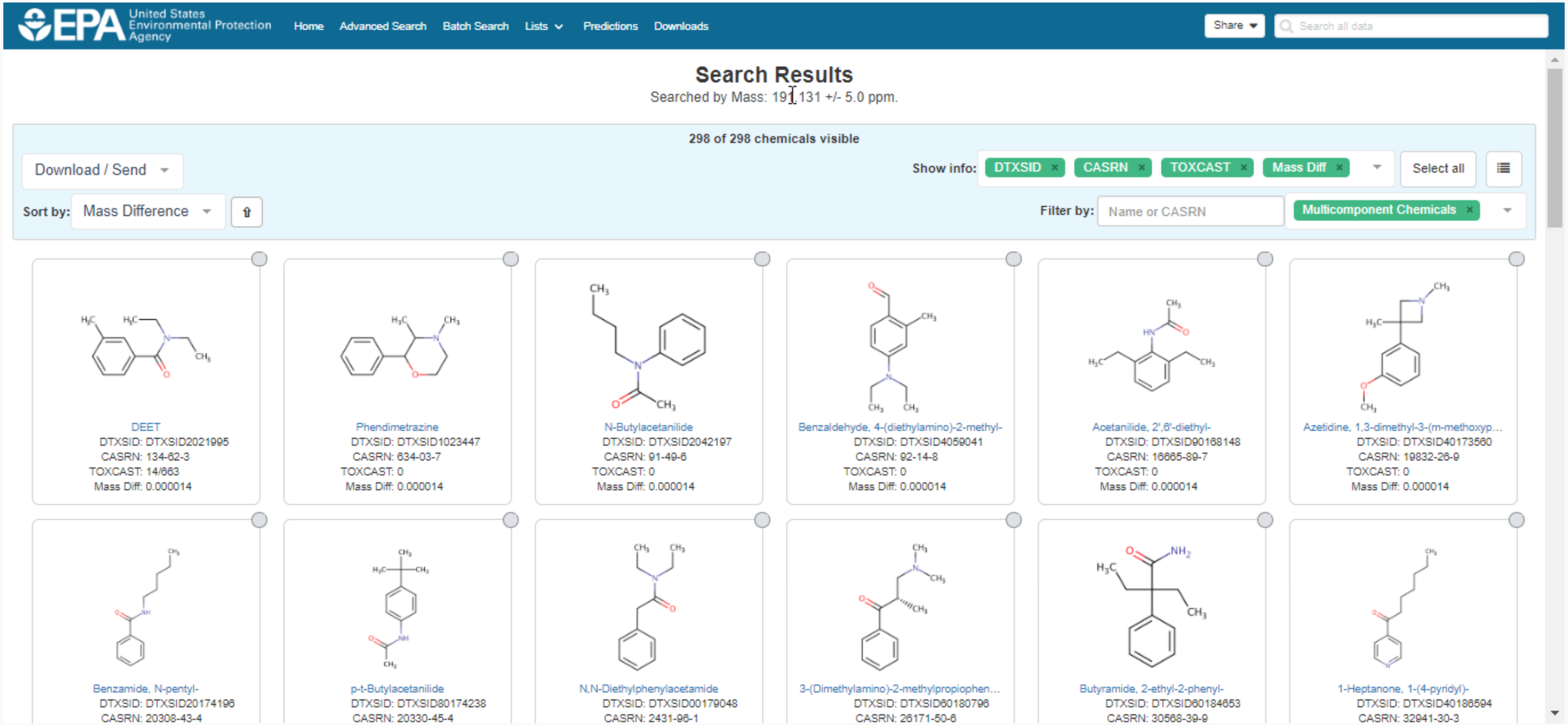
Default Options: C[1-50] H[0-100] O[0-20] N[0-20] P[0-20] S[0-10]

Include Halogens: □ F[0-20] Cl[0-20] Br[0-20] I[0-20]

Advanced Searches
Mass Based Search



191.131 Da ± 5 ppm



Search Results

Searched by Mass: 191.131 +/- 5.0 ppm.

298 of 298 chemicals visible

Download / Send
Show info: DTXSID × CASRN × TOXCAST × Mass Diff ×
Select all
Sort by: Mass Difference
Filter by: Name or CASRN
Multicomponent Chemicals ×

DEET
DTXSID: DTXSID2021995
CASRN: 134-62-3
TOXCAST: 14/663
Mass Diff: 0.000014

Phendimetrazine
DTXSID: DTXSID1023447
CASRN: 634-03-7
TOXCAST: 0
Mass Diff: 0.000014

N-Butylacetanilide
DTXSID: DTXSID2042197
CASRN: 91-49-6
TOXCAST: 0
Mass Diff: 0.000014

Benzaldehyde, 4-(diethylamino)-2-methyl-
DTXSID: DTXSID4059041
CASRN: 92-14-8
TOXCAST: 0
Mass Diff: 0.000014

Acetanilide, 2',6'-diethyl-
DTXSID: DTXSID90168148
CASRN: 16665-89-7
TOXCAST: 0
Mass Diff: 0.000014

Azetidine, 1,3-dimethyl-3-(m-methoxyp...
DTXSID: DTXSID40173560
CASRN: 19832-26-9
TOXCAST: 0
Mass Diff: 0.000014

Benzamide, N-pentyl-
DTXSID: DTXSID20174196
CASRN: 20308-43-4

p-t-Butylacetanilide
DTXSID: DTXSID80174238
CASRN: 20330-45-4

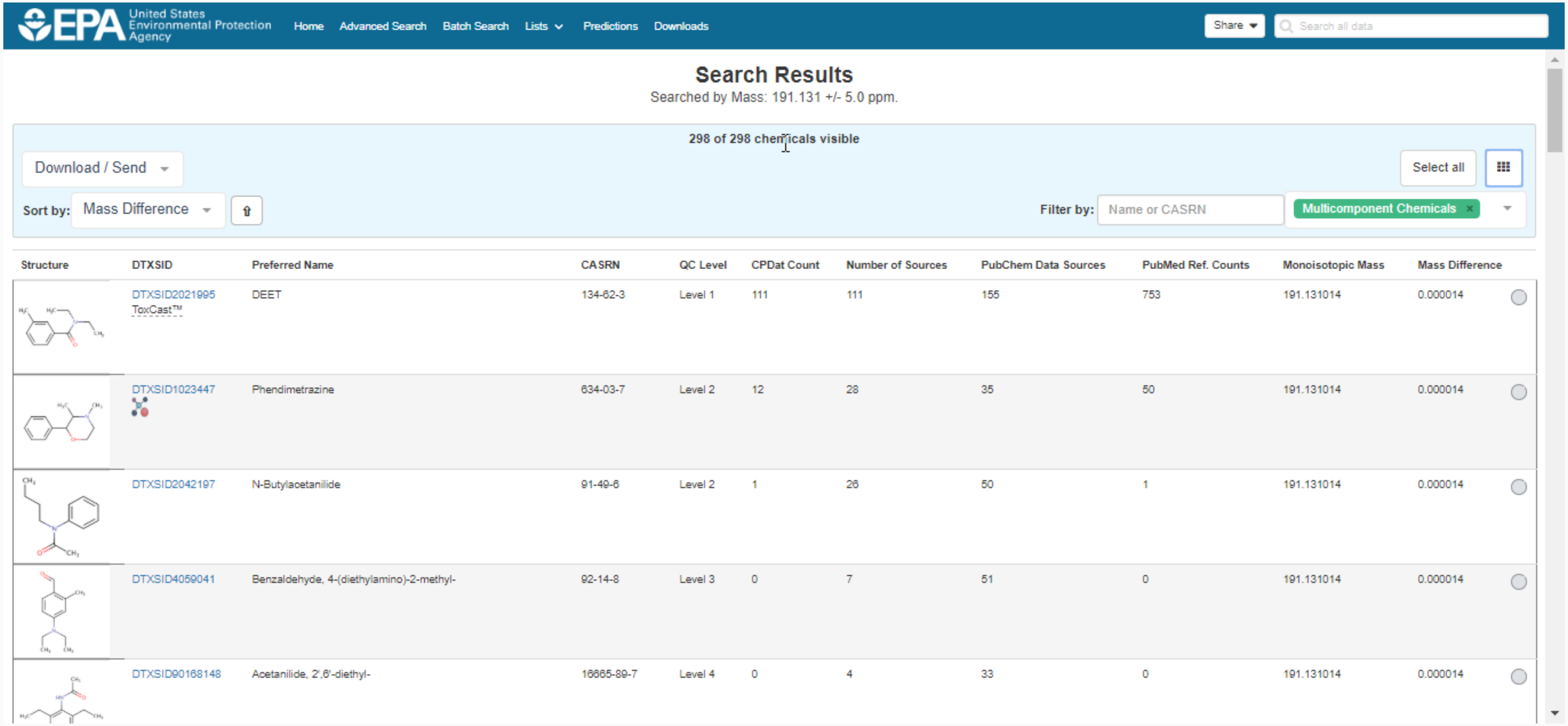
N,N-Diethylphenylacetamide
DTXSID: DTXSID00179048
CASRN: 2431-96-1

3-(Dimethylamino)-2-methylpropiophen...
DTXSID: DTXSID60180796
CASRN: 26171-50-6

Butyramide, 2-ethyl-2-phenyl-
DTXSID: DTXSID60184653
CASRN: 30568-39-9

1-Heptanone, 1-(4-pyridyl)-
DTXSID: DTXSID40186594
CASRN: 32941-30-3

Advanced Searches
Mass Based Search



Search Results

Searched by Mass: 191.131 +/- 5.0 ppm.

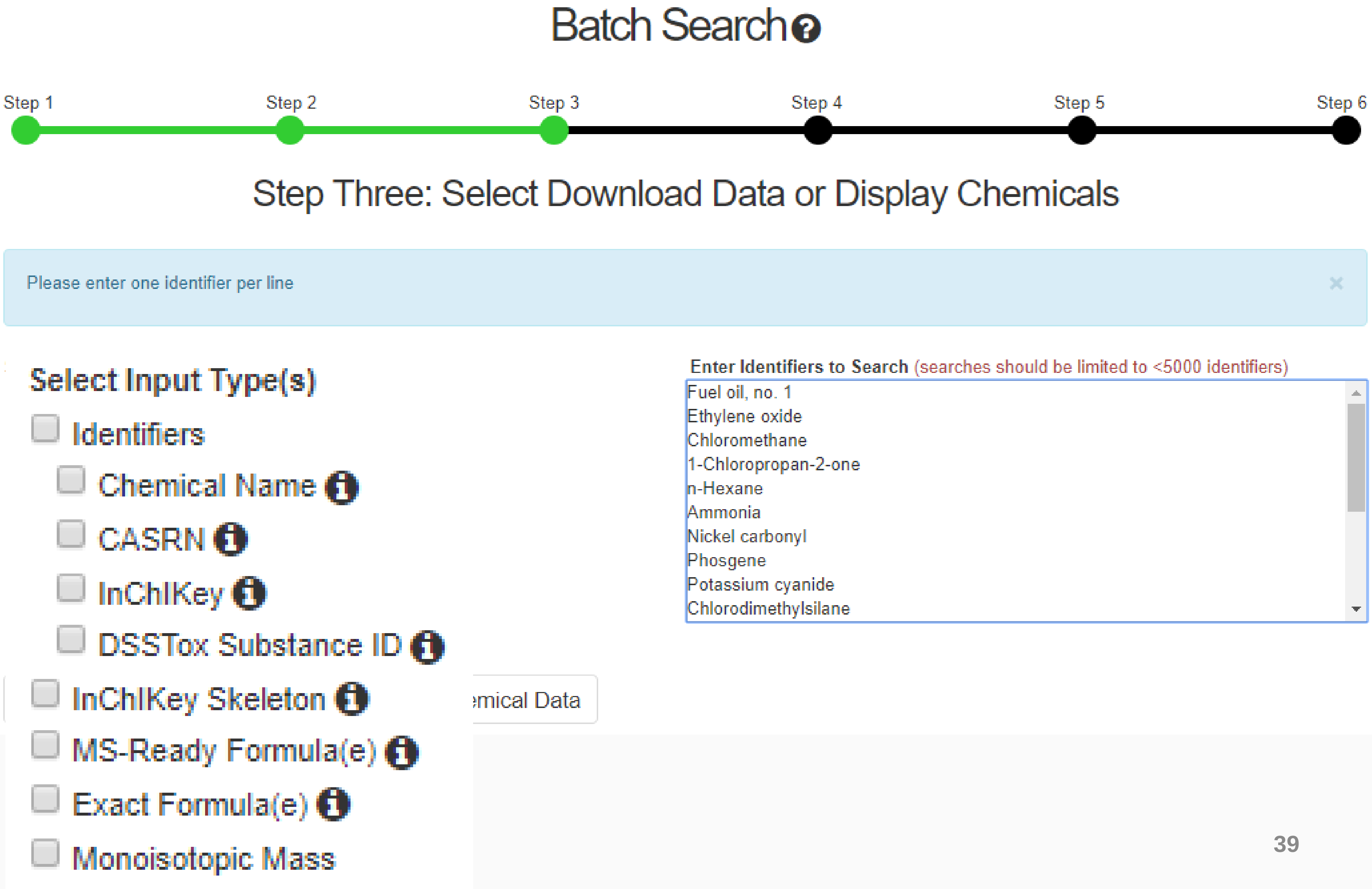
298 of 298 chemicals visible

Structure	DTXSID	Preferred Name	CASRN	QC Level	CPDat Count	Number of Sources	PubChem Data Sources	PubMed Ref. Counts	Monoisotopic Mass	Mass Difference	
	DTXSID2021995 ToxCast™	DEET	134-62-3	Level 1	111	111	155	753	191.131014	0.000014	○
	DTXSID1023447	Phendimetrazine	634-03-7	Level 2	12	28	35	50	191.131014	0.000014	○
	DTXSID2042197	N-Butylacetanilide	91-49-6	Level 2	1	26	50	1	191.131014	0.000014	○
	DTXSID4059041	Benzaldehyde, 4-(diethylamino)-2-methyl-	92-14-8	Level 3	0	7	51	0	191.131014	0.000014	○
	DTXSID90168148	Acetanilide, 2',6'-diethyl-	16665-89-7	Level 4	0	4	33	0	191.131014	0.000014	○

Batch Searching

- Singleton searches are useful but we work with thousands of chemicals!
- Typical questions
  - What are the SMILES strings for a list of 1000 chemicals?
  - Do any of this list of chemicals have XXX type of data?
  - What are the predicted logP values for a list of chemicals?
  - Can I get chemical lists in Excel files? In SDF files?

Batch Searching



Batch Search

Step 1 ● — Step 2 ● — Step 3 ● — Step 4 ● — Step 5 ● — Step 6 ●

Step Three: Select Download Data or Display Chemicals

Please enter one identifier per line ×

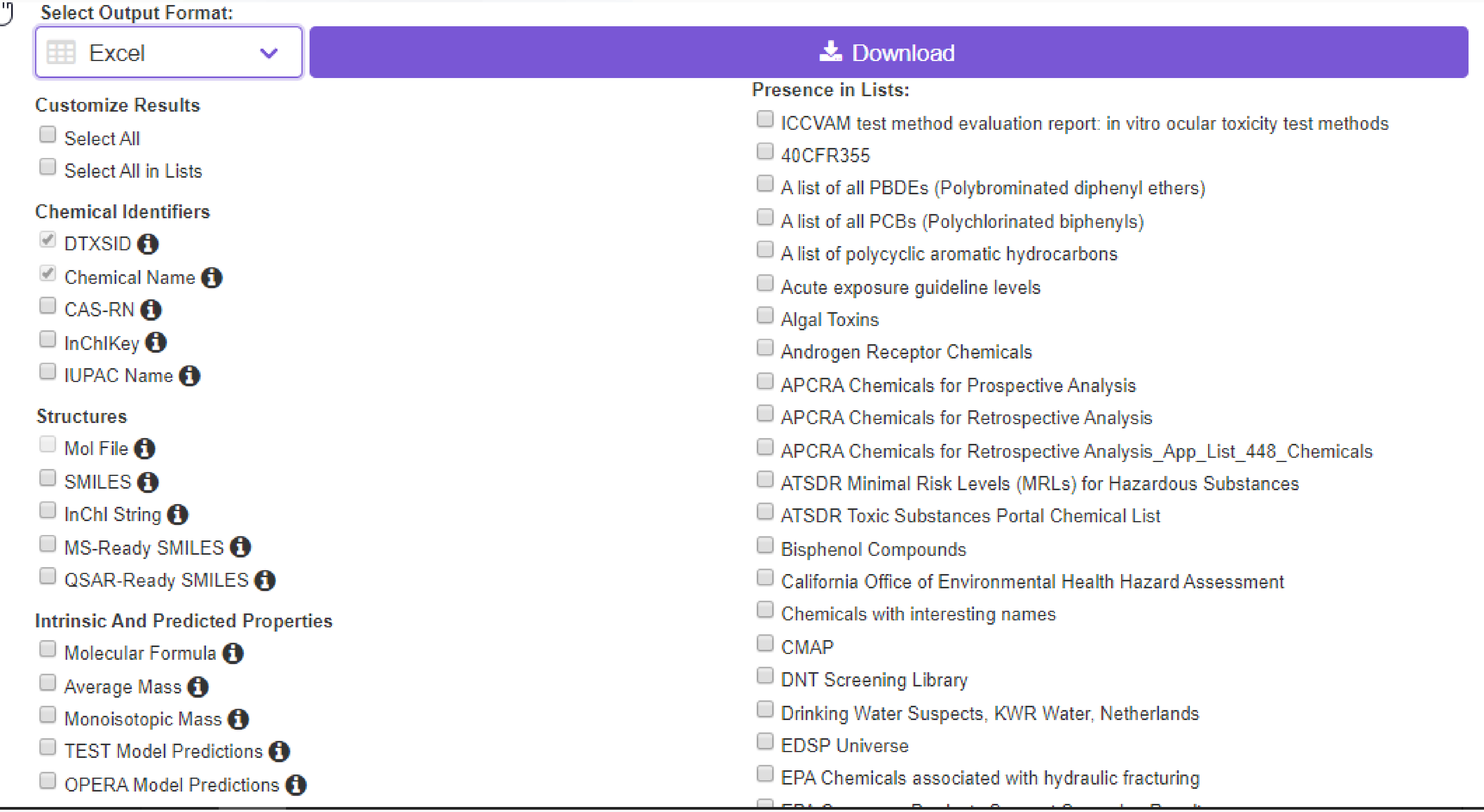
Select Input Type(s)

- □ Identifiers
  - □ Chemical Name
  - □ CASRN
  - □ InChIKey
  - □ DSSTox Substance ID
- □ InChIKey Skeleton
- □ MS-Ready Formula(e)
- □ Exact Formula(e)
- □ Monoisotopic Mass

Enter Identifiers to Search (searches should be limited to <5000 identifiers)

```
Fuel oil, no. 1
Ethylene oxide
Chloromethane
1-Chloropropan-2-one
n-Hexane
Ammonia
Nickel carbonyl
Phosgene
Potassium cyanide
Chlorodimethylsilane
```

Batch Searching



Select Output Format:

Customize Results

- □ Select All
- □ Select All in Lists

Chemical Identifiers

- ☑ DTXSID
- ☑ Chemical Name
- □ CAS-RN
- □ InChIKey
- □ IUPAC Name

Structures

- □ Mol File
- □ SMILES
- □ InChI String
- □ MS-Ready SMILES
- □ QSAR-Ready SMILES

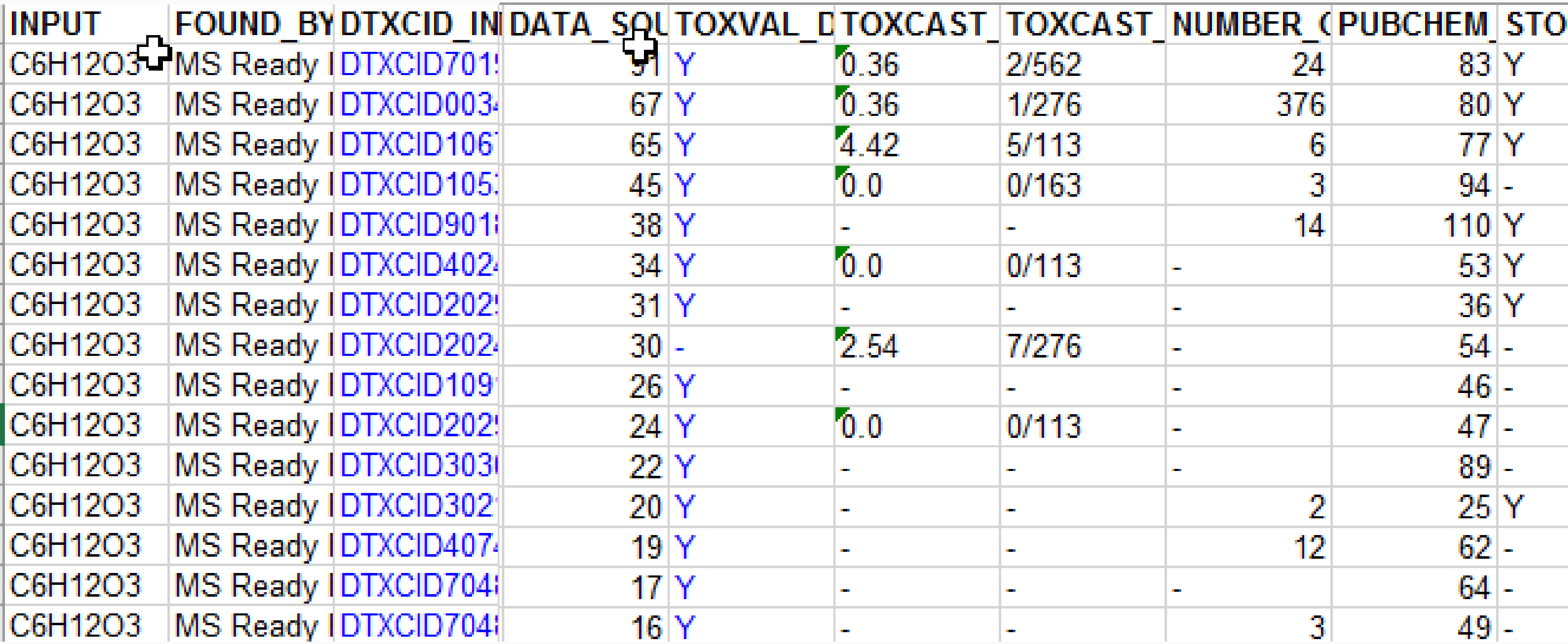
Intrinsic And Predicted Properties

- □ Molecular Formula
- □ Average Mass
- □ Monoisotopic Mass
- □ TEST Model Predictions
- □ OPERA Model Predictions

Presence in Lists:

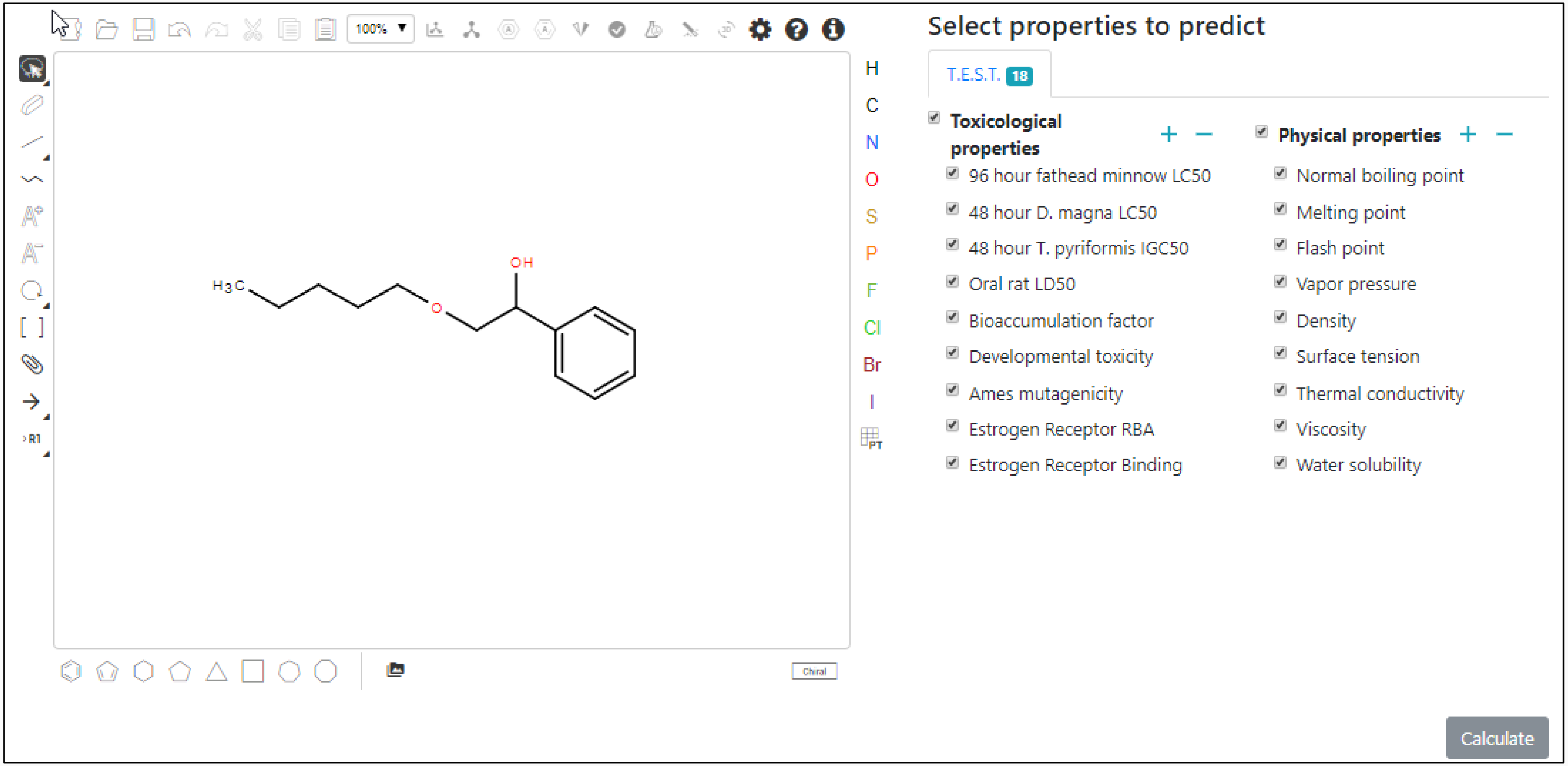
- □ ICCVAM test method evaluation report: in vitro ocular toxicity test methods
- □ 40CFR355
- □ A list of all PBDEs (Polybrominated diphenyl ethers)
- □ A list of all PCBs (Polychlorinated biphenyls)
- □ A list of polycyclic aromatic hydrocarbons
- □ Acute exposure guideline levels
- □ Algal Toxins
- □ Androgen Receptor Chemicals
- □ APCRA Chemicals for Prospective Analysis
- □ APCRA Chemicals for Retrospective Analysis
- □ APCRA Chemicals for Retrospective Analysis_App_List_448_Chemicals
- □ ATSDR Minimal Risk Levels (MRLs) for Hazardous Substances
- □ ATSDR Toxic Substances Portal Chemical List
- □ Bisphenol Compounds
- □ California Office of Environmental Health Hazard Assessment
- □ Chemicals with interesting names
- □ CMAP
- □ DNT Screening Library
- □ Drinking Water Suspects, KWR Water, Netherlands
- □ EDSP Universe
- □ EPA Chemicals associated with hydraulic fracturing

Excel Output



INPUT	FOUND_BY	DTXCID_IN	DATA_SOU	TOXVAL_D	TOXCAST_	TOXCAST_	NUMBER_(	PUBCHEM_	STO
C6H12O3	MS Ready I	DTXCID701	91	Y	0.36	2/562	24	83	Y
C6H12O3	MS Ready I	DTXCID003	67	Y	0.36	1/276	376	80	Y
C6H12O3	MS Ready I	DTXCID106	65	Y	4.42	5/113	6	77	Y
C6H12O3	MS Ready I	DTXCID105	45	Y	0.0	0/163	3	94	-
C6H12O3	MS Ready I	DTXCID901	38	Y	-	-	14	110	Y
C6H12O3	MS Ready I	DTXCID402	34	Y	0.0	0/113	-	53	Y
C6H12O3	MS Ready I	DTXCID202	31	Y	-	-	-	36	Y
C6H12O3	MS Ready I	DTXCID202	30	-	2.54	7/276	-	54	-
C6H12O3	MS Ready I	DTXCID109	26	Y	-	-	-	46	-
C6H12O3	MS Ready I	DTXCID202	24	Y	0.0	0/113	-	47	-
C6H12O3	MS Ready I	DTXCID303	22	Y	-	-	-	89	-
C6H12O3	MS Ready I	DTXCID302	20	Y	-	-	2	25	Y
C6H12O3	MS Ready I	DTXCID407	19	Y	-	-	12	62	-
C6H12O3	MS Ready I	DTXCID704	17	Y	-	-	-	64	-
C6H12O3	MS Ready I	DTXCID704	16	Y	-	-	3	49	-

Real-Time Predictions



Select properties to predict

T.E.S.T. 18

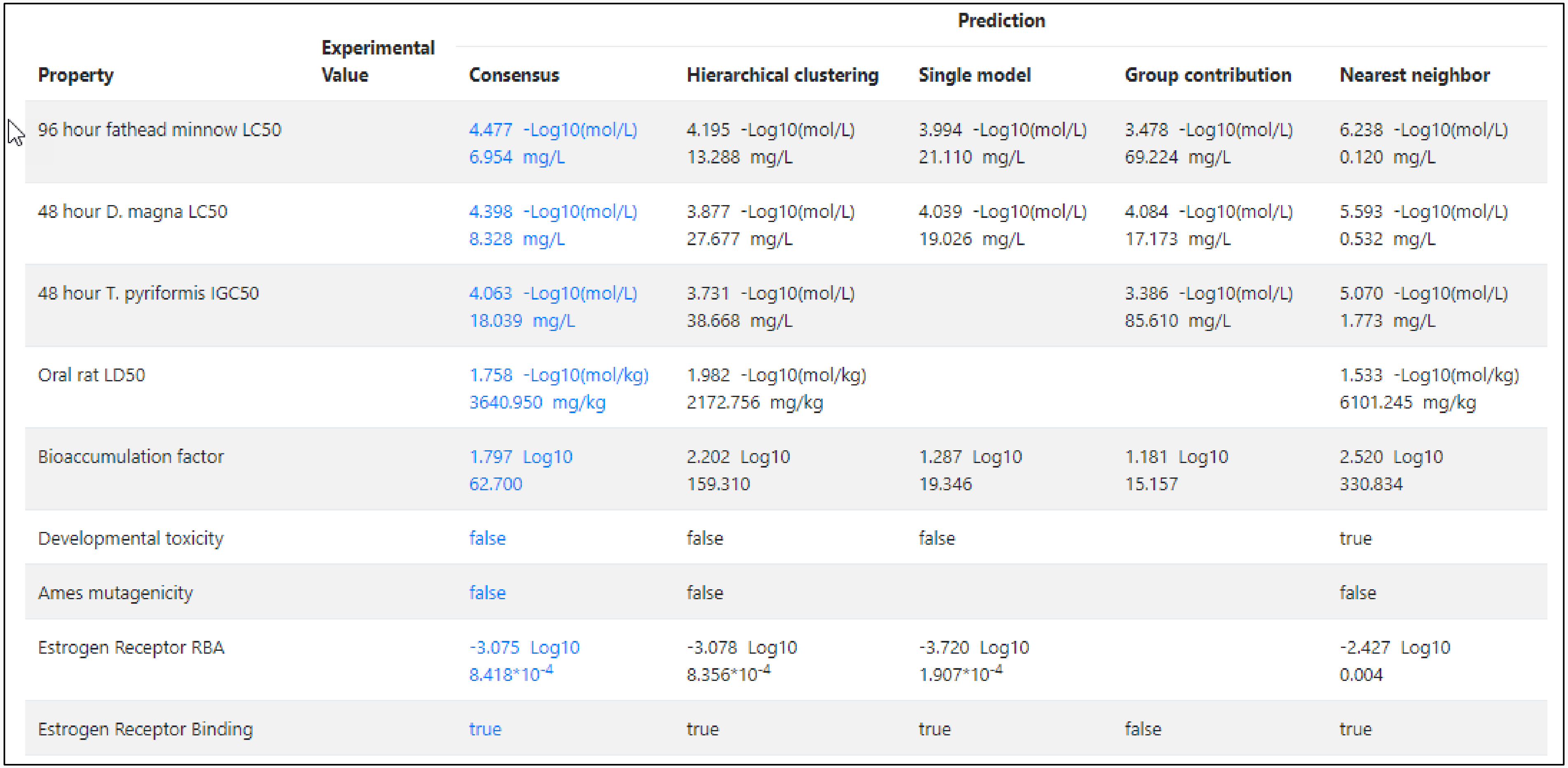
☑ **Toxicological properties**

- ☑ 96 hour fathead minnow LC50
- ☑ 48 hour D. magna LC50
- ☑ 48 hour T. pyriformis IGC50
- ☑ Oral rat LD50
- ☑ Bioaccumulation factor
- ☑ Developmental toxicity
- ☑ Ames mutagenicity
- ☑ Estrogen Receptor RBA
- ☑ Estrogen Receptor Binding

☑ **Physical properties**

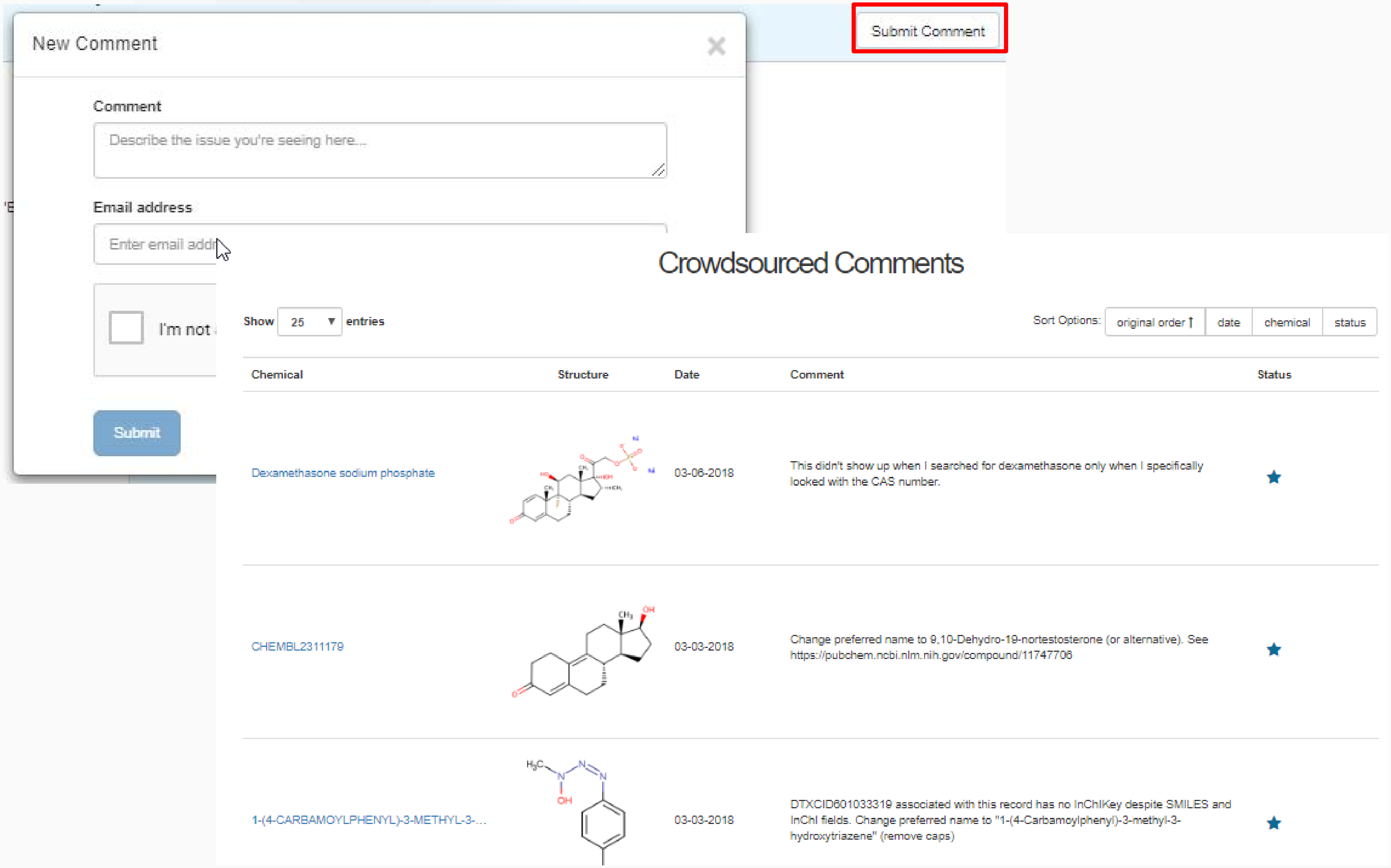
- ☑ Normal boiling point
- ☑ Melting point
- ☑ Flash point
- ☑ Vapor pressure
- ☑ Density
- ☑ Surface tension
- ☑ Thermal conductivity
- ☑ Viscosity
- ☑ Water solubility

Real-Time Predictions



Property	Experimental Value	Prediction				
		Consensus	Hierarchical clustering	Single model	Group contribution	Nearest neighbor
96 hour fathead minnow LC50		4.477 -Log10(mol/L) 6.954 mg/L	4.195 -Log10(mol/L) 13.288 mg/L	3.994 -Log10(mol/L) 21.110 mg/L	3.478 -Log10(mol/L) 69.224 mg/L	6.238 -Log10(mol/L) 0.120 mg/L
48 hour D. magna LC50		4.398 -Log10(mol/L) 8.328 mg/L	3.877 -Log10(mol/L) 27.677 mg/L	4.039 -Log10(mol/L) 19.026 mg/L	4.084 -Log10(mol/L) 17.173 mg/L	5.593 -Log10(mol/L) 0.532 mg/L
48 hour T. pyriformis IGC50		4.063 -Log10(mol/L) 18.039 mg/L	3.731 -Log10(mol/L) 38.668 mg/L		3.386 -Log10(mol/L) 85.610 mg/L	5.070 -Log10(mol/L) 1.773 mg/L
Oral rat LD50		1.758 -Log10(mol/kg) 3640.950 mg/kg	1.982 -Log10(mol/kg) 2172.756 mg/kg			1.533 -Log10(mol/kg) 6101.245 mg/kg
Bioaccumulation factor		1.797 Log10 62.700	2.202 Log10 159.310	1.287 Log10 19.346	1.181 Log10 15.157	2.520 Log10 330.834
Developmental toxicity		false	false	false		true
Ames mutagenicity		false	false			false
Estrogen Receptor RBA		-3.075 Log10 $8.418*10^{-4}$	-3.078 Log10 $8.356*10^{-4}$	-3.720 Log10 $1.907*10^{-4}$		-2.427 Log10 0.004
Estrogen Receptor Binding		true	true	true	false	true

Crowdsourced Curation



New Comment

Comment

Describe the issue you're seeing here...

Email address

Enter email addr

□ I'm not

Crowdsourced Comments

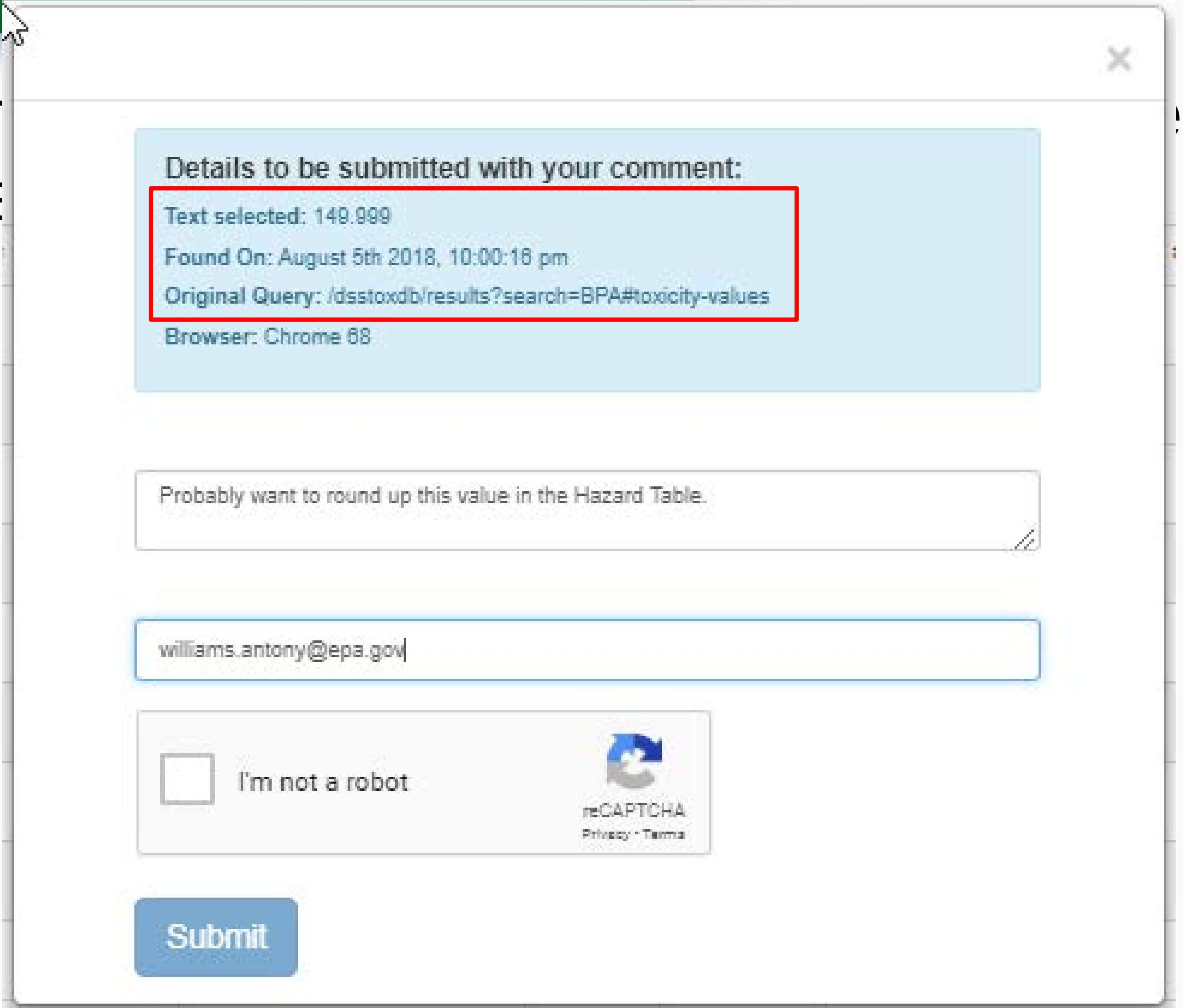
Show 25 entries

Sort Options: original order ↑ | date | chemical | status

Chemical	Structure	Date	Comment	Status
Dexamethasone sodium phosphate		03-06-2018	This didn't show up when I searched for dexamethasone only when I specifically looked with the CAS number.	★
CHEMBL2311179		03-03-2018	Change preferred name to 9,10-Dehydro-19-nortestosterone (or alternative). See https://pubchem.ncbi.nlm.nih.gov/compound/11747706	★
1-(4-CARBAMOYLPHENYL)-3-METHYL-3-...		03-03-2018	DTXCID601033319 associated with this record has no InChIKey despite SMILES and InChI fields. Change preferred name to "1-(4-Carbamoylphenyl)-3-methyl-3-hydroxytriazene" (remove caps)	★

Crowdsourced Curation

- Ar l
  vie



Details to be submitted with your comment:

Text selected: 149.999

Found On: August 5th 2018, 10:00:18 pm

Original Query: /dsstoxdb/results?search=BPA#toxicity-values

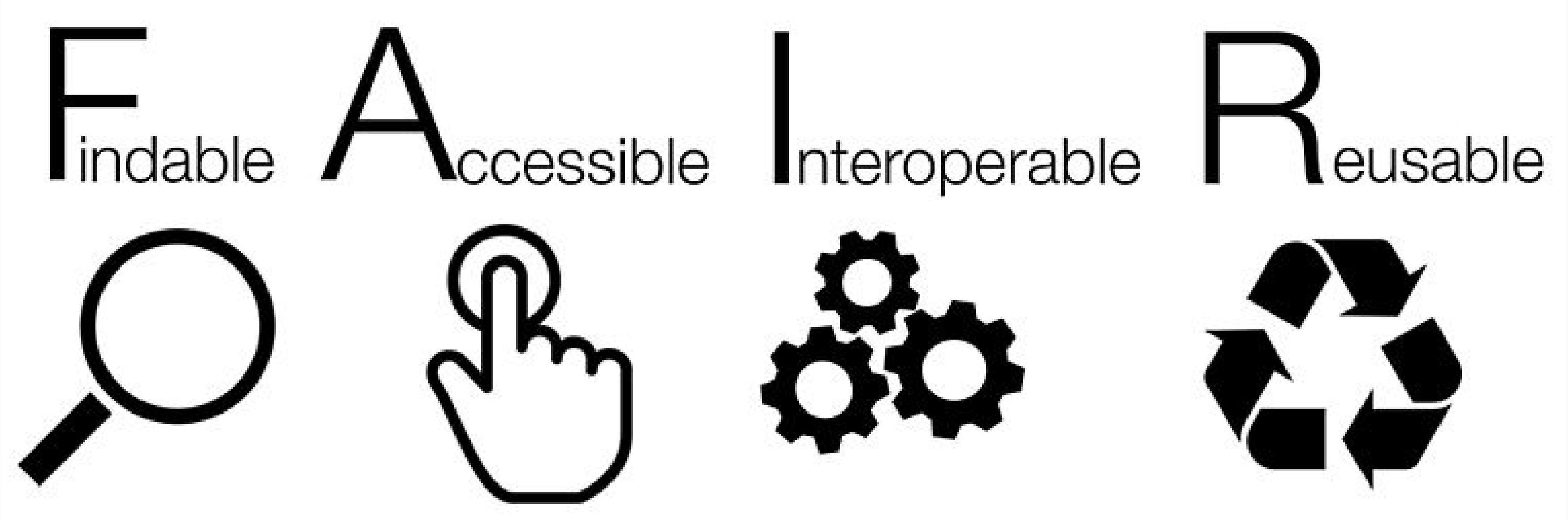
Browser: Chrome 68

Probably want to round up this value in the Hazard Table.

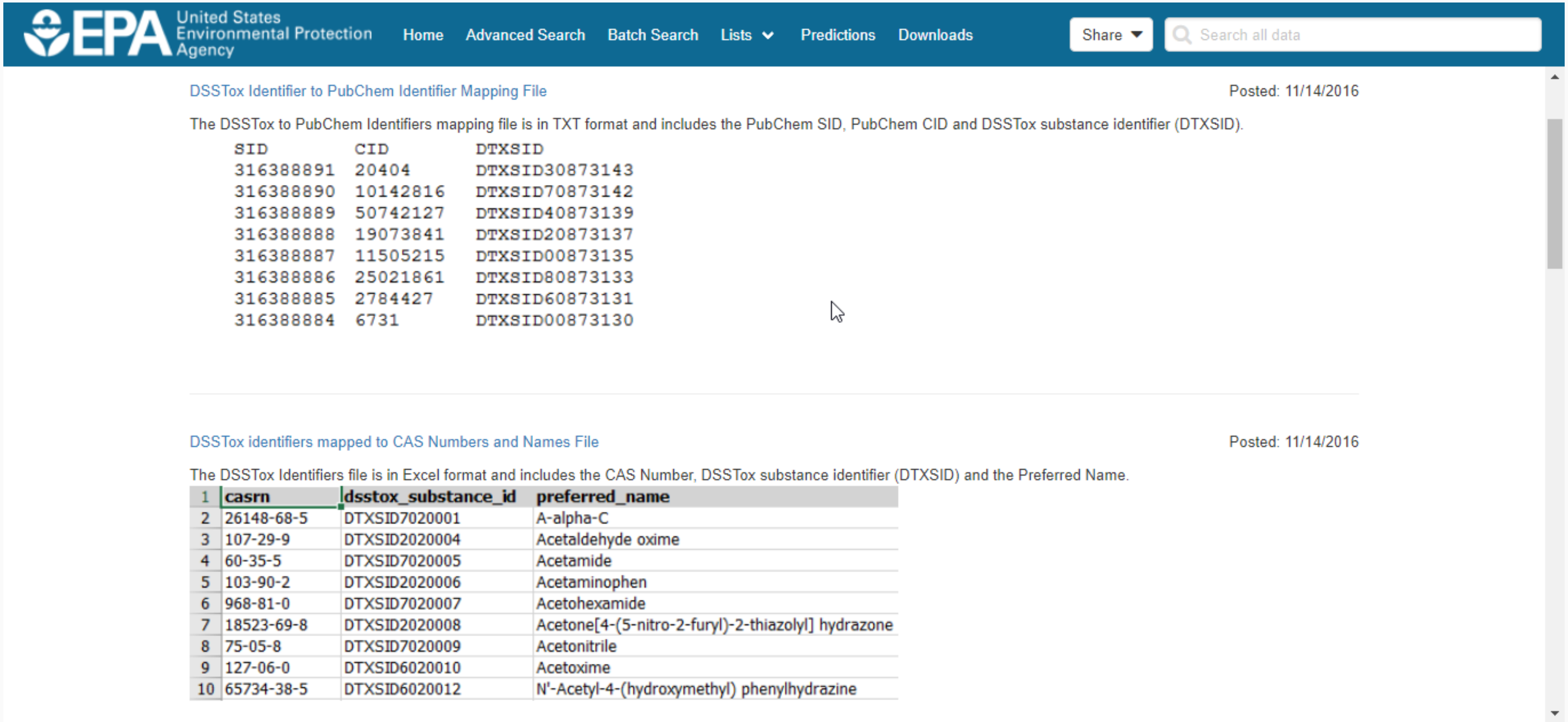
williams.antony@epa.gov

□ I'm not a robot

Our support for FAIR Data



Downloadable Data



DSSTox Identifier to PubChem Identifier Mapping File

Posted: 11/14/2016

The DSSTox to PubChem Identifiers mapping file is in TXT format and includes the PubChem SID, PubChem CID and DSSTox substance identifier (DTXSID).

```
SID        CID        DTXSID
316388891  20404      DTXSID30873143
316388890  10142816   DTXSID70873142
316388889  50742127   DTXSID40873139
316388888  19073841   DTXSID20873137
316388887  11505215   DTXSID00873135
316388886  25021861   DTXSID80873133
316388885  2784427    DTXSID60873131
316388884  6731       DTXSID00873130
```

DSSTox identifiers mapped to CAS Numbers and Names File

Posted: 11/14/2016

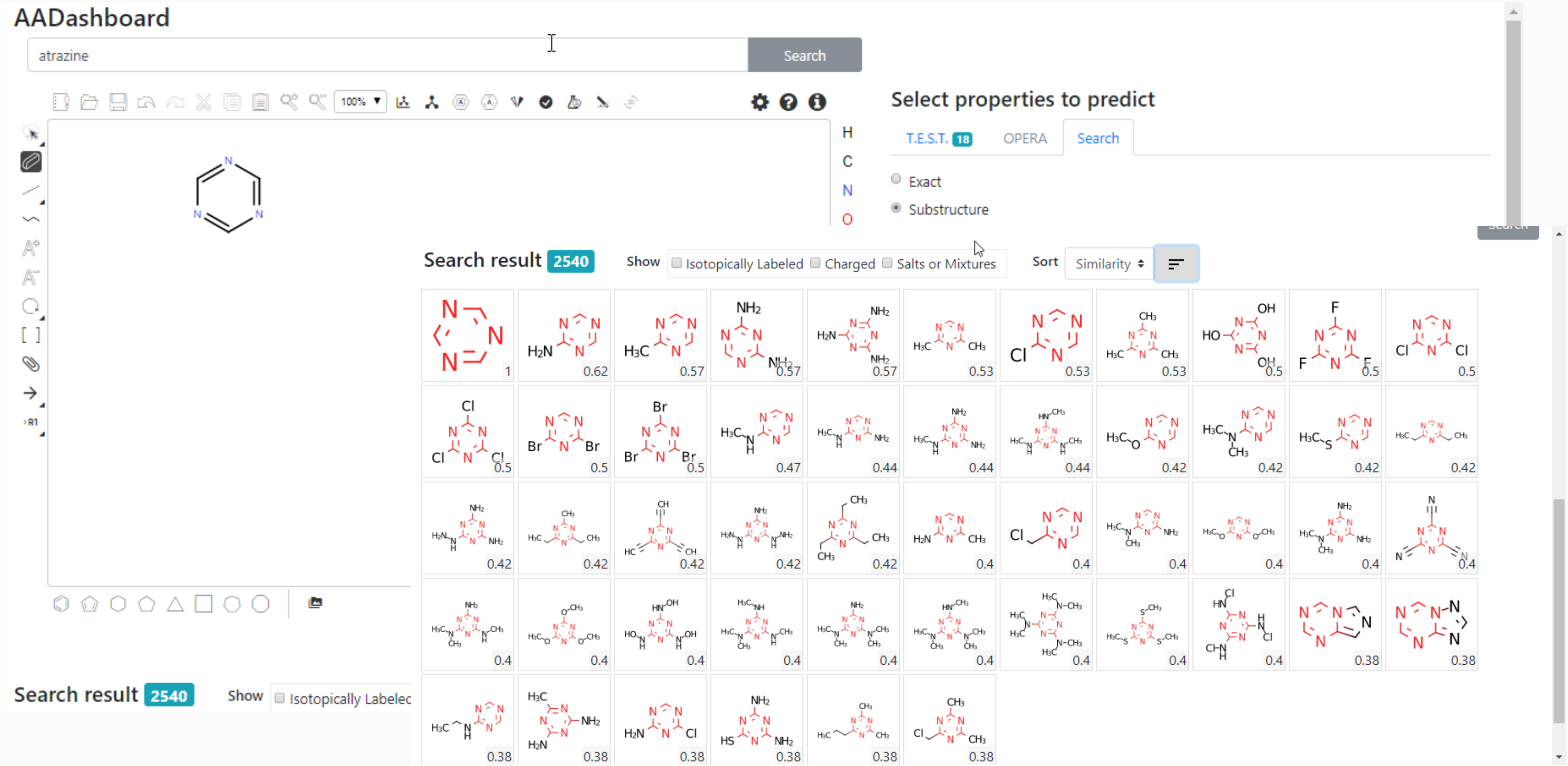
The DSSTox Identifiers file is in Excel format and includes the CAS Number, DSSTox substance identifier (DTXSID) and the Preferred Name.

1	casrn	dsstox_substance_id	preferred_name
2	26148-68-5	DTXSID7020001	A-alpha-C
3	107-29-9	DTXSID2020004	Acetaldehyde oxime
4	60-35-5	DTXSID7020005	Acetamide
5	103-90-2	DTXSID2020006	Acetaminophen
6	968-81-0	DTXSID7020007	Acetohexamide
7	18523-69-8	DTXSID2020008	Acetone[4-(5-nitro-2-furyl)-2-thiazolyl] hydrazone
8	75-05-8	DTXSID7020009	Acetonitrile
9	127-06-0	DTXSID6020010	Acetoxime
10	65734-38-5	DTXSID6020012	N'-Acetyl-4-(hydroxymethyl) phenylhydrazine

Work in Progress

- Present work in development
  - Real time prediction using OPERA models
  - Structure/substructure/similarity search integration
  - Ongoing expansion of chemicals
  - Release of new ToxCast database (v3_2018)
  - Addition of products data from 10s of thousands of MSDS sheets
  - Analytical Data support
    - Integration of analytical data for ToxCast/Tox21 data
    - Spectral searching against predicted Mass Spectra

Prototype Development



AADashboard

atrazine

Search

Select properties to predict

T.E.S.T. 18 | OPERA | Search

○ Exact

● Substructure

Search result 2540

Show □ Isotopically Labeled □ Charged □ Salts or Mixtures

Sort Similarity

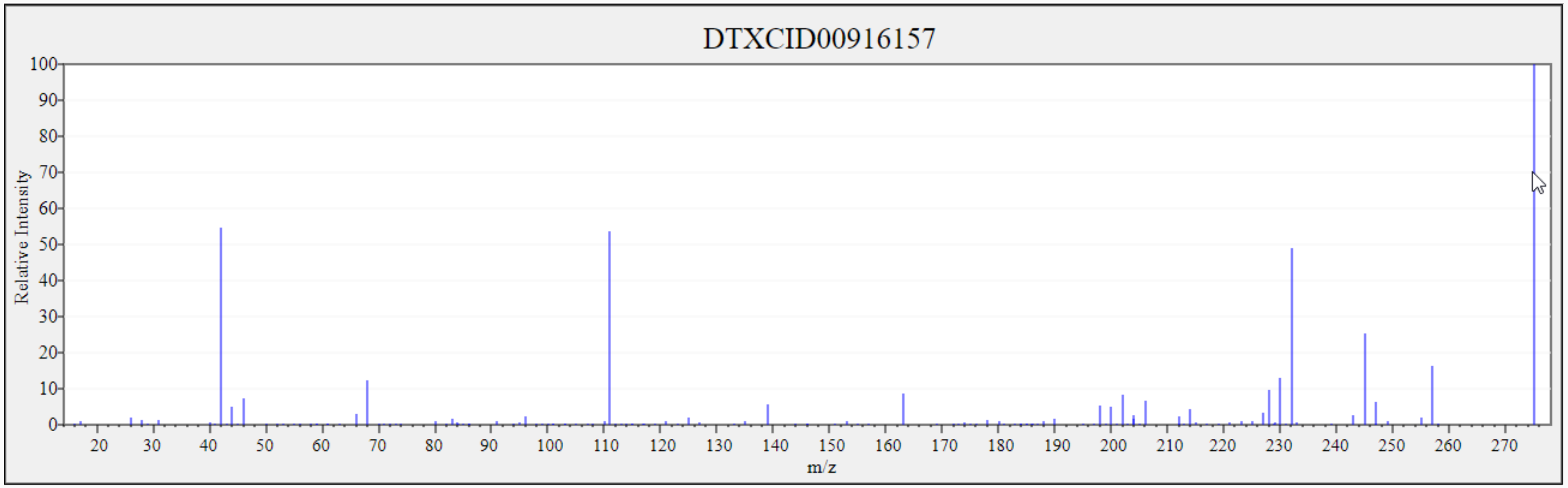
Predicted Mass Spectra

http://cfmid.wishartlab.com/

CFM-ID

Competitive Fragmentation Modeling for Metabolite Identification

- MS/MS spectra prediction for ESI+, ESI-, and EI
- Predictions generated and stored for >700,000 structures, to be accessible via Dashboard



Conclusion

- The EPA CompTox Dashboard provides access to data for ~762,000 chemicals, ToxCast assays and associated product use categories
- High quality data from ongoing curation efforts
- An integration hub for multiple “modules”
  - Experimental and predicted properties
  - Human and Ecological Hazard data
  - Exposure data – products, data in the environment
  - *In vitro* bioassay data – ToxCast/Tox21
  - Literature searching – Google Scholar and PubMed
  - Specialized searches – mass/formula for analytical support
  - Batch searching and Real Time Predictions
- Data and functionality increases with every release

Acknowledgments

- The NCCT CompTox Chemistry Dashboard Development Team
- NERL scientists (Jon Sobus, Elin Ulrich) – Mass Spectrometry
- Kamel Mansouri – OPERA models
- Todd Martin and Valery Tkachenko – TEST predictions
- Nancy Baker – Abstract Sifter

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