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

EPA United States Environmental Protection Agency

Delivering web-based access to data and algorithms to support computational toxicology: US EPA CompTox Chemicals Dashboard

Antony Williams, *Chris Grulke, Ann Richard, Richard Judson, Grace Patlewicz, Imran Shah, John Wambaugh, Katie Paul-Friedman, Jeremy Dunne and Jeff Edwards*

National Center for Computational Toxicology, U.S. Environmental Protection Agency, 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 2019

ACS Fall Meeting, San Diego

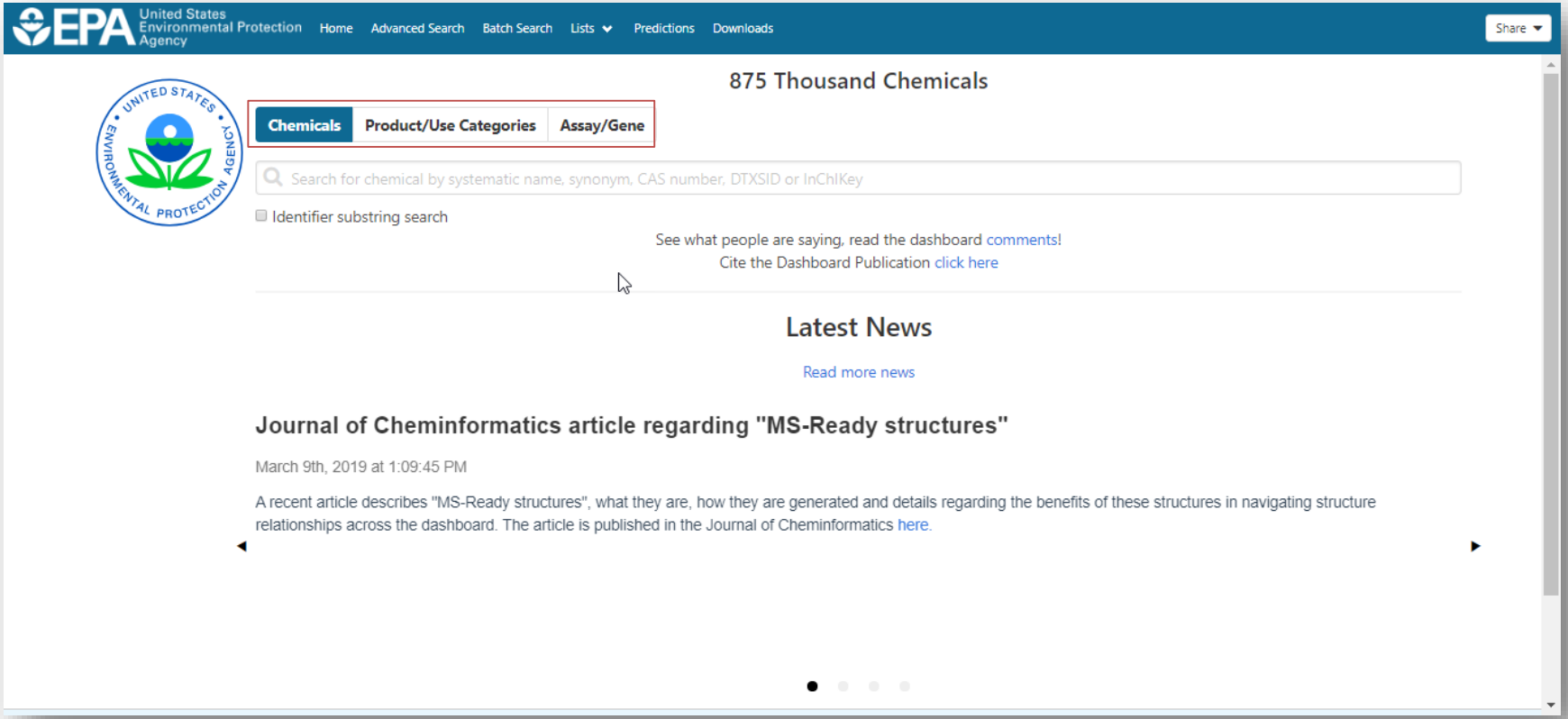
Overview

- The CompTox Chemicals Dashboard - web-based database of 875k substances
- Associated data including:
  - Experimental and predicted physicochemical data
  - *In vivo* hazard data
  - *In vitro* bioactivity screening data
  - Link farm to tens of public resources
- Integrated modules – read-across, lit search
- Data mappings and searches supporting Mass Spectrometry & structure identification

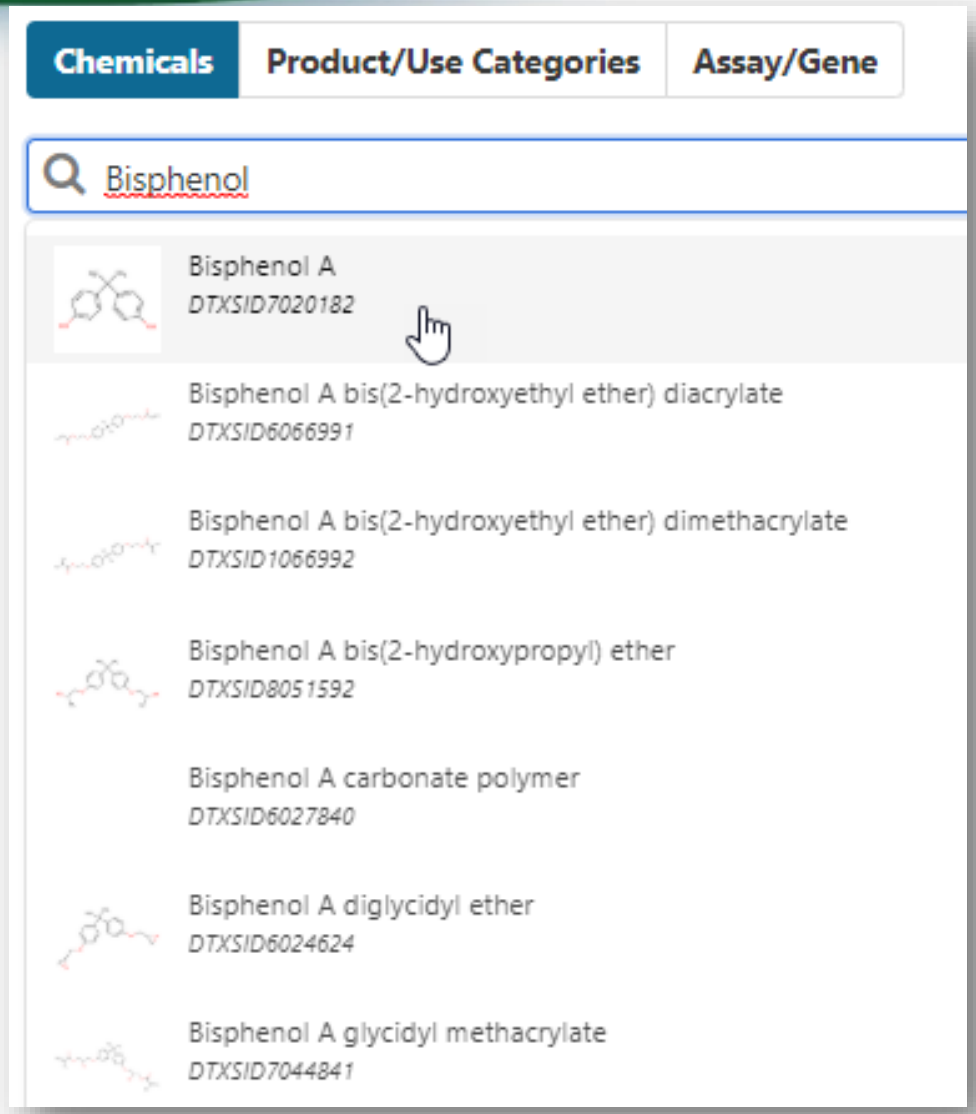
CompTox Chemicals Dashboard

https://comptox.epa.gov/dashboard

875k Chemical Substances



BASIC Search



Detailed Chemical Pages

EPA United States Environmental Protection Agency

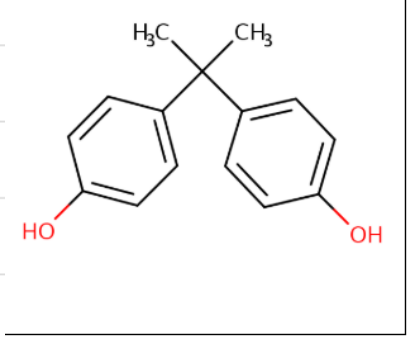
- **DETAILS**
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- ADME
- EXPOSURE
- BIOACTIVITY
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE
- LINKS
- COMMENTS

Advanced Search | Batch Search | Lists | Predictions | Downloads | Copy | Share | Submit Comment | Search all data

Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.



Wikipedia

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

Intrinsic Properties

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

Average Mass: 228.291 g/mol | Isotope Mass Distribution

Monoisotopic Mass: 228.11503 g/mol

Structural Identifiers

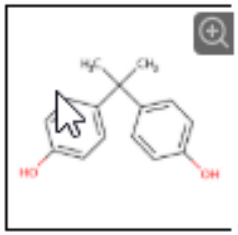
Linked Substances

Presence in Lists

Record Information

Quality Control Notes

Experimental and Predicted Data



Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

Property

Summary

Download Columns

Property	Experimental average	Predicted average
LogP: Octanol-Water	3.32 (1)	3.29
Melting Point	155 (7)	139
Boiling Point	200 (1)	363
Water Solubility	5.26e-4 (1)	9.62e-4
Vapor Pressure	-	8.37e-7
Flash Point	-	190

Transparency for prediction models

EPA United States Environmental Protection Agency

Predicted

Download Predicted Data

Source	Result	Calculation Details	QMRF
EPISUITE	3.64	Not Available	Not Available
NICEATM	2.40	Not Available	Available
ACD/Labs Consensus	3.63	Not Available	Not Available
ACD/Labs	3.43	Not Available	Not Available
OPERA	3.35	OPERA Model Report [Inside AD]	Available

OPERA Models: LogP: Octanol-Water

Bisphenol A

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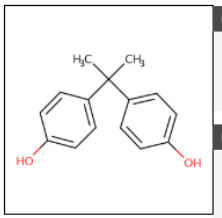
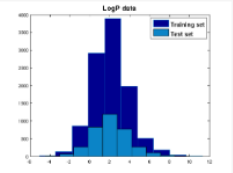
Print PDF

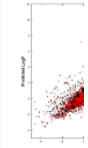


Model Results

Predicted value: 3.35
Global applicability domain: Inside
Local applicability domain index: 0.877
Confidence level: 0.813

Model Performance



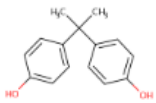


QMRF

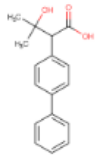
Weighted KNN model

5-fold CV (75%)		Training (75%)	
Q2	RMSE	R2	RMSE
0.850	0.690	0.860	0.670

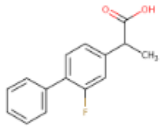
Nearest Neighbors from the Training Set



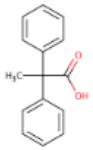
Bisphenol A
Measured:3.32
Predicted: 3.35076



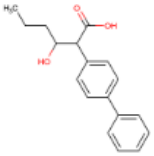
BUTANOIC ACID,2-(4-BIPHENYLYL)-3-HYDROXY-3-METHY
Measured:3.25
Predicted: 3.39062



Flurbiprofen
Measured:4.16
Predicted: 3.94445



2,2-Diphenylpropionic acid
Measured:2.69
Predicted: 2.84603



3-OH-2-(4-BIPHENYLYL)HEXANOIC ACID
Measured:3.75
Predicted: 3.70322

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

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

Journal of Cheminformatics

RESEARCH ARTICLE Open Access

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]

OPERA Models: https://github.com/kmansouri/OPERA

Access to Chemical Hazard Data

EPA United States Environmental Protection Agency

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

Hazard

DataType: Toxicity Value

Human | Eco

Download | Columns | Search query

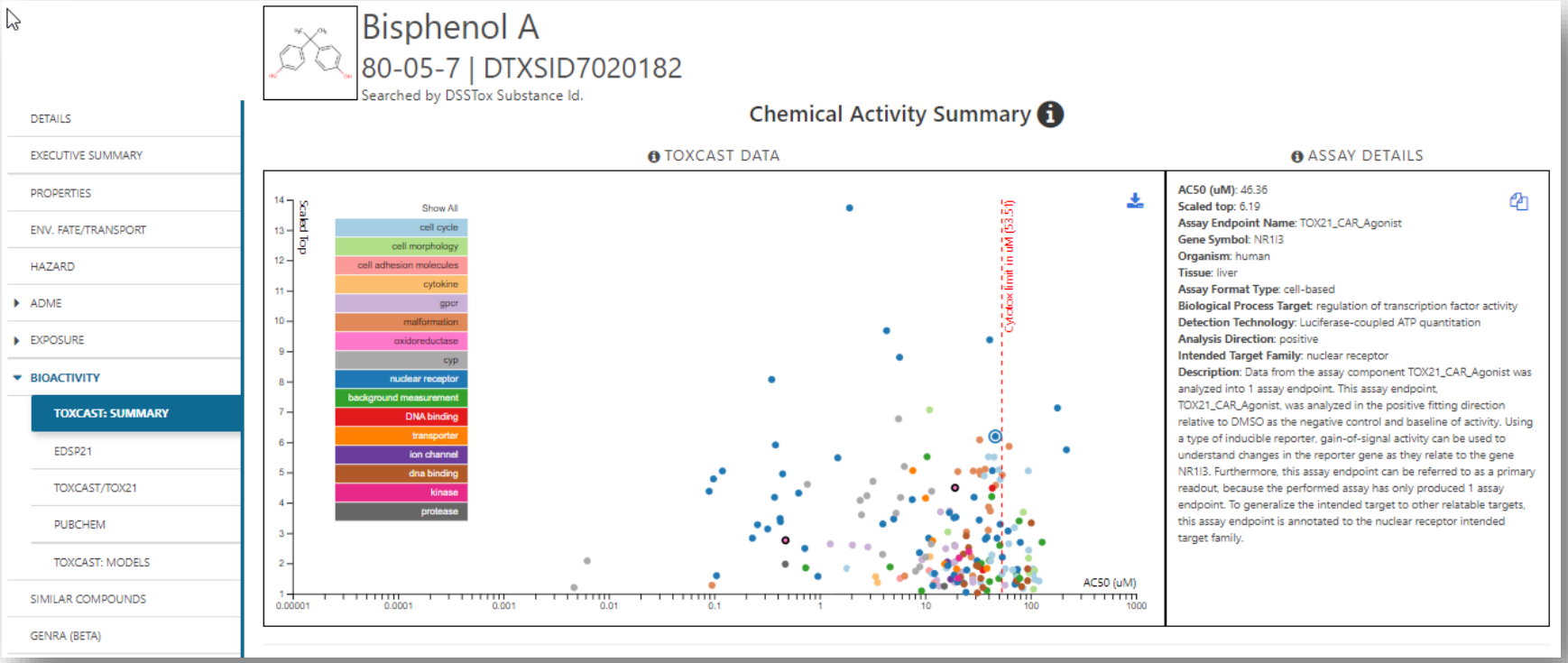
More	Priority	Type	Subtype	Risk assessment class	Value	Units	Study type	Exposure route	Species	Subsource	Source
	7	MEG	Short-term Critical Air	short-term	500	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Short-term Marginal Air	short-term	100	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Short-term Negligible Air	short-term	15	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Soil Negligible Soil	chronic	106000	mg/kg	-	soil	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Long-Term, 5L/d Negligible Water	chronic	7	mg/L	-	oral	-	TG 230 Military Exposure Guidelines Table	DOD
	6	RfD	-	chronic	0.05	mg/kg-day	-	oral	rat	Wignall	Wignall
	5	RfD	-	chronic	0.05	mg/kg-day	-	-	-	MSC Table 5	Pennsylvania DEP ToxValues
	4	RfD	-	chronic	0.05	mg/kg-day	chronic	oral	rat	IRIS	Chiu
	3	RfD	-	chronic	0.6	mg/kg-day	-	oral	rat	EPA/ORNL/OLEM	HEAST
	1	RfD	-	chronic	0.05	mg/kg-day	-	oral	-	EPA NCEA	IRIS

Hazard Data from “ToxVal_DB”

- ToxVal Database contains following data:
  - ~800,000 toxicity values
  - ~30 sources of data
  - ~22,000 sub-sources
  - ~5000 journals cited
  - ~70,000 literature citations

In Vitro Bioassay Screening

ToxCast and Tox21



In Vitro Bioassay Screening

ToxCast and Tox21

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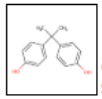
EPA United States Environmental Protection Agency | Home | Advanced Search | Batch Search | Lists | Predictions | Downloads | Copy | Share | Submit Comment | Search all data



Bisphenol A

80-05-7 | DTXSID7020182

Searched by Expert Validated Synonym.

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- ADME
- EXPOSURE
- BIOACTIVITY
  - TOXCAST: SUMMARY
  - EDSP21
  - TOXCAST/TOX21
  - PUBCHEM
  - TOXCAST: MODELS
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE
- LINKS
- COMMENTS

ToxCast/Tox21

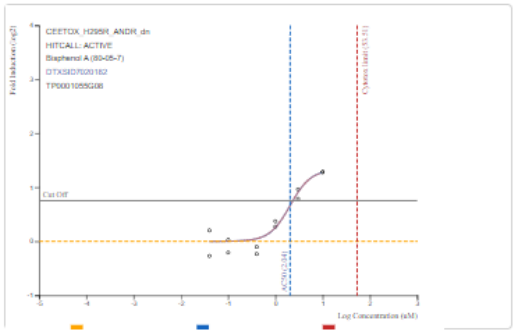
QC Data ID	Grade	Description
Tox21_202992	Pass	Purity>90% and MW confirmed
Tox21_400088	Pass	Purity>90% and MW confirmed

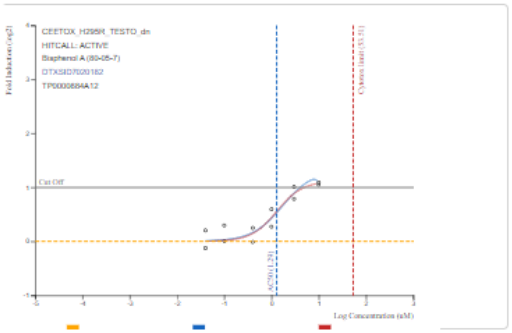
Assay Selection 136 Selected | A Single Assay Can Have Multiple Charts | Representative Samples Only | Bioactivity Summary | Number of Charts: 136

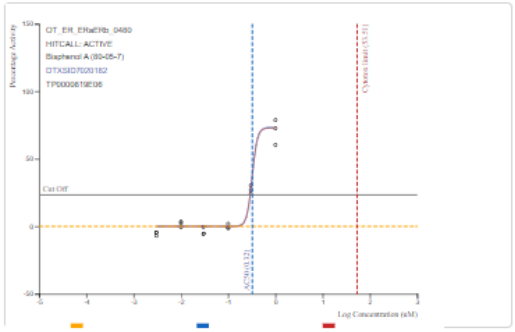
Active | Inactive | All

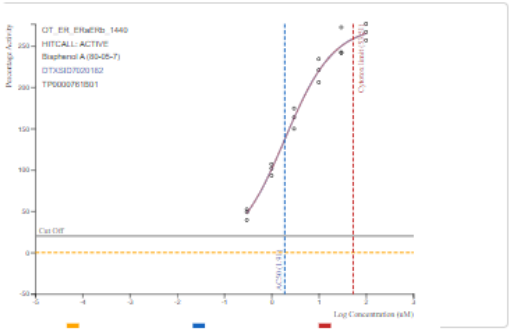
Filter assays

- Ceetox/OpAns (2 of 24 selected)
- Odyssey Thera (6 of 17 selected)
- Attagene (4 of 165 selected)
- Tox21/NCGC (44 of 211 selected)
- CellzDirect (3 of 48 selected)
- Bioseek (4 of 174 selected)
- Apredica (8 of 107 selected)
- NHEERL Padilla Lab (1 of 1 selected)
- Novascreen (46 of 167 selected)
- NHEERL's Hunter Lab (0 of 4 selected)
- NCCT's Lab (4 of 4 selected)
- ACEA Biosciences (4 of 6 selected)
- Tanguay Lab (9 of 19 selected)
- NHEERL Stoker & Laws Lab (1 of 2 selected)









Bioactivity: Downloadable Data

https://www.epa.gov/chemical-research/exploring-toxcast-data-downloadable-data

EPA United States Environmental Protection Agency

Exploring ToxCast Data: Downloadable Data

The results after processing through the Pipeline are available on the ToxCast Dashboard, and for most users EPA recommends accessing the data there.

- ToxCast Chemicals
- ToxCast Assays

Resources

- Toxicity Forecaster (ToxCast) Fact Sheet
- ToxCast Publications
- ToxCast Citation
- About ToxCast

ToxCast Data and Information

- **ToxCast & Tox21 Summary Files.** Data for a single chemical endpoint pair for thousands of chemicals and assay endpoints for 20 variables such as the activity or hit call, activity concentrations, whether the chemical was tested in a specific assay, etc.
  - Download ToxCast Summary Information
  - Download ReadMe
- **ToxCast & Tox21 Data Spreadsheet.** A spreadsheet of EPA's analysis of the chemicals screened through ToxCast and the Tox21 collaboration which includes EPA's activity calls from the screening of over 1,800 chemicals.
  - Download Data
  - Download ReadMe
- **ToxCast Data Pipeline R Package.** The R computer programming package used to process and model all EPA ToxCast and Tox21 chemical screening data. The files include the R programming package as well as documents that provide overviews of the data analysis pipeline used and the R package. Users will need experience with R to use these files.
  - Download Package
  - TCPL Overview

Sources of Exposure to Chemicals

EPA United States Environmental Protection Agency

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Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

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

Product and Use Categories (PUCs)

Download | Columns | 10 | Search query

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

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

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  - PRODUCTION VOLUME
- BIOACTIVITY

Toxics Release Inventory

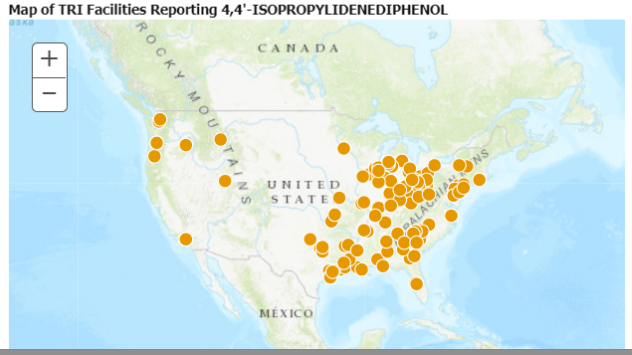
Print Page

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

An "Executive Summary" Quick Look Tox Info

EPA United States Environmental Protection Agency

Executive Summary

Quantitative Risk Assessment Values
- IRIS values available
- No PPRTV values
- EPA RSL values available
- Minimum RfD: **0.050 mg/kg-day** (chronic, IRIS, oral, 8)
- No RfC calculated
- IVIVE POD not calculated

Quantitative Hazard Values
- Minimum oral POD: **3.8 mg/kg-day** (reproductive, HPVIS, oral, 6)
- No inhalation POD values
- Lowest Observed Bioactivity Equivalent Level: CYP1A1, CYP1A2, Tpo, ESR2, ESR1, ESR1, NR1I3, PPARA, NR1I2, Cyp2c11, MMP3, Esr1

Cancer Information
- No cancer slope factor
- No inhalation unit risk value
- Carcinogenicity data available: University of Maryland carcinogenicity warning;
- No genotoxicity findings reported

Reproductive Toxicology
- 200 Reproductive toxicity PODs available

Chronic Toxicology
- 340 Chronic toxicity PODs available

Subchronic Toxicology
- 12 Subchronic toxicity PODs available

Developmental Toxicology
- 6 Developmental toxicity PODs available

Acute Toxicology
- 391 Acute toxicity PODs available

Subacute Toxicology
- 1 subacute toxicity PODs available

Neurotoxicology
- No neurotoxicology data available.

Endocrine System
- Endocrine Disruption Potential. Significant Estrogen and Androgen Receptor activity seen. Chemical was positive in **21 ER assays (out of 35)** and was positive in **9 AR assays (tested in 19)**.

ADME
- HTTK Css data are available

Fate and Transport
- No bioaccumulation concern.
- No volatility concern.
- Biodegradation predictions are available
- BCF predictions are available
- Vapor Pressure predictions are available

Exposure
- Exposure estimates are available based on NHANES and SEEM

AOP Information
- AOP Links: 13, 33, 36, 58, 60, 61, 66, 107, 124, 150, 163, 175, 187, 200

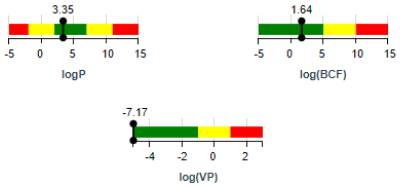
Other Notes
- No water quality values available.
- No air quality values available.
- 14 Occupational exposure values available.

POINT-OF-DEPARTURE PLOTS

REGIONAL SCREENING

Class	THQ	Value
risk-based SSL (mg/kg)	THQ = 0.1	5.8
GIABS (unspecified)	THQ = 1	1
GIABS (unspecified)	THQ = 0.1	1
ABS (unspecified)	THQ = 0.1	0.1
RFDo (mg/kg-day)	THQ = 0.1	0.05
screening level (residential Soil) (mg/kg)	THQ = 0.1	320
screening level (industrial soil) (mg/kg)	THQ = 0.1	4100
screening level (tap water) (ug/L)	THQ = 0.1	77
RFDo (mg/kg-day)	THQ = 1	0.05
screening level (residential Soil) (mg/kg)	THQ = 1	3200
screening level (industrial soil) (mg/kg)	THQ = 1	41000
ABS (unspecified)	THQ = 1	0.1
risk-based SSL (mg/kg)	THQ = 1	58
screening level (tap water) (ug/L)	THQ = 1	770

PHYSCHEM PARAMETERS



ASSAY PLOTS

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- Minimum RfD: **0.050 mg/kg-day** (chronic, IRIS, oral, 8)
- No RfC calculated
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Quantitative Hazard Values
- Minimum oral POD: **3.8 mg/kg-day** (reproductive, HPVIS, oral, 6)
- No inhalation POD values
- Lowest Observed Bioactivity Equivalent Level: CYP1A1, CYP1A2, Tpo, NR1I3, PPARA, NR1I2, Cyp2c11, MMP3, Esr1

Identifiers to Support Searches

EPA United States Environmental Protection Agency

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- GENRA (BETA)
- RELATED SUBSTANCES
- **SYNONYMS**
- LITERATURE
- LINKS
- COMMENTS

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*

Quality Control of the Database

- We have full time curators checking data

Record Information

Citation: U.S. Environmental Protection Agency. Chemistry Dashboard. https://comptox.epa.gov/dashboard/DTXSID7020007 (accessed Apr 1st, 2019), Acetohexamide

Data Quality:

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

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

Level 3: Programmatically curated from high quality EPA source, unique chemical identifiers have no conflicts in ChemID and PubChem

Level 4: Programmatically curated from ChemID, unique chemical identifiers have no conflicts in PubChem

Level 5: Programmatically curated from ACToR or PubChem, unique chemical identifiers with low confidence, single public source

Built-in “Modules”

Abstract Sifter for Excel

F1000Research
Open for Science

Search

BROWSE GATEWAYS HOW TO PUBLISH ABOUT BLOG

Check for updates

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.

METRICS

629 VIEWS

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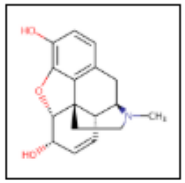
Abstract

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

Literature Searching



Morphine

57-27-2 | DTXSID9023336

Searched by Approved Name.

Abstract Sifter

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

Select a Query Term

Retrieve Articles

- 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
- Disaster / Emergency

Optionally, edit the query before retrieving.

"57-27-2" OR "Morphine"

Literature Searching

Child (infant through adolescent)
Dust and Exposure
Food and Exposure
Water and Exposure
Algae
Disaster / Emergency

Optionally, edit the query before retrieving.

("57-27-2" OR "Morphine") AND ((water OR groundwater OR drinking water) AND Environmental Exposure)

Literature Searching

37 of 37 articles loaded...

To find articles quickly, enter terms to sift abstracts.

wastewater | Spectrometry | EPA | Clear Terms

Download / Send to... | Download Sifter for Excel

	wastewater	Spectrometry	EPA	Total	PMID	Year	Title	Authors	Journal	Rev
	4	2	0	6	29274731	2017	Simultaneous analysis of opioid analgesics and thei...	Krizman-Matasic; Kostanjevecki; Ahel; Terzic	Journal of chromatography. A	
	0	1	0	1	25768972	2015	Evaluating external contamination of polybrominate...	Poon; Aleksa; Carnevale; Kapur; Goodyer; Koren	Therapeutic drug monitoring	
	0	1	0	1	22544551	2012	Spatial distribution of illicit drugs in surface waters o...	Vazquez-Roig; Andreu; Blasco; Morillas; Picó	Environmental science and pollution research inter...	
	1	1	0	2	20801487	2010	Analysis of llicit and illicit drugs in waste, surface an...	Berset; Brenneisen; Mathieu	Chemosphere	
	1	1	0	2	17935751	2007	Illicit drugs, a novel group of environmental contami...	Zuccato; Castiglioni; Bagnati; Chiabrando; Grassi; ...	Water research	
	2	1	1	4	17607391	2007	Using environmental analytical data to estimate lev...	Bones; Thomas; Paull	Journal of environmental monitoring : JEM	
	3	1	2	6	17180984	2006	Simultaneous determination of psychoactive drugs ...	Hummel; Löffler; Fink; Ternes	Environmental science & technology	
	6	0	0	6	30583189	2018	Assessment of drugs of abuse in a wastewater trea...	Kumar; Tscharke; O'Brien; Mueller; Wilkins; Padhye	The Science of the total environment	
	0	0	3	3	30488421	2018	Effect of enriched environment during adolescence ...	Mohammadian; Najafi; Miladi-Gorji	Developmental psychobiology	
	3	0	0	3	29574368	2018	Estimation of the consumption of illicit drugs during ...	Foppe; Hammond-Weinberger; Subedi	The Science of the total environment	
	1	0	0	1	28787791	2017	Evaluation of in-sewer transformation of selected illi...	Gao; Banks; Li; Jiang; Lai; Mueller; Thai	The Science of the total environment	
	9	0	0	9	28472697	2017	Occurrence and fate of illicit drugs and pharmaceuti...	Causanilles; Ruepert; Ibáñez; Emke; Hernández; d...	The Science of the total environment	
	0	0	0	0	28010888	2016	Dose-dependent effects of morphine on lipopolysac...	Mottaz; Schönenberger; Fischer; Eggen; Schirmer; ...	Environmental pollution (Barking, Essex : 1987)	
	0	0	0	0	27746311	2016	Effects of voluntary exercise on the viability, prolifer...	Haydari; Safari; Zarbakhsh; Bandegi; Miladi-Gorji	Neuroscience letters	
	0	0	0	0	27261879	2016	Genotoxic effects induced by the exposure to an en...	Parolini; Magni; Castiglioni; Binelli	Ecotoxicology and environmental safety	
	3	0	0	3	27179320	2016	Temporal trends in drug use in Adelaide, South Aus...	Tscharke; Chen; Gerber; White	The Science of the total environment	

Generalized Read-Across (GenRA)

EPA United States Environmental Protection Agency

Bisphenol A

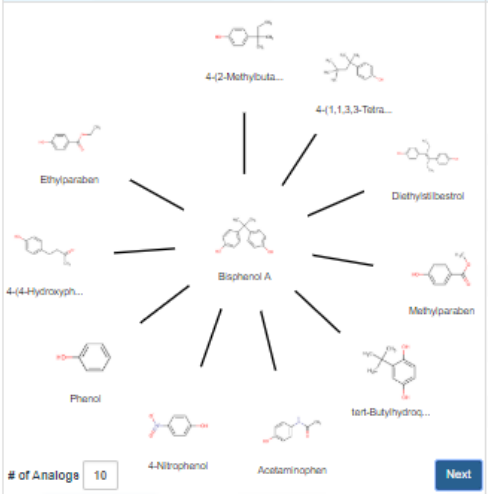
80-05-7 | DTXSID7020182

Searched by Expert Validated Synonym.

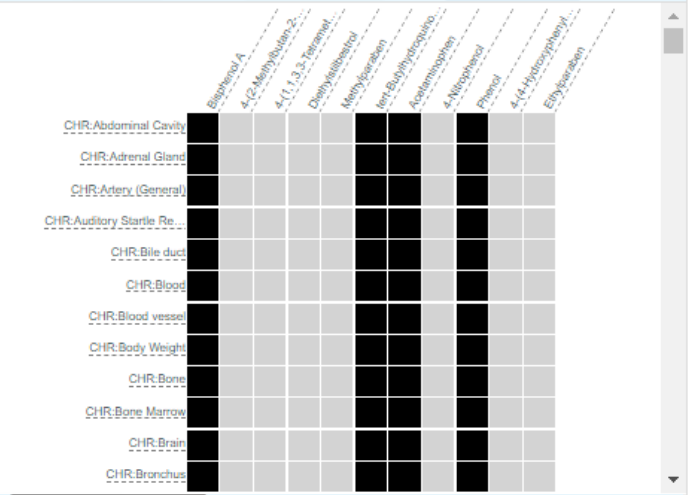
- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- ADME
- EXPOSURE
- BIOACTIVITY
  - TOXCAST: SUMMARY
  - PUBCHEM
  - TOXCAST: DATA
  - TOXCAST: MODELS
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE
- LINKS
- COMMENTS

Step Two: Data Gap Analysis & Generate Data Matrix

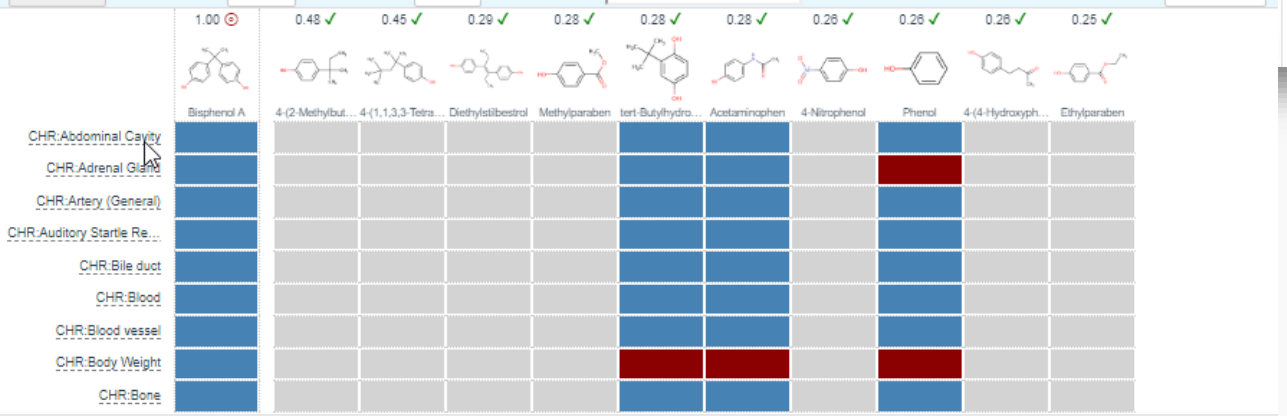
Neighbors by: Chem: Morgan Fgrprts | Filter by: Invivo data | Summary Data Gap Analysis | Group: ToxRef | By: Tox Fingerprint | Generate Data Matrix



	bio_b21	bio_brd	chm_c1	tox_brd
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	85
Ethylparaben	3	714	8	48



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



Related Publications

Chemical Research in Toxicology

Article

Cite This: Chem. Res. Toxicol. 2017, 30, 2046-2059 pubs.acs.org/crt

Predicting Organ Toxicity Using *in Vitro* Bioactivity Data and Chemical Structure

Jie Liu,[‡,§] Grace Patlewicz,[†] Antony J. Williams,[†] Russell S. Thomas,[†] and Imran Shah*[,†]

[†]National Center for Computational Toxicology, Office of Research and Development, U.S. Environmental Protection Agency, Research Triangle Park, Durham, North Carolina 27711, United States

[‡]Department of Information Science, University of Arkansas at Little Rock, Arkansas 72204, United States

[§]Oak Ridge Institute for Science Education, National Center for Computational Toxicology, Office of Research and Development, U.S. Environmental Protection Agency, Research Triangle Park, Durham, North Carolina 27711, United States

ELSEVIER

Regulatory Toxicology and Pharmacology

Volume 79, August 2016, Pages 12-24

Systematically evaluating read-across prediction and performance using a local validity approach characterized by chemical structure and bioactivity information

Imran Shah [a], Jie Liu [b, c], Richard S. Judson [a], Russell S. Thomas [a], Grace Patlewicz [a]

ELSEVIER

Computational Toxicology

Available online 23 July 2018

In Press, Corrected Proof

Extending the Generalised Read-Across approach (GenRA): A systematic analysis of the impact of physicochemical property information on read-across performance

George Helman [a, b], Imran Shah [b], Grace Patlewicz [b]

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Contents lists available at ScienceDirect

Computational Toxicology

journal homepage: www.elsevier.com

Journal Cover Image

Navigating through the minefield of read-across frameworks: A commentary perspective

Grace Patlewicz[a, *], Mark T.D. Cronin[b], George Helman[a, c], Jason C. Lambert[d], Lucina E. Lizarraga[d], Imran Shah[a]

[a] National Center for Computational Toxicology (NCCT), Office of Research and Development, US Environmental Protection Agency (US EPA), 109 TW Alexander Dr, Research Triangle Park (RTP), NC 27711, USA

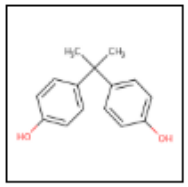
[b] School of Pharmacy and Biomolecular Sciences, Liverpool John Moores University, Byrom Street, Liverpool L3 3AF, UK

[c] Oak Ridge Institute for Science and Education (ORISE), 1299 Bethel Valley Road, Oak Ridge, TN 37830, USA

[d] National Center for Evaluation Assessment (NCEA), US Environmental Protection Agency (US EPA), 26 West Martin Luther King Dr, Cincinnati, OH 45268, USA

Mapped Relationships

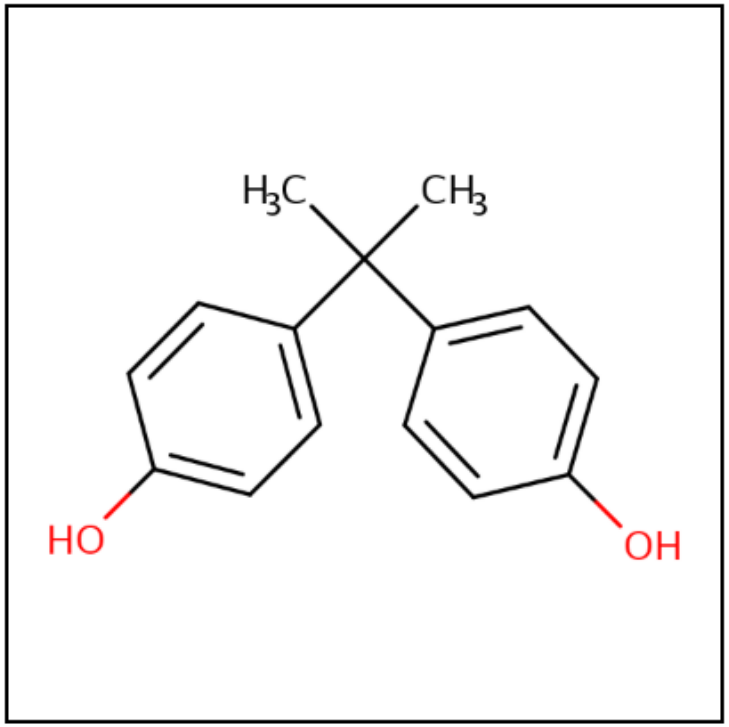
Relationships in the Data



Bisphenol A

80-05-7 | DTXSID7020182

Searched by Expert Validated Synonym.



Wikipedia

Intrinsic Properties

Structural Identifiers

Linked Substances

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

Mixtures, Components and Neutralized Forms: 9 records (based on QSAR ready mappings and with the compound as a component of a mixture)

MS-Ready Mappings: DTXCID30182: 27 records;

Similar Compounds: 390 records (based on Tanimoto coefficient >0.8)

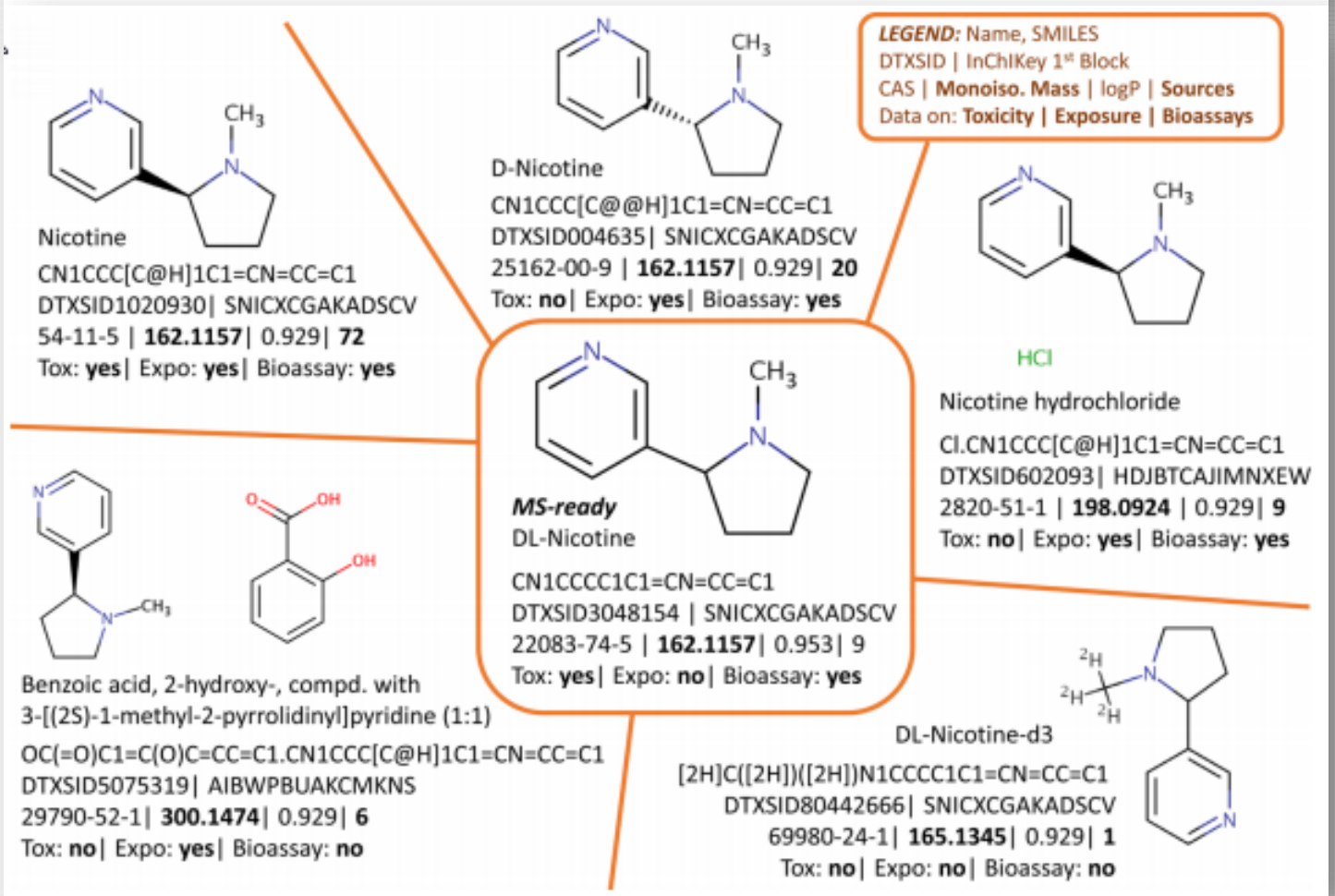
Presence in Lists

Environmental Science & Technology
Viewpoint
pubs.acs.org/est

EPA United States Environmental Protection Agency

Open Science for Identifying "Known Unknown" Chemicals

Emma L. Schymanski*,† and Antony J. Williams*,‡



“MS-Ready Structures”

https://doi.org/10.1186/s13321-018-0299-2

McEachran *et al. J Cheminform (2018) 10:45*
https://doi.org/10.1186/s13321-018-0299-2

Journal of Cheminformatics

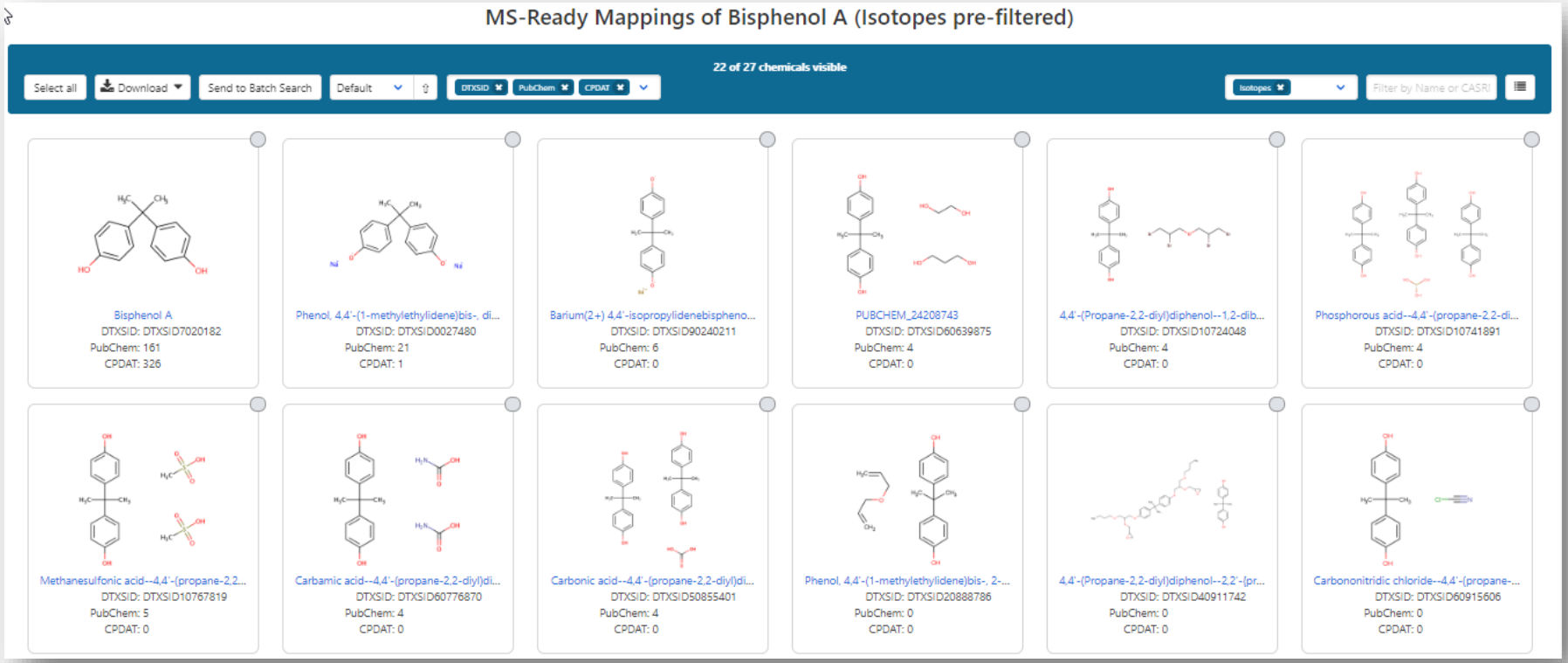
METHODOLOGY

Open Access

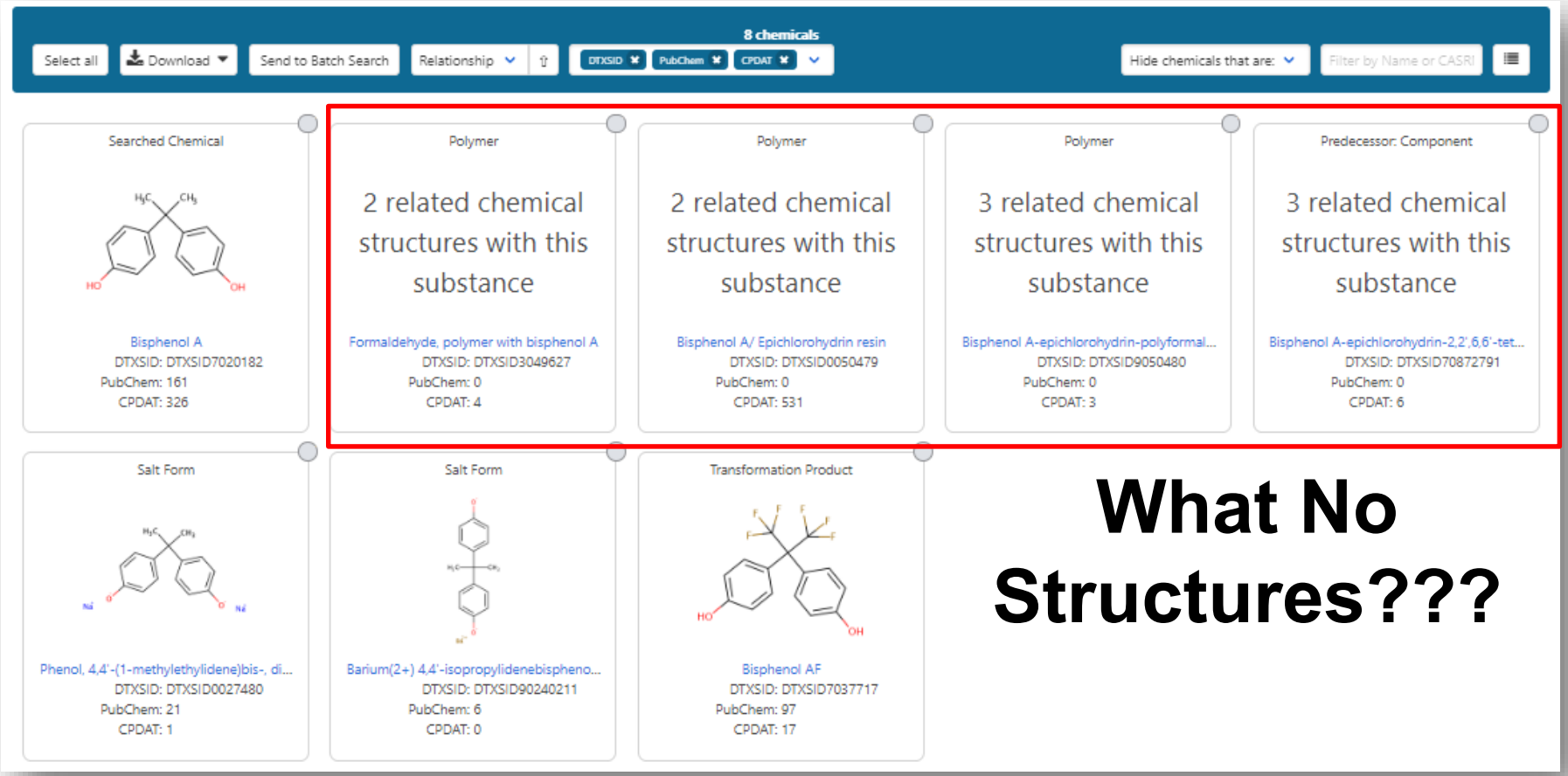
“MS-Ready” structures for non-targeted high-resolution mass spectrometry screening studies

Andrew D. McEachran[1,2*], Kamel Mansouri[1,2,3], Chris Grulke[2], Emma L. Schymanski[4], Christoph Ruttkies[5] and Antony J. Williams[2*]

Bisphenol A
27 Total MS-Ready Mappings



Related Substances – Transformation Products, “Monomer-Polymer”



What No Structures???

“UVCB” Chemical Substances

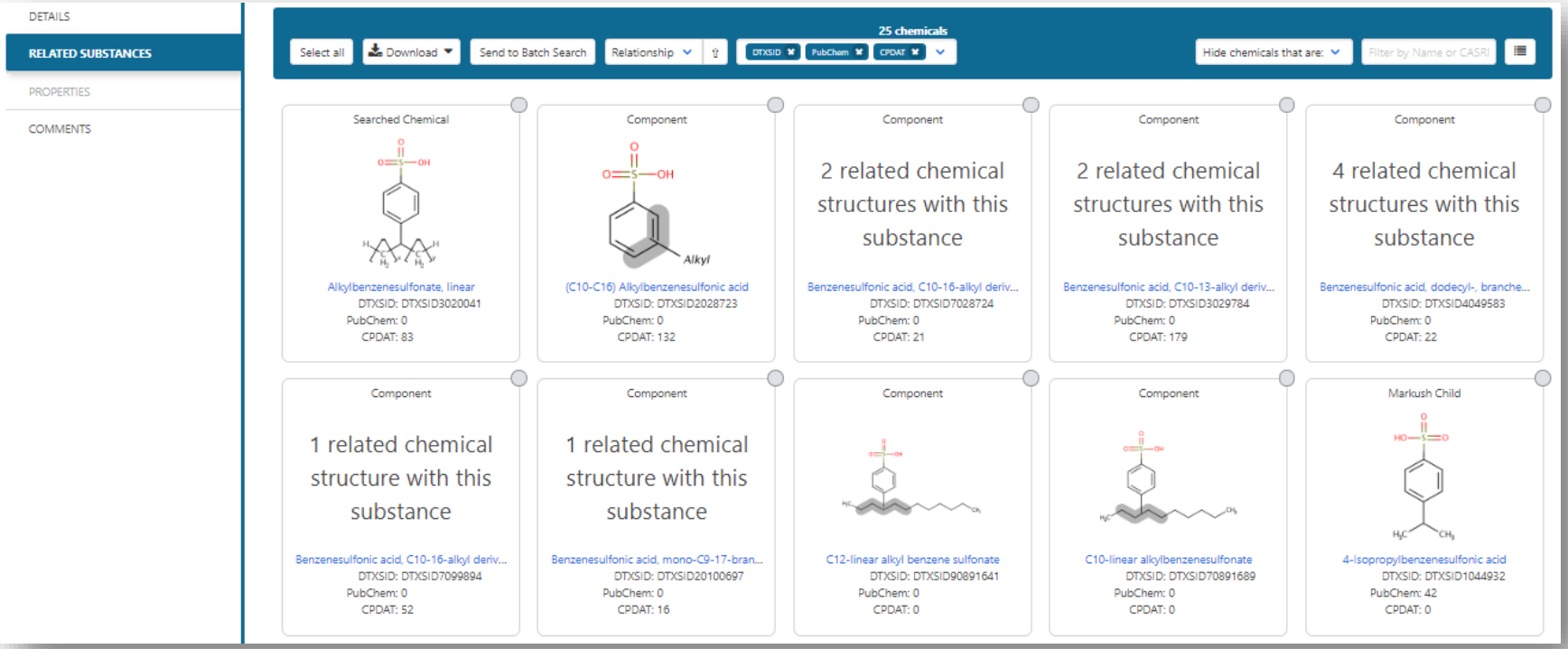
UVCB Chemicals

EPA United States Environmental Protection Agency

Chemical Substances of Unknown or Variable Composition, Complex Reaction Products and Biological Materials (UVCB Substance) on the TSCA Inventory

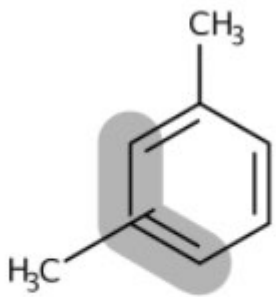
This paper is a compendium of information related to the broad class of chemical substances referred to as UVCBs for the Toxic Substances Control Act (TSCA) Chemical Substance Inventory. These chemical substances cannot be represented by unique structures and molecular formulas.

UVCB: Complex Surfactants

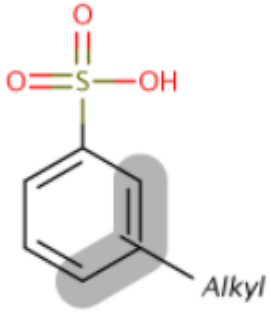


“Markush Structures”

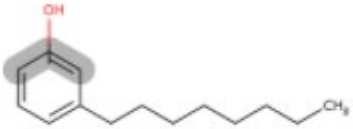
https://en.wikipedia.org/wiki/Markush_structure



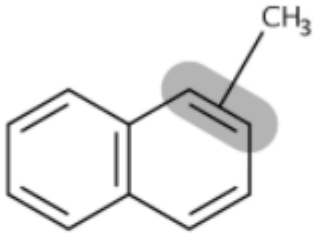
Xylenes
1330-20-7



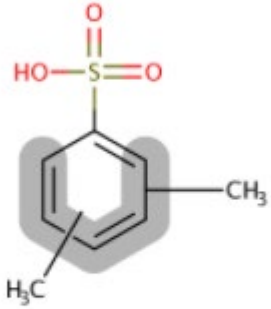
(C10-C16) Alkylbenzenesulfonic acid
68584-22-5



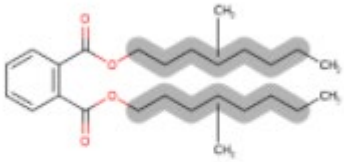
n-Nonylphenol
25154-52-3



Methylnaphthalene
1321-94-4

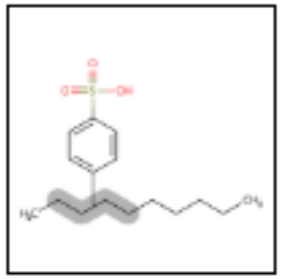


Sodium xylenesulfonate
1300-72-7



Diisononyl phthalate
28553-12-0

UVCB: Complex Surfactants

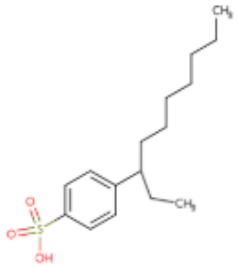


C10-linear alkylbenzenesulfonate

NOCAS_891689 | DTXSID70891689

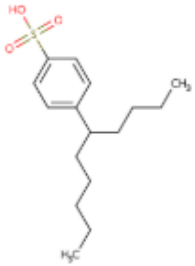
Searched by DSSTox Substance Id.

Markush Child



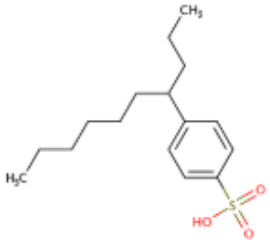
4-(Decan-3-yl)benzene-1-sulfonic acid
DTXSID: DTXSID20859618
PubChem: 0
CPDAT: 0

Markush Child



4-(decan-5-yl)benzene-1-sulfonic acid
DTXSID: DTXSID70881146
PubChem: 0
CPDAT: 0

Markush Child



4-(decan-4-yl)benzenesulfonic acid
DTXSID: DTXSID40891333
PubChem: 0
CPDAT: 0

Chemical Lists and Categories

Category example – PAHs

EPA United States Environmental Protection Agency

Polycyclic aromatic hydrocarbons

130498-29-2 | DTXSID3044043

Searched by DSSTox Substance Id.

Wikipedia

Polycyclic aromatic hydrocarbons (**PAHs**, also ***polyaromatic hydrocarbons*** or ***polynuclear aromatic hydrocarbons***) are hydrocarbons—organic compounds containing only carbon and hydrogen—that are composed of multiple aromatic rings (organic rings in which the electrons are delocalized). The simplest such chemicals are naphthalene, having two aromatic rings, and the three-ring compounds anthracene and phenanthrene.
PAHs are uncharged, non-polar molecules found

...

Read more

Presence in Lists

Federal

ATSDR: Toxic Substar

EPA: Toxicity Values

US State

None.

Polycyclic aromatic hydrocarbons

130498-29-2 | DTXSID3044043

Searched by DSSTox Substance Id.

DETAILS
RELATED SUBSTANCES
SYNONYMS
LINKS
BIOACTIVITY
EXPOSURE
HAZARD
COMMENTS
PROPERTIES
LITERATURE

73 chemicals

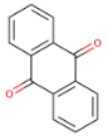
Select all | Download | Send to Batch Search | Relationship | DTXSID | PubChem | CPDAT | Hide chemicals that are: | Filter by Name or CASRI

Searched Chemical

73 related chemical structures with this substance

Polycyclic aromatic hydrocarbons
DTXSID: DTXSID3044043
PubChem: 0
CPDAT: 87

Component

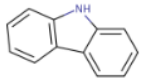


Anthraquinone
DTXSID: DTXSID3020095
PubChem: 138
CPDAT: 34

Component

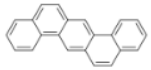
Benzo(a)pyrene
DTXSID: DTXSID2020139
PubChem: 161
CPDAT: 81

Component



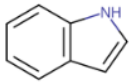
Carbazole
DTXSID: DTXSID4020248
PubChem: 147
CPDAT: 2

Component



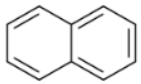
Dibenz(a,h)anthracene
DTXSID: DTXSID9020409
PubChem: 73
CPDAT: 28

Component



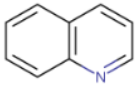
Indole
DTXSID: DTXSID0020737

Component



Naphthalene
DTXSID: DTXSID8020913

Component

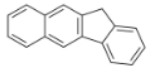


Quinoline
DTXSID: DTXSID1021798

Component

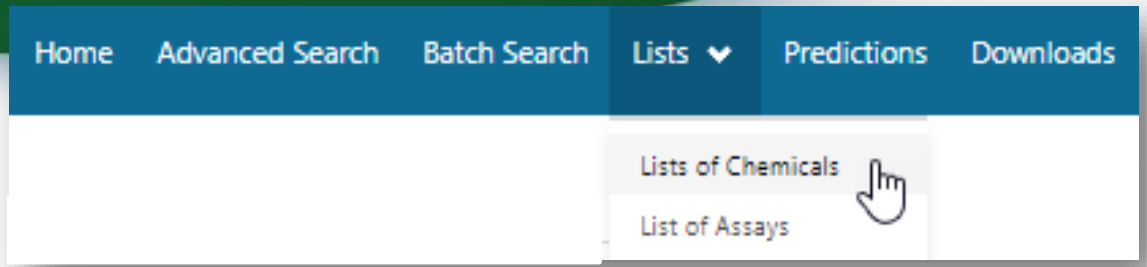
Chrysene
DTXSID: DTXSID0022432

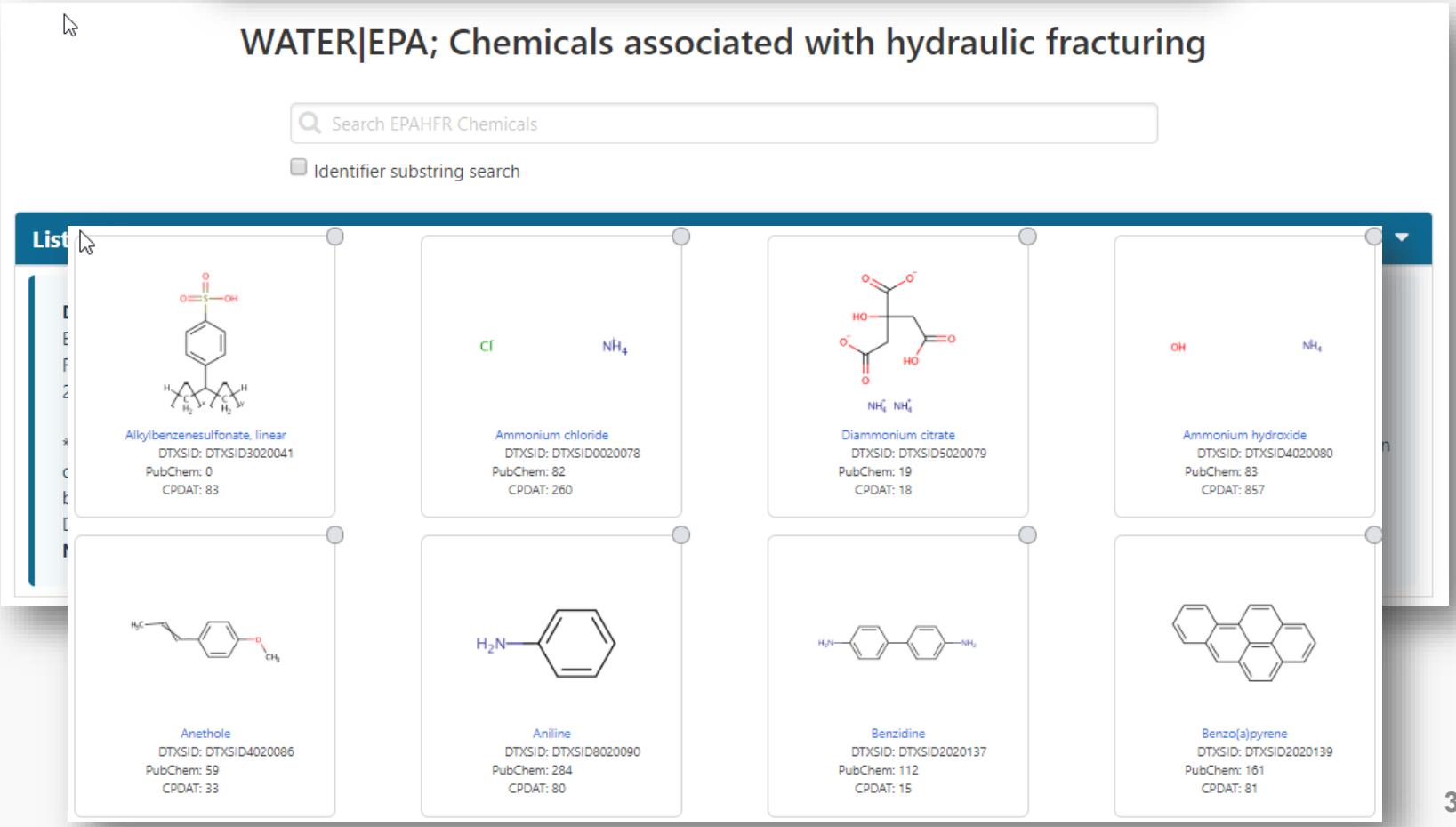
Component



2,3-Benzofluorene
DTXSID: DTXSID1022477

EPAHFR: Hydraulic Fracturing





List of Assays

EPA United States Environmental Protection Agency

Assay List

Download | 10 | ATG × | OT × | NHEERL_PADILLA × | Search query | Copy page URL

ACEA Biosciences
Apredica
Attagene
Bioseek
Novascreen
Odyssey Thera
Tox21/NCGC
Ceetox/OpAns
CellzDirect
NHEERL Padilla Lab
NCCT's Lab
Tanguay Lab
NHEERL's Hunter Lab
NHEERL Stoker & Laws Lab
NHEERL Med Lab

Assay Component Endpoint Name	Details	Active Hits	Description	Gene Symbols
ATG_Ahr_CIS_up		573 / 3807	Data from the assay component ATG_A assay endpoint. This assay endpoint, ATG_Ahr_CIS_up, was analyz ction relative to DMSO as the negative control and baseline of activi reporter, measures of mRNA for gain-of-signal activity can be used to u e at the transcription factor-level as they relate to the gene AHR. Furtherm be referred to as a primary readout, because this assay has produ s where this one serves a reporter gene function. To generalize the intend targets, this assay endpoint is annotated to the "dna binding" intend subfamily is "basic helix-loop-helix protein".	AHR
ATG_AP_1_CIS_up		658 / 3807	Data from the assay component ATG_A assay endpoint. This assay endpoint, ATG_AP_1_CIS_up, was analy ection relative to DMSO as the negative control and baseline of activi reporter, measures of mRNA for gain-of-signal activity can be used to u e at the transcription factor-level as they relate to the gene FOS and JUN. F oint can be referred to as a primary readout, because this assay has produ s where this one serves a reporter gene function. To generalize the intend targets, this assay endpoint is annotated to the "dna binding" intended target family, where the subfamily is "basic leucine zipper".	FOS JUN
ATG_AP_2_CIS_up		47 / 3807	Data from the assay component ATG_AP_2_CIS was analyzed into 1 assay endpoint. This assay endpoint, ATG_AP_2_CIS_up, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of inducible reporter, measures of mRNA for	TFAP2A TFAP2B TFAP2D

From Assay to Chemicals…

EPA United States Environmental Protection Agency

Assay Endpoint Name: ACEA_ER_80hr

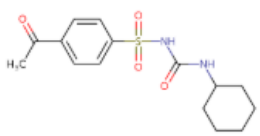
Assay Details

Assay Endpoint Name: ACEA_ER_80hr

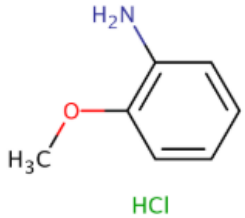
Assay Source Description: ACEA Biosciences, Inc. (ACEA) is a privately owned biotechnology company that developed a real-time, label-free, cell-based assay system based on a microelectronic readout called xCELLigence.

425 of 3031 chemicals visible

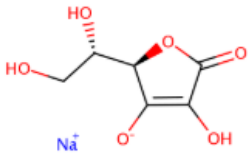
Select all | Download | Send to Batch Search | Default | CASRN ✕ | TOXCAST ✕ | PubMed ✕ | Inactive ✕ | Filter by Name or CASRN



Acetohexamide
CASRN: 968-81-0
TOXCAST: 4/376
PubMed: 235



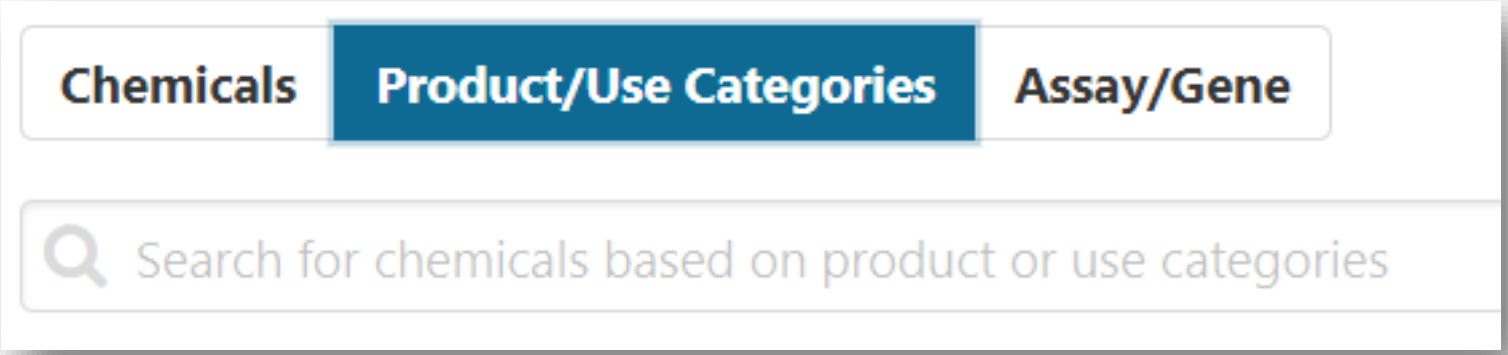
2-Methoxyaniline hydrochloride
CASRN: 134-29-2
TOXCAST: 17/385
PubMed: 46



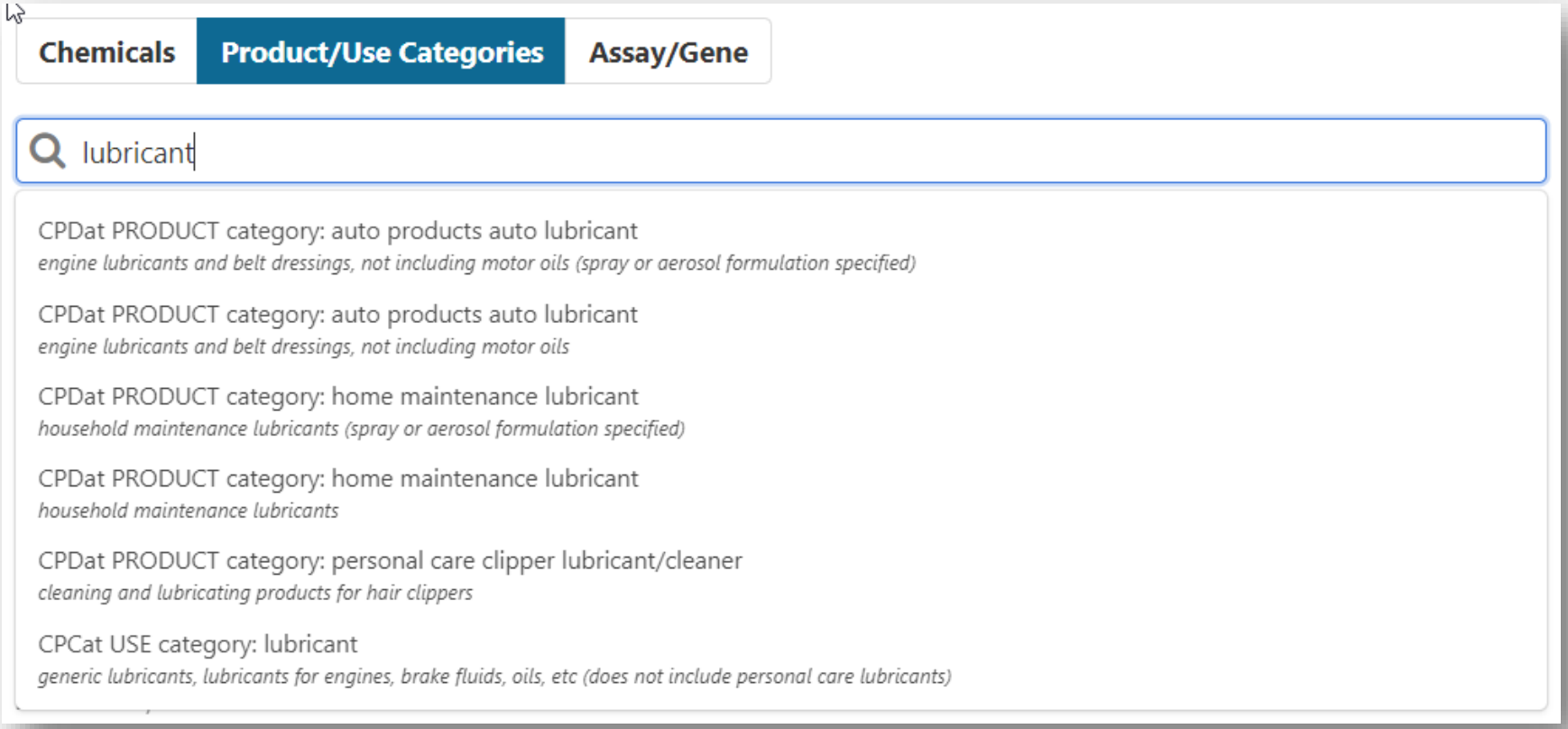
Sodium L-ascorbate
CASRN: 134-03-2
TOXCAST: 20/662
PubMed: 38756

Sodium azide
CASRN: 26628-22-8
TOXCAST: 26/644
PubMed: 1866

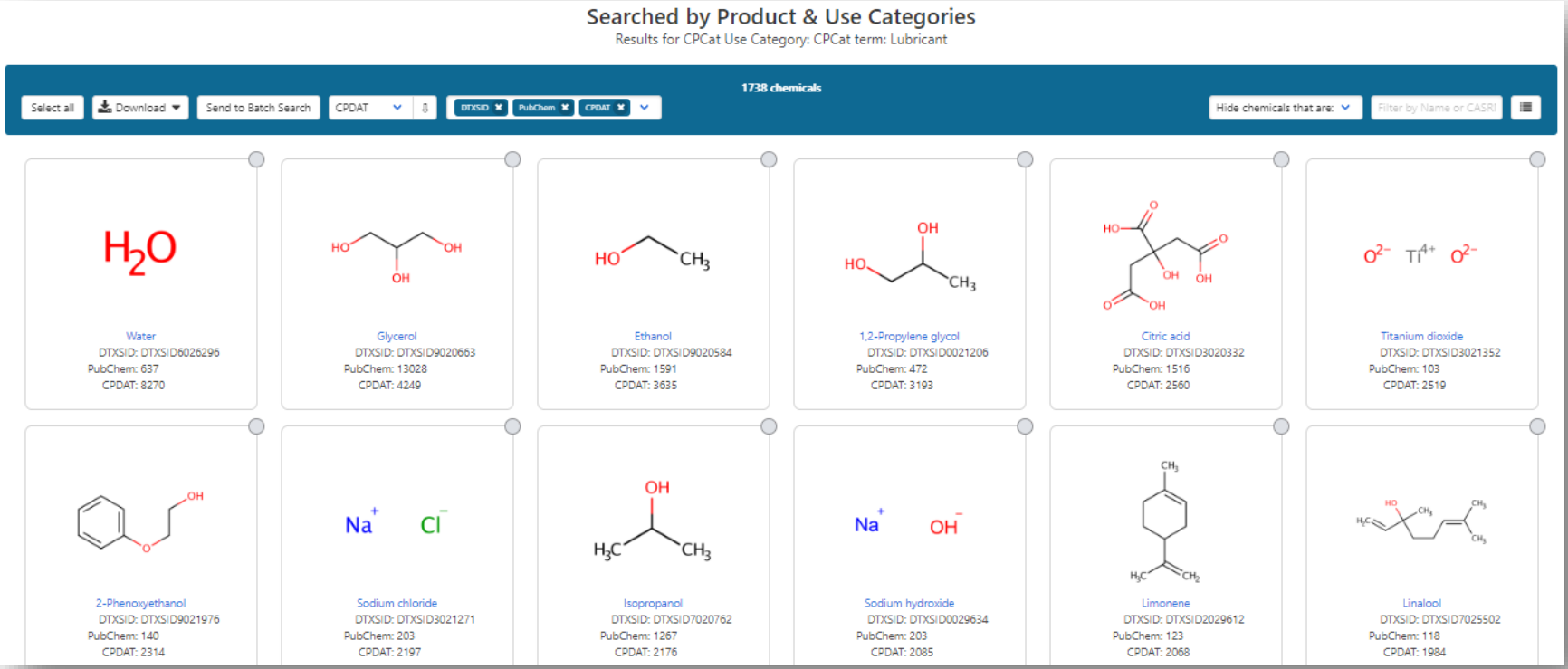
Other Searches



Product/Use Categories



Lubricant


Searched by Product & Use Categories
Results for CPCat Use Category: CPCat term: Lubricant
1738 chemicals
Select all
Download
Send to Batch Search
CPDAT
DTXSID
PubChem
CPDAT
Hide chemicals that are:
Filter by Name or CASRN
Water
DTXSID: DTXSID6026296
PubChem: 637
CPDAT: 8270
Glycerol
DTXSID: DTXSID9020663
PubChem: 13028
CPDAT: 4249
Ethanol
DTXSID: DTXSID9020584
PubChem: 1591
CPDAT: 3635
1,2-Propylene glycol
DTXSID: DTXSID0021206
PubChem: 472
CPDAT: 3193
Citric acid
DTXSID: DTXSID3020332
PubChem: 1516
CPDAT: 2560
Titanium dioxide
DTXSID: DTXSID3021352
PubChem: 103
CPDAT: 2519
2-Phenoxyethanol
DTXSID: DTXSID9021976
PubChem: 140
CPDAT: 2314
Sodium chloride
DTXSID: DTXSID3021271
PubChem: 203
CPDAT: 2197
Isopropanol
DTXSID: DTXSID7020762
PubChem: 1267
CPDAT: 2176
Sodium hydroxide
DTXSID: DTXSID0029634
PubChem: 203
CPDAT: 2085
Limonene
DTXSID: DTXSID2029612
PubChem: 123
CPDAT: 2068
Linalool
DTXSID: DTXSID7025502
PubChem: 118
CPDAT: 1984

Lots of UVCBS in Commerce….

1 related chemical structure with this substance

Butoxypolypropylene glycol
DTXSID: DTXSID3034404
PubChem: 0
CPDAT: 437

0 related chemical structures with this substance

Fatty acids, tall-oil
DTXSID: DTXSID0028088
PubChem: 0
CPDAT: 436

Poly(oxy-1,2-ethanediyl), alpha-tridecyl-...
DTXSID: DTXSID8043993
PubChem: 0
CPDAT: 435

1 related chemical structure with this substance

Polyoxyethylene (20) oleylether
DTXSID: DTXSID1027714
PubChem: 0
CPDAT: 435

0 related chemical structures with this substance

Soy oil
DTXSID: DTXSID8027660
PubChem: 0
CPDAT: 435

0 related chemical structures with this substance

Bentonite
DTXSID: DTXSID6030782
PubChem: 0
CPDAT: 433

0 related chemical structures with this substance

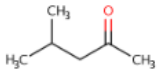
Distillates, petroleum, hydrotreated heav...
DTXSID: DTXSID3028217
PubChem: 0
CPDAT: 433

1 related chemical structure with this substance

Edifas B
DTXSID: DTXSID2020555
PubChem: 0
CPDAT: 433

0 related chemical structures with this substance

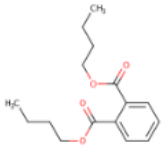
Coconut oil
DTXSID: DTXSID8027664
PubChem: 0
CPDAT: 432



4-Methyl-2-pentanone
DTXSID: DTXSID5021889
PubChem: 173
CPDAT: 428

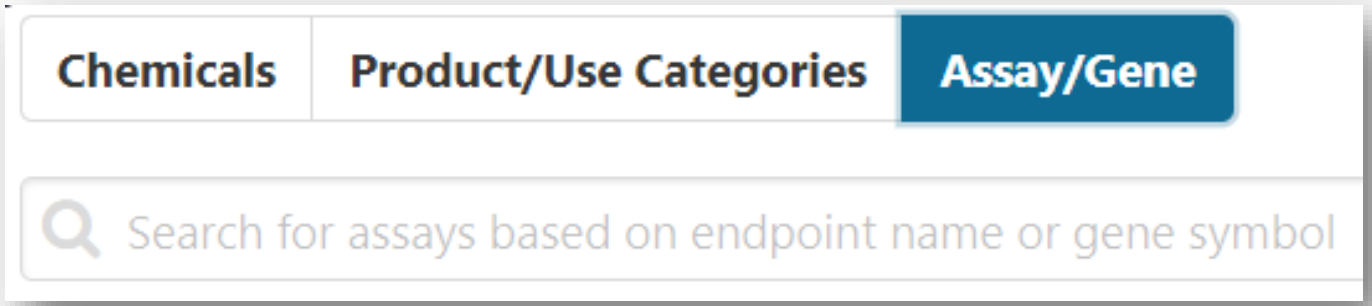
0 related chemical structures with this substance

Distillates, petroleum, solvent-refined he...
DTXSID: DTXSID9028172
PubChem: 0
CPDAT: 426



Dibutyl phthalate
DTXSID: DTXSID2021781
PubChem: 138
CPDAT: 421

Other Searches



Chemical-Biology

Assay/Gene Search

Chemicals | Product/Use Categories | **Assay/Gene**

ESR

ASSAY: TOX21_ESRE_BLA_ch1
Data from the assay component TOX21_ESRE_BLA_ch1 was analyzed into 1 a...

ASSAY: TOX21_ESRE_BLA_ch2
Data from the assay component TOX21_ESRE_BLA_ch2 was analyzed into 1 a...

ASSAY: TOX21_ESRE_BLA_ratio
Data from the assay component TOX21_ESRE_BLA_ratio was analyzed into 1...

ASSAY: TOX21_ESRE_BLA_viability
TOX21_ESRE_BLA_viability used a type of growth reporter where loss-of-...

GENE: ESR1
estrogen receptor 1

GENE: esr1.L
estrogen receptor 1 L homeolog

GENE: ESR2
estrogen receptor 2 (ER beta)

GENE: esr2.L
estrogen receptor 2 L homeolog

Assay/Gene Search
Finds associated assays/chemicals

EPA United States Environmental Protection Agency

Assay List

Download | 10 | Filter by vendor | ESR1 | Copy Filtered Lists URL

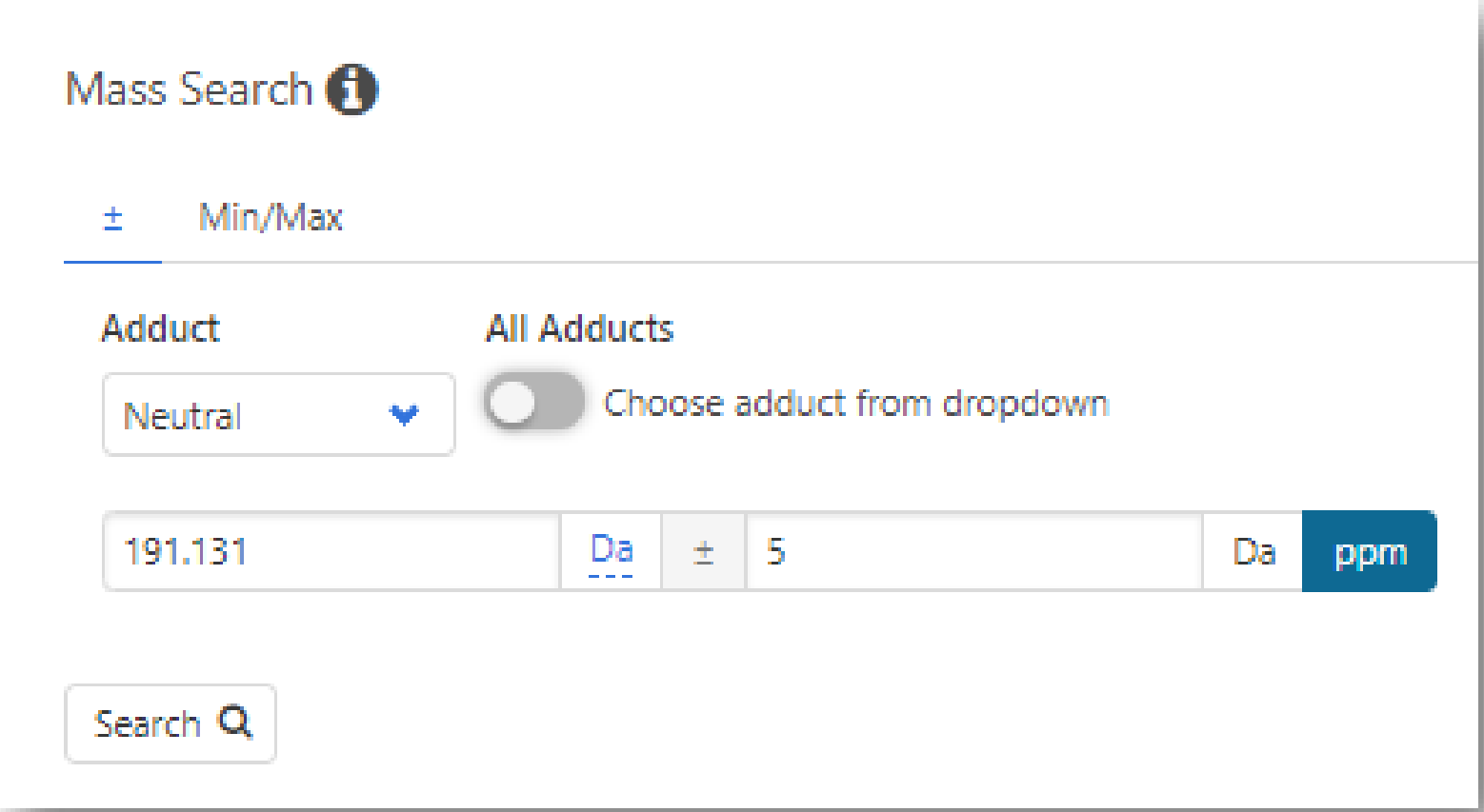
Assay Component Endpoint Name	Details	Active Hits	Description	Gene Symbols
ACEA_ER_80hr		425 / 3031	Data from the assay component ACEA_ER_80hr was analyzed into 2 assay endpoints. This assay endpoint, ACEA_ER_80hr_Positive, was analyzed in the positive fitting direction relative to DMSO as the negative 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 ESR1. 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".	ESR1
ATG_ERE_CIS_up		992 / 3807	Data from the assay component ATG_ERE_CIS was analyzed into 1 assay endpoint. This assay endpoint, ATG_ERE_CIS_up, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of inducible reporter, measures of mRNA for gain-of-signal activity can be used to understand the reporter gene at the transcription factor-level as they relate to the gene ESR1. 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 reporter gene 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".	ESR1

<< < 1 2 3 4 > >>

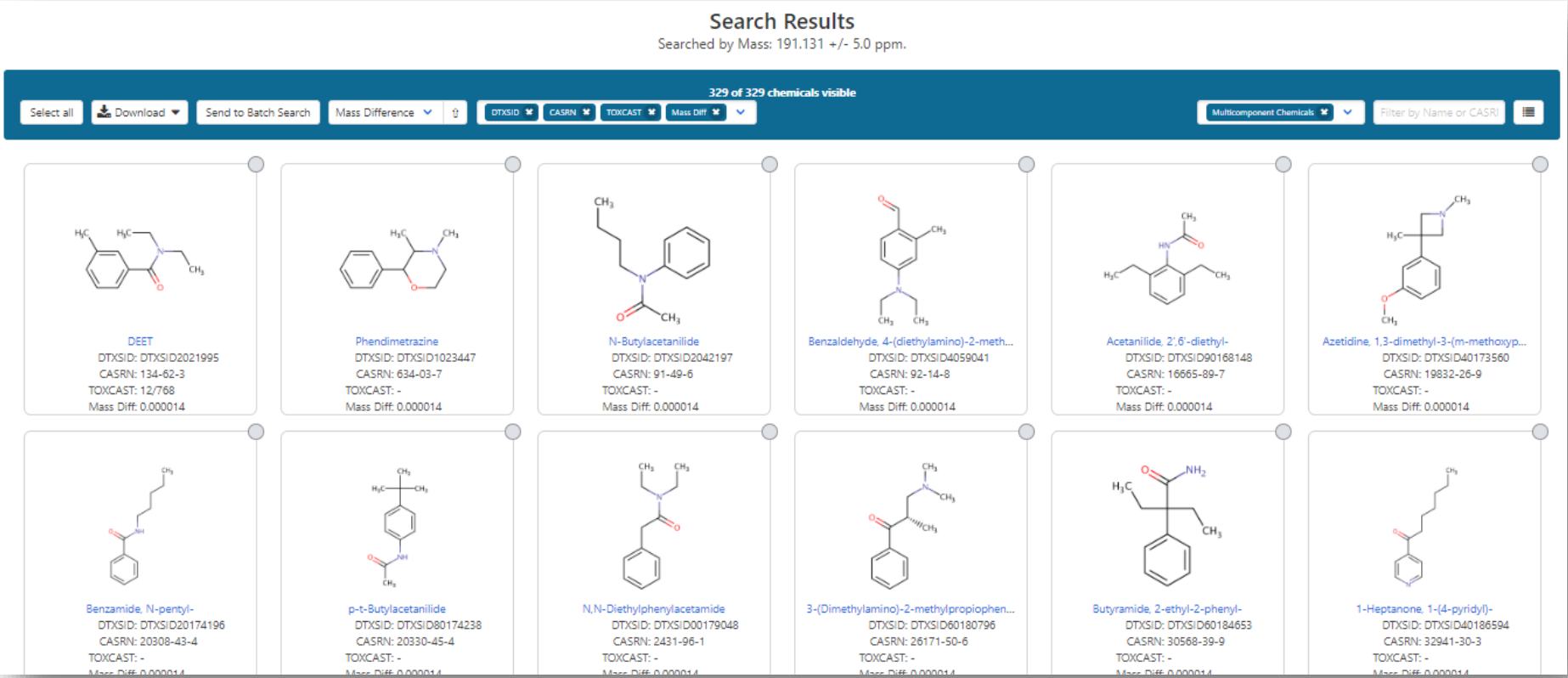
Showing 1 to 10 of 32 records

Mass/Formula Searching and Metadata Ranking

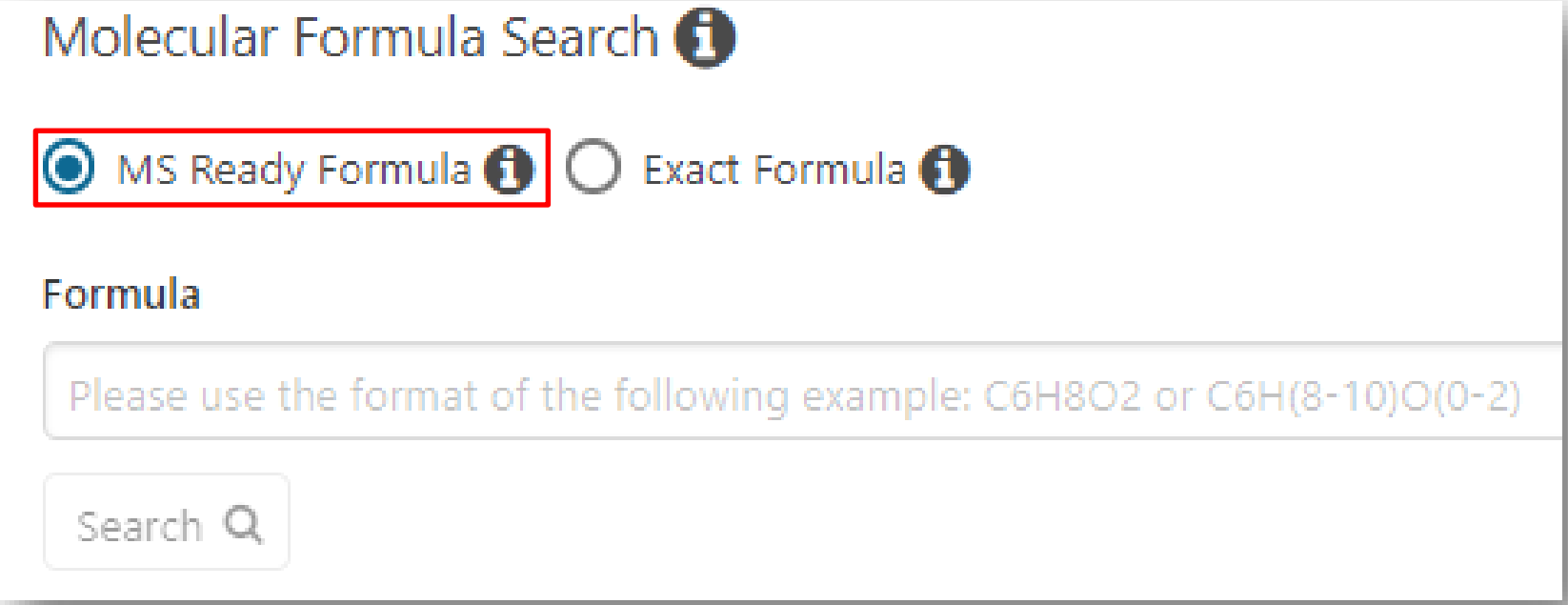
Advanced Searches
Mass Search



Advanced Searches
Mass Search

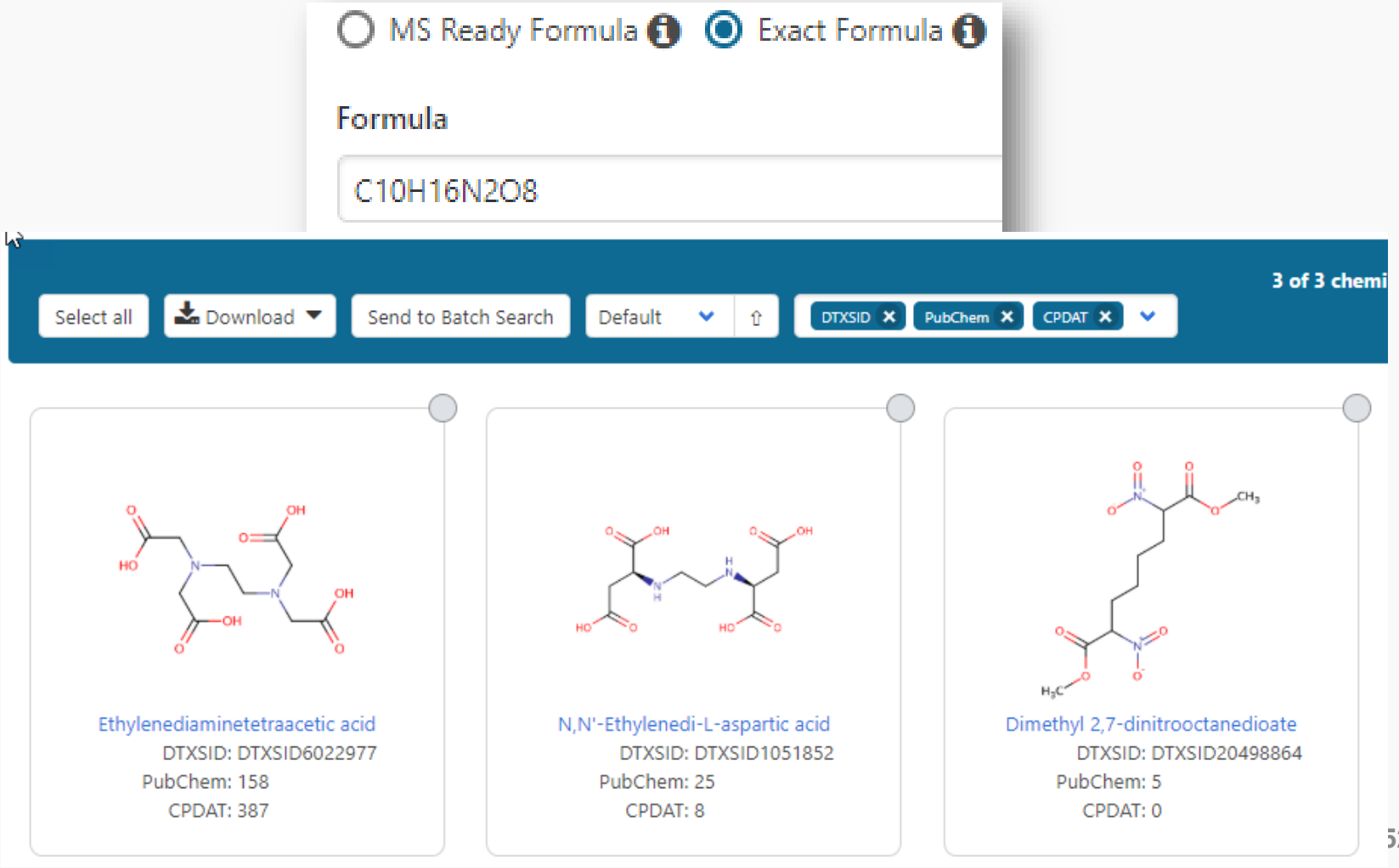


MS-Ready Structures for **Formula Search**



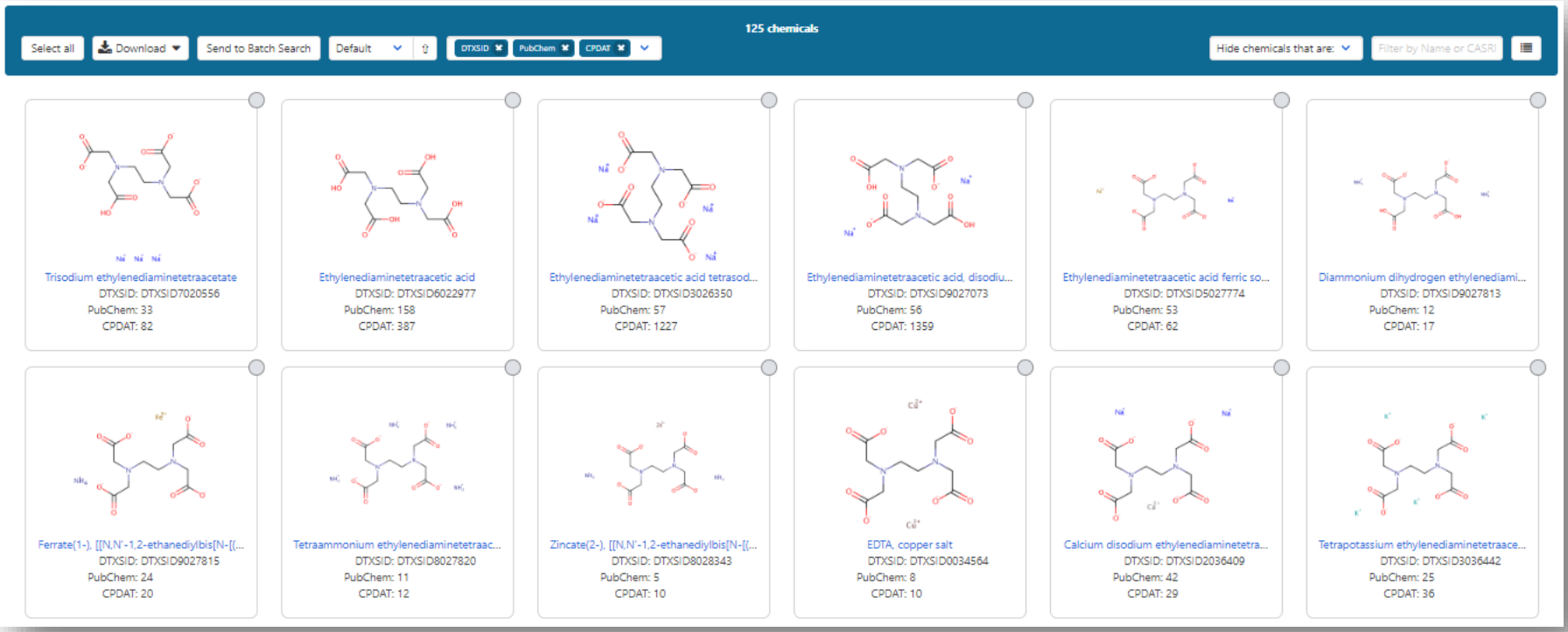
MS-Ready Mappings

- **EXACT Formula**: C10H16N2O8: 3 Hits



MS-Ready Mappings

- **Same** Input Formula: C10H16N2O8
- **MS Ready Formula** Search: **125** Chemicals



Mass Spec Focused Applications

Analytical and Bioanalytical Chemistry (2019) 411:853–866
https://doi.org/10.1007/s00216-018-1435-6

RESEARCH PAPER

EPA's non-targeted analysis collaborative trial (ENTACT): genesis, design, and initial findings

Elin M. Ulrich[1] · Jon R. Sobus[1] · Christopher M. Grulke[2] · Ann M. Richard[2] · Seth R. Newton[1] · Mark J. Strynar[1] · Kamel Mansouri[3,4] · Antony J. Williams[2]

Analytical and Bioanalytical Chemistry (2019) 411:835–851
https://doi.org/10.1007/s00216-018-1526-4

RESEARCH PAPER

Using prepared mixtures of ToxCast chemicals to evaluate non-targeted analysis (NTA) method performance

Jon R. Sobus[1] · Jarod N. Grossman[2,3] · Alex Chao[2] · Randolph Singh[4] · Antony J. Williams[5] · Christopher M. Grulke[5] · Ann M. Richard[5] · Seth R. Newton[1] · Andrew D. McEachran[4] · Elin M. Ulrich[1]

Mass Spec Focused Applications

EPA United States Environmental Protection Agency

Journal of Exposure Science & Environmental Epidemiology (2018) 28:411–426
https://doi.org/10.1038/s41370-017-0012-y

REVIEW ARTICLE

Integrating tools for non-targeted analysis research and chemical safety evaluations at the US EPA

Jon R. Sobus[1] · John F. Wambaugh[2] · Kristin K. Isaacs[1] · Antony J. Williams[2] · Andrew D. McEachran[3] · Ann M. Richard[2] · Christopher M. Grulke[2] · Elin M. Ulrich[1] · Julia E. Rager[3,4] · Mark J. Strynar[1] · Seth R. Newton[1]

Environmental Science & Technology

Article

Cite This: *Environ. Sci. Technol.* 2018, 52, 3125–3135

pubs.acs.org/est

Suspect Screening Analysis of Chemicals in Consumer Products

Katherine A. Phillips,[†] Alice Yau,[‡] Kristin A. Favela,[‡] Kristin K. Isaacs,[†] Andrew McEachran,[§,∥] Christopher Grulke,[∥] Ann M. Richard,[∥] Antony J. Williams,[∥] Jon R. Sobus,[†] Russell S. Thomas,[∥] and John F. Wambaugh*[,∥]

Batch Searching

Batch Searching

- Singleton searches are useful but people generally want data on LOTS of chemicals!

- Typical questions
  - What is the list of chemicals for the formula $C_xH_yO_z$
  - What is the list of chemicals for a mass +/- error
  - Can I get chemical lists in Excel files? In SDF files?
  - Can I include properties in the download file?

Aggregate data for a list of chemicals

ELSEVIER

Trends in Environmental Analytical Chemistry

Volume 20, October 2018, e00059

TrEAC

Opioid occurrence in environmental water samples—A review

Marina Celia Campos-Mañas [a], Imma Ferrer [b], E.Michael Thurman [b], Ana Agüera [a]

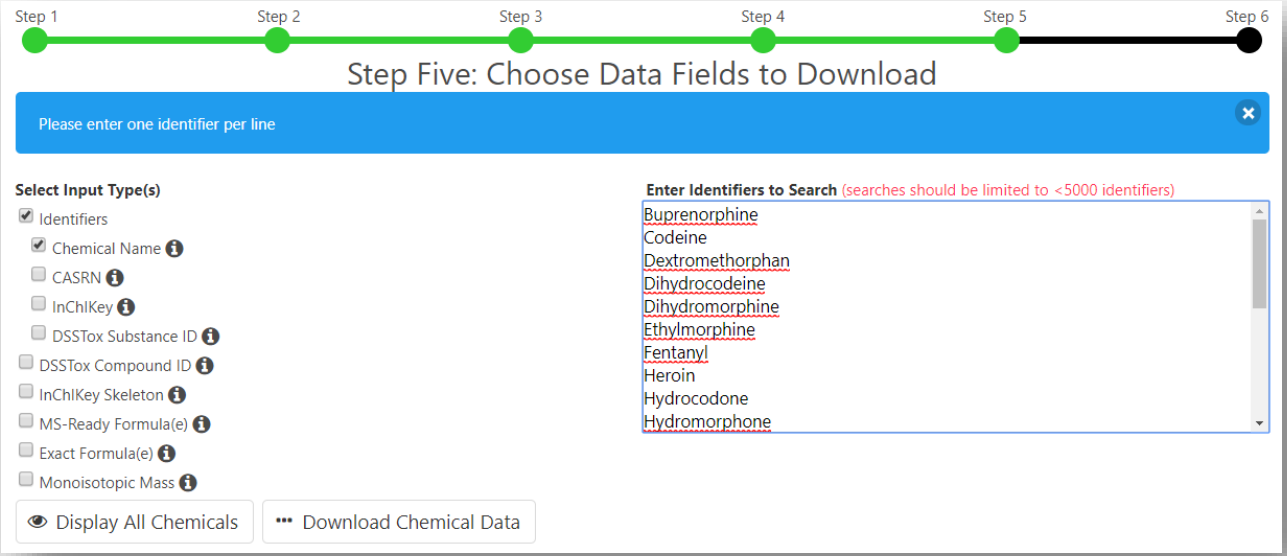
Show more

https://doi.org/10.1016/j.teac.2018.e00059

Get rights and content

Batch Search Names

Buprenorphine
Codeine
Dextromethorphan
Dihydrocodeine
Dihydromorphine
Ethylmorphine
Fentanyl
Heroin
Hydrocodone
Hydromorphone
Ketamine
Meperidine
Methadone
Morphine
Morphinone
Naloxone
Naltriben
Oxycodone
Oxymorphone
Propoxyphene
Sufentanil
Tramadol



Excel Download

INPUT	FOUND_BY	DTXSID
Buprenorphine	Approved Name	DTXSID2022705
Codeine	Approved Name	DTXSID2020341
Dextromethorphan	Approved Name	DTXSID3022908
Dihydrocodeine	Approved Name	DTXSID5022936
Dihydromorphine	Approved Name	DTXSID7048908
Ethylmorphine	Approved Name	DTXSID1046760
Fentanyl	Approved Name	DTXSID9023049
Heroin	Synonym	DTXSID6046761
Hydrocodone	Approved Name	DTXSID8023131
Hydromorphone	Approved Name	DTXSID8023133
Ketamine	Approved Name	DTXSID8023187
Meperidine	Approved Name	DTXSID9023253
Methadone	Approved Name	DTXSID7023273
Morphine	Approved Name	DTXSID9023336

Add Other Data of Interest

EPA United States Environmental Protection Agency

Chemical Identifiers

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

Structures

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

Intrinsic And Predicted Properties

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

INPUT	DTXSID	CASRN	MOLECULAR_F(	MONOISOTOPIC	MS_READY_SMI
Buprenorph	DTXSID202	52485-79-7	C29H41NO4	467.3035588	[H]C12CC3=C4C(
Codeine	DTXSID202	76-57-3	C18H21NO3	299.1521435	[H]C12CC3=C4C(
Dextrometh	DTXSID302	125-71-3	C18H25NO	271.1936144	[H]C12CC3=C(C=
Dihydrocod	DTXSID502	125-28-0	C18H23NO3	301.1677936	[H]C12CC3=C4C(
Dihydromor	DTXSID704	509-60-4	C17H21NO3	287.1521435	[H]C12CC3=C4C(
Ethylmorph	DTXSID104	76-58-4	C19H23NO3	313.1677936	[H]C12CC3=C4C(
Fentanyl	DTXSID902	437-38-7	C22H28N2O	336.2201635	CCC(=O)N(C1CC
Heroin	DTXSID604	561-27-3	C21H23NO5	369.1576228	[H]C12CC3=C4C(
Hydrocodor	DTXSID802	125-29-1	C18H21NO3	299.1521435	[H]C12CC3=C4C(
Hydromorpl	DTXSID802	466-99-9	C17H19NO3	285.1364935	[H]C12CC3=C4C(
Ketamine	DTXSID802	6740-88-1	C13H16ClNO	237.0920418	CNC1(CCCCC1=(
Meperidine	DTXSID902	57-42-1	C15H21NO2	247.1572289	CCOC(=O)C1(CC
Methadone	DTXSID702	76-99-3	C21H27NO	309.2092645	CCC(=O)C(CC(C)
Morphine	DTXSID902	57-27-2	C17H19NO3	285.1364935	[H]C12CC3=C4C(
Morphinone	DTXSID501	467-02-7	C17H17NO3	283.1208434	[H]C12CC3=C4C(
Naloxone	DTXSID802	465-65-6	C19H21NO4	327.1470582	[H]C12CC3=C4C(
Naltriben	-	-	-	-	-
Oxycodone	DTXSID502	76-42-6	C18H21NO4	315.1470582	[H]C12CC3=C4C(
Oxymorpho	DTXSID502	76-41-5	C17H19NO4	301.1314081	[H]C12CC3=C4C(
Propoxyphe	DTXSID102	469-62-5	C22H29NO2	339.2198292	CCC(=O)OC(CC1
Sufentanil	DTXSID602	56030-54-7	C22H30N2O2S	386.2027994	CCC(=O)N(C1=C
Tramadol	DTXSID908	27203-92-5	C16H25NO2	263.188529	COC1=CC=CC(=

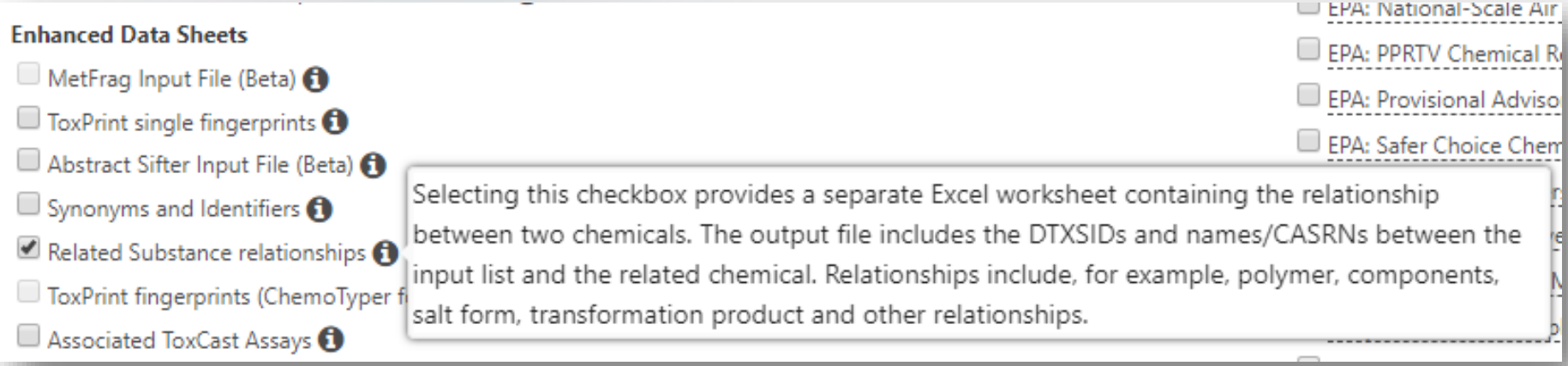
Batch Search in specific lists

INPUT	DTXSID	MASSBANKREF	NEMILIST	WRTMSD	NORMANPRI	SUSDAT
Buprenorph	DTXSID202	-	-	Y	-	Y
Codeine	DTXSID202	Y	Y	Y	Y	Y
Dextrometh	DTXSID302	Y	Y	Y	-	Y
Dihydrocod	DTXSID502	Y	-	Y	Y	Y
Dihydromor	DTXSID704	-	-	-	-	Y
Ethylmorph	DTXSID104	-	-	Y	-	Y
Fentanyl	DTXSID902	Y	-	Y	-	Y
Heroin	DTXSID604	Y	-	Y	Y	Y
Hydrocodor	DTXSID802	Y	Y	Y	Y	Y
Hydromorpl	DTXSID802	-	-	Y	-	Y
Ketamine	DTXSID802	Y	-	Y	-	Y
Meperidine	DTXSID902	Y	-	Y	-	Y
Methadone	DTXSID702	Y	Y	Y	-	Y
Morphine	DTXSID902	Y	Y	Y	Y	Y
Morphinone	DTXSID501	-	-	-	-	Y
Naloxone	DTXSID802	-	-	Y	-	Y
Naltriben	-	-	-	-	-	-
Oxycodone	DTXSID502	Y	Y	Y	Y	Y
Oxymorpho	DTXSID502	-	-	Y	-	Y
Propoxyphe	DTXSID102	Y	Y	Y	-	Y
Sufentanil	DTXSID602	-	-	Y	-	Y
Tramadol	DTXSID908	Y	Y	Y	Y	Y

Built in Checks…

Ingredient Name	Cas Number	FIXED C	FOUND_BY
D-Glucitol, 1-deoxy-1(methylamino)-, N-C12 acyl derivs.	87246-72-8	87246-72-8	Alternate CAS-RN
6-Acetyl-1,1,2,4,4,7-hexamethyl tetralin	1506-02-1	1506-02-1	Alternate CAS-RN
Spiro(isobenzofuran-1(3H),9'-(9H)xanthen)-3-one,3',6'-dihydroxy-2',4',5',7'-tetrai	568-63-8	568-63-8	Alternate CAS-RN
2-Propenoic acid, 2-methyl-, 2-((2,3,3a,4,7,7a(or 3a,4,5,6,7,7a)-hexahydro-4,7-met	68586-19-6	68586-19-	Alternate CAS-RN
Sodium N-cis-9-octadecenyl-N-methyltaurine	7346-80-7	7346-80-7	Alternate CAS-RN
Oxirane, methyl-, polymer with oxirane, ether with oxybis(propanol) (2:1)	63466-93-3	63466-93-	Alternate CAS-RN
Spiro(isobenzofuran-1(3H),9'-(9H)xanthen)-3-one, 2',4',5',7',-tetrabromo-3',6'-dih	548-26-5	548-26-5	Alternate CAS-RN
1-Octadecene	111-88-9	111-88-9	Checksum Failed
1,2,4-Benzenetricarboxylic acid, tris(decyl) ester,mixt. with 2-[[3-[(1-oxodecyl)ox	187273-40-6	187273-40	Checksum Failed
Acetic acid ethenyl ester, polymer with ethenol	24213-24-5	24213-24-	Checksum Failed
1,4-Benzenedicarbixylic acid, dimethyl ester,polymer with 1,4-cyclohexanedimet	25640-14-0	25640-14-	Checksum Failed
Poly(oxy-1,2-ethanediyl), .alpha.,.alpha.'-[[methyl[3-(tridecyloxy)propyl]imino]d	68601-19-5	68601-19-	Checksum Failed
Cyclohexanol, 5-methyl-2-(1-methylethyl)-, acetate, (1.alpha.,2.beta.,5.alpha.)-(.	29066-34-0	29066-34-	Deleted CAS-RN
Ethoxylated lanolin	9/6/8039	8039-09-6	Deleted CAS-RN
1-Octanaminium, N-methyl-N,N-dioctyl-, chloride	76925-99-0	76925-99-	Deleted CAS-RN
Nitric acid, copper(2+) salt	10031-43-3; 3251-23	10031-43-	Not CAS Number Format
Fatty acids, coco, reaction products with 2-{(2-aminoethyl)amino}ethanol, bis(2-c	132647-09-7; 68411-	132647-09	Not CAS Number Format
Mixture of 2,2'-Dimorpholinodiethyl ether with 1,2-dimorpholinoethane	1723-94-0; 6425-39-	1723-94-0	Not CAS Number Format
(Chloropropyl)trimethoxysilane	2530-87-2; 25512-39	2530-87-2	Not CAS Number Format

Related Substance Relationships



	A	B	C	D	E	
1	INPUT	DTXSID	PREFERRED_NAME	HAS_RELATIONSHIP_WITH	RELATED_DTXSID	RELATED_PREFERRED_NAM
2	xylenes	DTXSID2021446	Xylenes	Transformation Product	DTXSID40176394	N-Benzoylalanine
3	xylenes	DTXSID2021446	Xylenes	Component	DTXSID6026298	m-Xylene
4	xylenes	DTXSID2021446	Xylenes	Component	DTXSID3021807	o-Xylene
5	xylenes	DTXSID2021446	Xylenes	Component	DTXSID2021868	p-Xylene
6	xylenes	DTXSID2021446	Xylenes	Predecessor: Component	DTXSID9021421	Xylenes; defined mixture 1
7	xylenes	DTXSID2021446	Xylenes	Predecessor: Component	DTXSID7021447	Xylenes; defined mixture 2
8	xylenes	DTXSID2021446	Xylenes	Predecessor: Component	DTXSID30891529	Total Petroleum Hydrocarbons
9	xylenes	DTXSID2021446	Xylenes	Markush Child	DTXSID3021807	o-Xylene
10	xylenes	DTXSID2021446	Xylenes	Markush Child	DTXSID6026298	m-Xylene
11	xylenes	DTXSID2021446	Xylenes	Markush Child	DTXSID2021868	p-Xylene

Batch Searching Formula/Mass

Batch Search

Step 1 Step 2 Step 3 Step 4 Step 5 Step 6

Step Five: Choose Data Fields to Download

Please enter one identifier per line

Select Input Type(s)

+/- 5 ppm

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

Display All Chem

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

41.0265
56.02621
53.0265
58.0418
93.0578
113.9639
151.8754
69.9377
77.9872

This search is based on what we refer to as "Mass Spec (MS) Ready" structures. All chemicals within the database are treated in a manner such that all are desalted, mixtures are separated, and stereochemistry is removed as Mass Spectrometry detects the major components of a salt or mixture and is insensitive to stereochemistry. As an example, a search for the monoisotopic mass of phenol will return phenol, sodium phenolate and calcium phenoxide. See the publication for more details: https://doi.org/10.1186/s13321-018-0299-2.

Searching batches using MS-Ready Formula (or mass) searching

	A	B	C	D	E	F	G
1	INPUT	DTXSID	CASRN	PREFERRED NAME	MOL FORMULA	MONOISOTOPIC MASS	DATA SOURCES
2	C14H22N2O3	DTXSID2022628	29122-68-7	Atenolol	C14H22N2O3	266.163042576	46
3	C14H22N2O3	DTXSID0021179	6673-35-4	Practolol	C14H22N2O3	266.163042576	32
4	C14H22N2O3	DTXSID4048854	841-73-6	Bucolome	C14H22N2O3	266.163042576	20
5	C14H22N2O3	DTXSID1045407	13171-25-0	Trimetazidine dihydrochloride	C14H24Cl2N2O3	338.116398	19
6	C14H22N2O3	DTXSID0045753	56715-13-0	R-(+)-Atenolol	C14H22N2O3	266.163042576	19
7	C14H22N2O3	DTXSID2048531	5011-34-7	Trimetazidine	C14H22N2O3	266.163042576	14
8	C14H22N2O3	DTXSID10239405	93379-54-5	Esatenolol	C14H22N2O3	266.163042576	12
9	C14H22N2O3	DTXSID50200634	52662-27-8	N-(2-Diethylaminoethyl)-2-(4-hydroxyphenoxy)acetamide	C14H22N2O3	266.163042576	7
10	C14H22N2O3	DTXSID4020111	51706-40-2	dl-Atenolol hydrochloride	C14H23ClN2O3	302.1397203	6
11	C14H22N2O3	DTXSID1068693	51963-82-7	Benzenamine, 2,5-diethoxy-4-(4-morpholinyl)-	C14H22N2O3	266.163042576	5
12	C18H34N2O6S	DTXSID3023215	154-21-2	Lincomycin	C18H34N2O6S	406.213757997	35
13	C18H34N2O6S	DTXSID7047803	859-18-7	Lincomycin hydrochloride	C18H35ClN2O6S	442.1904357	22
14	C18H34N2O6S	DTXSID20849438	1398534-62-7	PUBCHEM_71432748	C18H35ClN2O6S	442.1904357	1
15	C10H12N2O	DTXSID1047576	486-56-6	Cotinine	C10H12N2O	176.094963014	40
16	C10H12N2O	DTXSID8075330	50-67-9	Serotonin	C10H12N2O	176.094963014	22
17	C10H12N2O	DTXSID8044412	2654-57-1	4-Methyl-1-phenylpyrazolidin-3-one	C10H12N2O	176.094963014	18
18	C10H12N2O	DTXSID80165186	153-98-0	Serotonin hydrochloride	C10H13ClN2O	212.0716407	11
19	C10H12N2O	DTXSID2048870	29493-77-4	(4R,5S)-4-methyl-5-phenyl-4,5-dihydro-1,3-oxazol-2-amine	C10H12N2O	176.094963014	10
20	C10H12N2O	DTXSID10196105	443-31-2	6-Hydroxytryptamine	C10H12N2O	176.094963014	9
21	C10H12N2O	DTXSID90185693	31822-84-1	1,4,5,6-Tetrahydro-5-phenoxypyrimidine	C10H12N2O	176.094963014	7
22	C10H12N2O	DTXSID40178777	2403-66-9	2-Benzimidazolepropanol	C10H12N2O	176.094963014	7
23	C10H12N2O	DTXSID80157026	13140-86-8	N-Cyclopropyl-N'-phenylurea	C10H12N2O	176.094963014	6
24	C10H12N2O	DTXSID30205607	570-14-9	4-Hydroxytryptamine	C10H12N2O	176.094963014	6
25	C14H18N4O3	DTXSID5023900	17804-35-2	Benomyl	C14H18N4O3	290.137890456	68
26	C14H18N4O3	DTXSID3023712	738-70-5	Trimethoprim	C14H18N4O3	290.137890456	51
27	C14H18N4O3	DTXSID40209671	60834-30-2	Trimethoprim hydrochloride	C14H19ClN4O3	326.1145682	8
28	C14H18N4O3	DTXSID70204210	55687-49-5	Benzenemethanol, 4-((2,4-diamino-5-pyrimidinyl)methyl)-2,	C14H18N4O3	290.137890456	5
29	C14H18N4O3	DTXSID20152671	120075-57-2	6-Methoxy-4-(3-(N,N-dimethylamino)propylamino)-5,8-quin	C14H18N4O3	290.137890456	4
30	C14H18N4O3	DTXSID30213742	63931-79-3	1H-1,2,4-Benzotriazepine-3-carboxylic acid, 4,5-dihydro-4-	C14H18N4O3	290.137890456	3
31	C14H18N4O3	DTXSID30219608	69449-07-6	2,4-Pyrimidinediamine, 5-((3,4,5-trimethoxyphenyl)methyl)-	C14H20N4O4	308.14845514	3
32	C14H18N4O3	DTXSID20241155	94232-27-6	L-Aspartic acid, compound with 5-((3,4,5-trimethoxyphenyl	C18H25N5O7	423.175398165	3
33	C14H18N4O3	DTXSID80241156	94232-28-7	L-Glutamic acid, compound with 5-((3,4,5-trimethoxypheny	C19H27N5O7	437.191048229	3
34	C14H18N4O3	DTXSID20143781	101204-93-7	1H-Pyrido(2,3-e)-1,4-diazepine-2,3,5-trione, 4-(2-(diethylam	C14H18N4O3	290.137890456	3
35	C12H11N7	DTXSID6021373	396-01-0	Triamterene	C12H11N7	253.107593382	52
36	C12H11N7	DTXSID00204465	5587-93-9	Ampyrimine	C12H11N7	253.107593382	7
37	C12H11N7	DTXSID5064621	7300-26-7	Benzenamine, 4-azido-N-(4-azidophenyl)-	C12H9N7	251.091943318	4
38	C12H11N7	DTXSID00848025	90293-82-6	Sulfuric acid--6-phenylpteridine-2,4,7-triamine (1/1)	C12H13N7O4S	351.074973101	1
39	C12H11N7	DTXSID50575293	92310-83-3	(1E)-N-Phenyl-1,2-bis(1H-1,2,4-triazol-1-yl)ethan-1-imine	C12H11N7	253.107593382	1
40	C8H9NO2	DTXSID2020006	103-90-2	Acetaminophen	C8H9NO2	151.063328534	75
41	C8H9NO2	DTXSID6025567	134-20-3	Methyl 2-aminobenzoate	C8H9NO2	151.063328534	60

Real-Time Predictions

Real-Time Predictions

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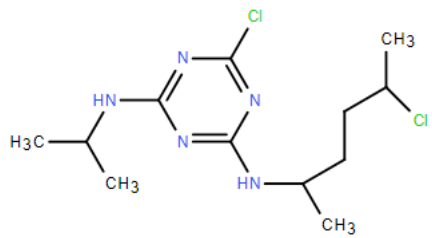
Atrazine

100%



H
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PT

Select properties to predict

T.E.S.T.

- 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

Calculate

Chiral

Real-Time Predictions with detailed calculation reports

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Provider: T.E.S.T.

Download Summary

Property	Experimental Value	Consensus	Hierarchical clustering	Single model	Group contribution	Nearest neighbor
96 hour fathead minnow LC50		4.951 -Log10(mol/L) 3.425 mg/L	5.198 -Log10(mol/L) 1.943 mg/L	5.257 -Log10(mol/L) 1.693 mg/L	5.287 -Log10(mol/L) 1.581 mg/L	4.064 -Log10(mol/L) 26.452 mg/L
48 hour D. magna LC50		4.430 -Log10(mol/L) 11.374 mg/L	4.764 -Log10(mol/L) 5.269 mg/L	5.006 -Log10(mol/L) 3.020 mg/L	4.430 -Log10(mol/L) 11.386 mg/L	3.521 -Log10(mol/L) 92.353 mg/L
48 hour T. pyriformis IGC50			5.272 -Log10(mol/L) 1.639 mg/L			
Oral rat LD50		1.989 -Log10(mol/kg) 3141.571 mg/kg	1.867 -Log10(mol/kg) 4157.591 mg/kg			2.111 -Log10(mol/kg) 2373.843 mg/kg
Bioaccumulation factor		1.321 Log10 20.956	1.209 Log10 16.192	1.585 Log10 38.452	1.517 Log10 32.923	0.974 Log10 9.409
Developmental toxicity		true	true	true		
Ames mutagenicity		false	false			false
Estrogen Receptor RBA						
Estrogen Receptor Binding		false	false	false	false	
Normal boiling point		357.4 °C	334.0 °C		432.8 °C	305.5 °C
Melting point		111.3 °C	98.3 °C		99.1 °C	136.7 °C
Flash point		219.9 °C	272.7 °C		211.4 °C	175.7 °C
Vapor pressure		-6.849 Log10(mmHg) 1.417*10^-7 mmHg	-6.471 Log10(mmHg) 3.382*10^-7 mmHg		-7.617 Log10(mmHg) 2.415*10^-8 mmHg	-6.458 Log10(mmHg) 3.486*10^-7 mmHg
Density		1.211 g/cm³	1.157 g/cm³		1.278 g/cm³	1.197 g/cm³

Real-Time Predictions with detailed calculation reports

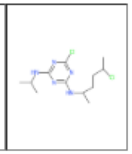
Predicted Vapor pressure at 25°C for ClC=1N=C(N=C(N1)NC(C)CCC(Cl)C)NC(C)C from Consensus method

Prediction results

Endpoint	Experimental value	Predicted value
Vapor pressure at 25°C Log10(mmHg)	N/A	-6.85
Vapor pressure at 25°C mmHg	N/A	1.42E-07

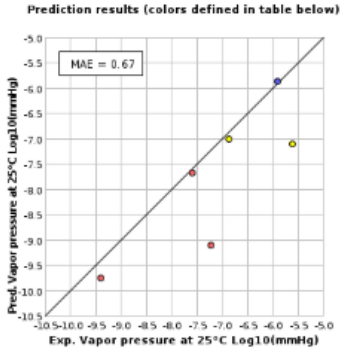
Individual Predictions

Method	Predicted value Log10(mmHg)
Hierarchical clustering	-6.47
Group contribution	-7.62
Nearest neighbor	-6.46



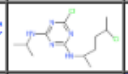
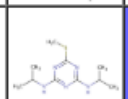
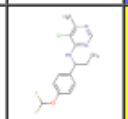
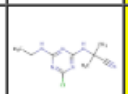
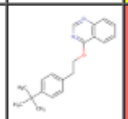
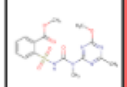
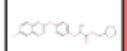
Predictions for the test chemical and for the most similar chemicals in the external tes

If the predicted value matches the experimental values for similar chemicals in the test set (and the similar che



Chemicals	MAE*
Entire set	0.47
Similarity coefficient ≥ 0.5	0.67

*Mean absolute error in Log10(mmHg)

CAS	Structure	Similarity Coefficient	Experimental value Log10(mmHg)	Predicted value Log10(mmHg)
ClC=1N=C(N=C(N1)NC(C)CCC(Cl)C)NC(C)C (test chemical)			N/A	-6.85
7287-19-6		0.83	-5.91	-5.86
130339-07-0		0.77	-5.62	-7.11
21725-46-2		0.76	-6.86	-7.01
120928-09-8		0.58	-7.59	-7.67
101200-48-0		0.56	-9.41	-9.76
119738-06-6		0.55	-7.23	-9.11

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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.

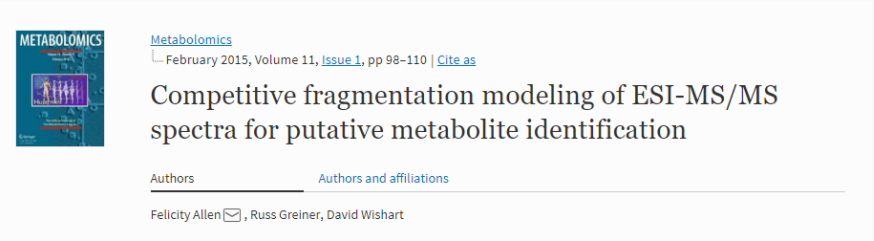
1	casrn	dsstox_substance_id	preferred_name
2	26148-68-5	DTXSID7020001	A-alpha-C
3	107-29-9	DTXSID2020004	Acetaldehyde oxime
4	60-35-5	DTXSID7020005	Acetamide
5	103-90-2	DTXSID2020006	Acetaminophen
6	968-81-0	DTXSID7020007	Acetohexamide
7	18523-69-8	DTXSID2020008	Acetone[4-(5-nitro-2-furyl)-2-thiazolyl] 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

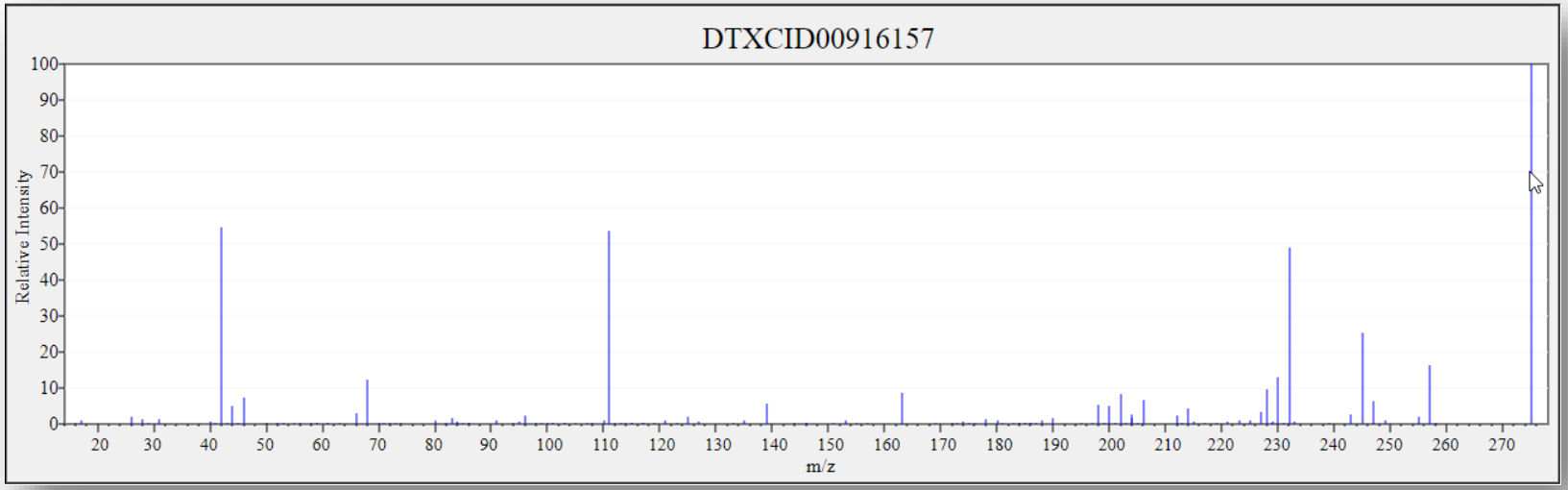
Prototypes in Development

Predicted Mass Spectra

http://cfmid.wishartlab.com/



- MS/MS spectra prediction for ESI+, ESI-, and EI
- Predictions generated and stored for >800,000 structures, to be accessible via Dashboard



Search Expt. vs. Predicted Spectra

EPA United States Environmental Protection Agency

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

Non Target Analysis Prototype

Mass Search

± | Min/Max

321.136493476 Da ± 0.0000002 Da ppm

Molecular Formula Search

Molecular Formula

Mass or Formula must be entered before searching spectrum

Ionization Type

ESI+
- ESI+
- ESI-
- EI

Spectra Input

Single Energy | Multiple

```
304.1332052 11.6199475
198.0913404 7.306439699
123.0440559 6.538348292
196.0756904 5.269463115
216.1019051 4.700461978
```

Peak Match Window: 0.02 Da ppm

Search

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Spectra Inpu

Single Ener

304.1332052 11.61
198.0913404 7.30
123.0440559 6.53
196.0756904 5.26
216.1019051 4.70

Peak Match

Search

TSV | CSV | Excel

Chemical Structure ID
DTXCID101048191
DTXCID101181567
DTXCID50879086
DTXCID60686349
DTXCID00830900
DTXCID10971176
DTXCID60301242
DTXCID40703048
DTXCID60349982
DTXCID10316649

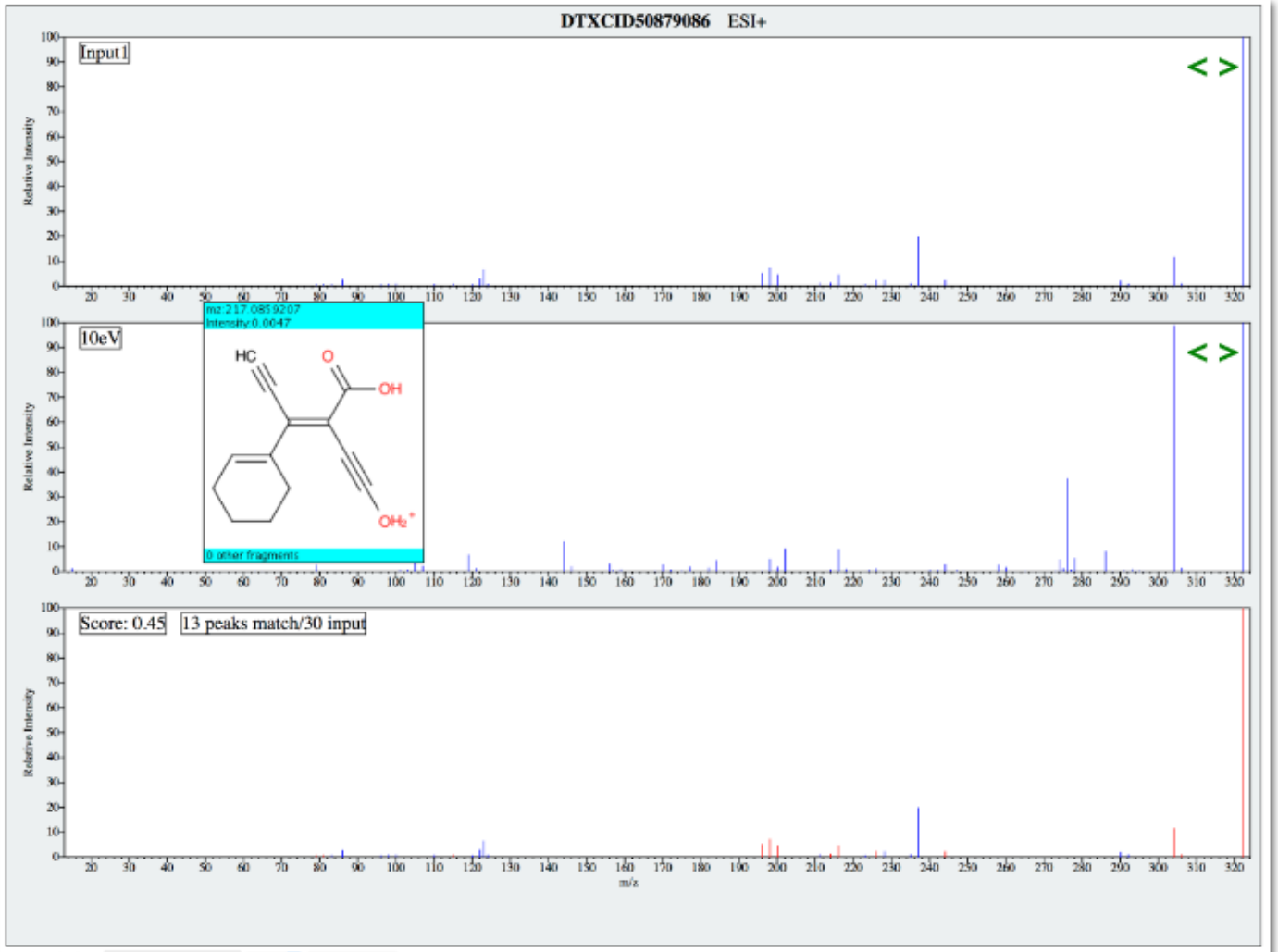
Showing 1 to 10 of 38 entries

m of Scores

1 2 3 4 Next

Chemical Structure ID	Score (10eV)
DTXCID101048191	0.22
DTXCID101181567	0.19
DTXCID50879086	0.17
DTXCID60686349	0.14
DTXCID00830900	0.13
DTXCID10971176	0.12
DTXCID60301242	0.12
DTXCID40703048	0.11
DTXCID60349982	0.11
DTXCID10316649	0.09

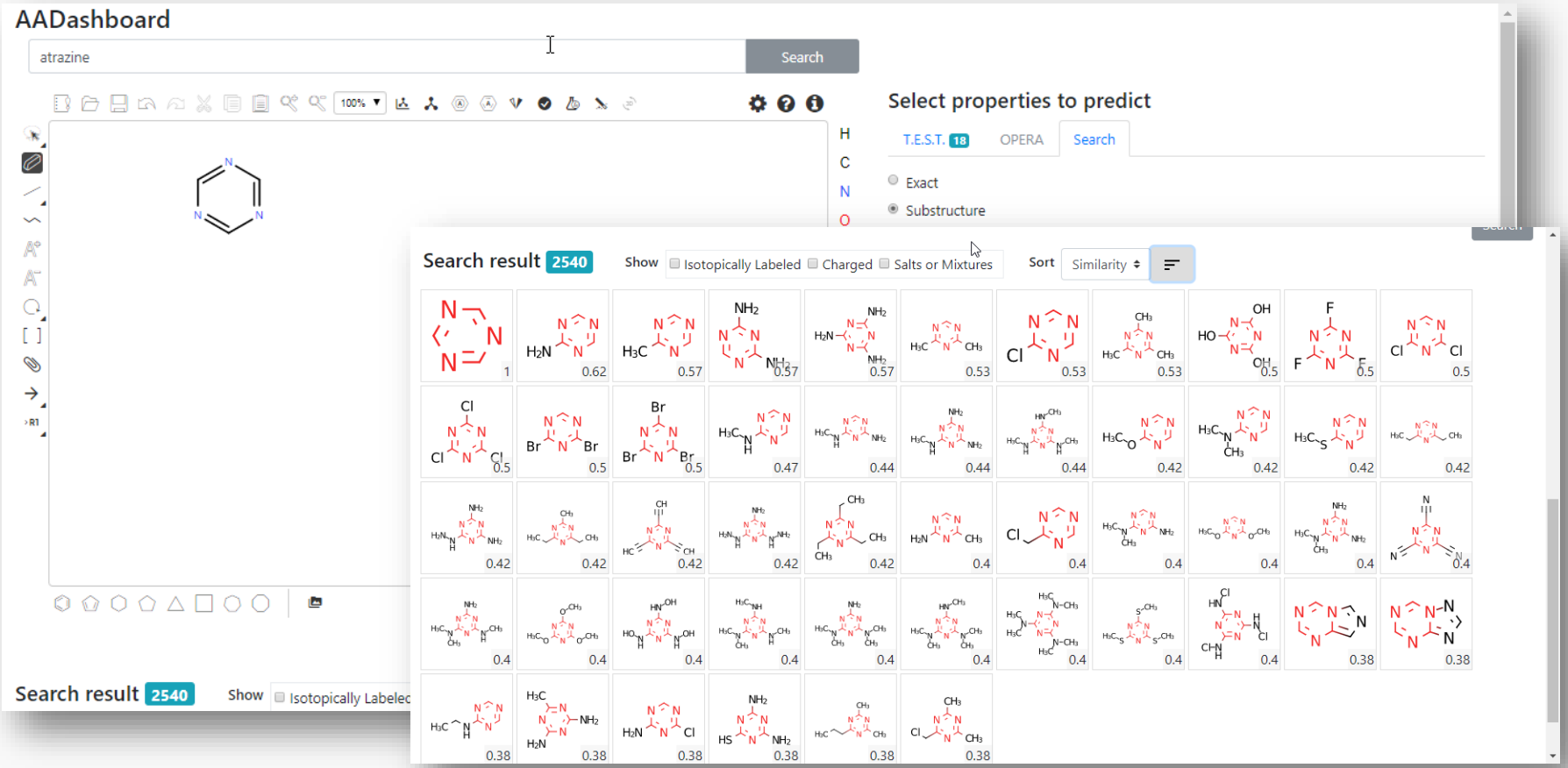
Spectral Viewer Comparison



Peak Window: 2.0 ppm Update Score

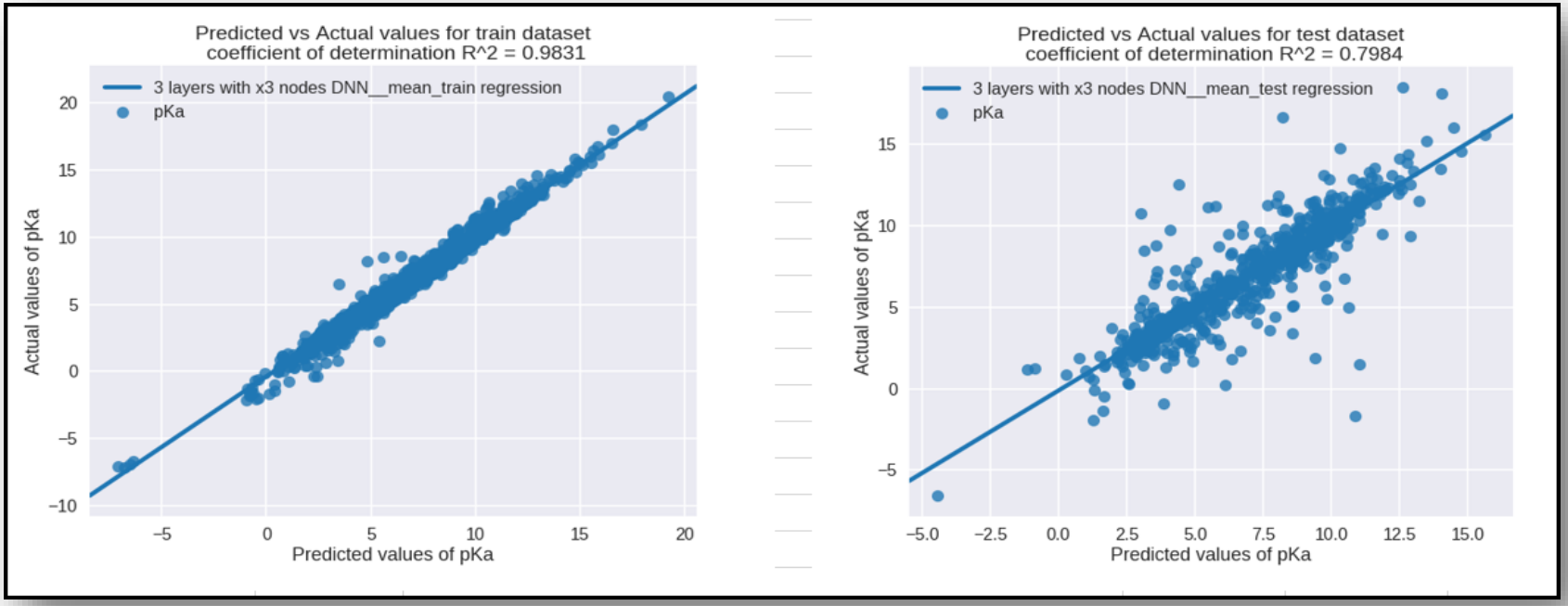
Input	10eV	20eV	40eV
1	0.45	0.16	0.029
2	0.45	0.16	0.029
3	0.45	0.16	0.029

Prototype Development



In Progress : pKa Prediction Model

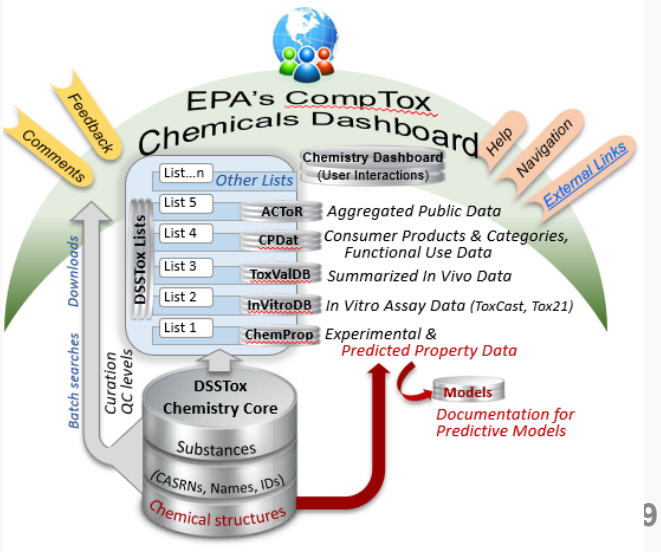
- pKa prediction models based on Open Data Set of 8000 chemicals – acidic, basic and amphoteric chemicals



- *Accepted for publication to Journal of Cheminformatics*

Conclusion

- Building an integrated hub for environmental chemistry data to serve computational toxicology
- Transparent access to data and models – file downloads, SQL data dumps and web services
- Expansion of functionality to serve all data streams generated by NCCT across the agency & community
- Data **QUALITY** is a key focus - ongoing curation
- Ongoing API development will provide enhanced access to data streams



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- *Many public domain databases and open data contributors*

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Journal of Cheminformatics

DATABASE

Open Access

The CompTox Chemistry Dashboard: a community data resource for environmental chemistry

Antony J. Williams[1*], Christopher M. Grulke[1], Jeff Edwards[1], Andrew D. McEachran[2], Kamel Mansouri[1,2,4], Nancy C. Baker[3], Grace Patlewicz[1], Imran Shah[1], John F. Wambaugh[1], Richard S. Judson[1] and Ann M. Richard[1]

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