

US EPA CompTox Chemicals Dashboard

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Conflict of Interest Statement

This work was reviewed by EPA and approved for presentation but does not necessarily reflect official Agency policy.

Abbreviations

- CompTox - Computational Toxicology
- DSSTox - Distributed Structure Searchable Toxicity DB
- CASRN - Chemical Abstracts Registry Number
- InChI - International Chemical Identifier
- QMRF – QSAR Model Report Format
- ToxVal - Toxicity Value Database
- OPERA - OPEn structure–activity Relationship App
- TEST - Toxicity Estimation Software Tool
- ToxCAST - Toxicity Forecaster
- CERAPP - Collaborative Estrogen Receptor Activity Prediction Project
- CoMPARA - Collaborative Modeling Project for Androgen Receptor Activity
- SDF - Structure data file

CompTox Chemicals Dashboard

<https://comptox.epa.gov/dashboard>

875k Chemical Substances

The screenshot shows the EPA CompTox Chemicals Dashboard. At the top left is the EPA logo with the text "United States Environmental Protection Agency". To the right of the logo are navigation links: "Home", "Advanced Search", "Batch Search", "Lists" (with a dropdown arrow), "Predictions", and "Downloads". In the top right corner, there is a "Share" button with a dropdown arrow. Below the navigation bar, the main content area features the EPA seal on the left and the heading "875 Thousand Chemicals" on the right. Under the heading, there are three tabs: "Chemicals" (which is selected and highlighted in blue), "Product/Use Categories", and "Assay/Gene". Below the tabs is a search bar with a magnifying glass icon and the placeholder text "Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey". Below the search bar is a checkbox labeled "Identifier substring search". To the right of the search bar, there are two links: "See what people are saying, read the dashboard [comments!](#)" and "Cite the Dashboard Publication [click here](#)". Below this is a section titled "Latest News" with a link "Read more news". The first news item is titled "Journal of Cheminformatics article regarding 'MS-Ready structures'" and is dated "March 9th, 2019 at 1:09:45 PM". The text of the article states: "A recent article describes 'MS-Ready structures', what they are, how they are generated and details regarding the benefits of these structures in navigating structure relationships across the dashboard. The article is published in the Journal of Cheminformatics [here](#)." At the bottom of the news section, there are four small circular indicators, with the first one being filled, indicating the current position in a carousel.

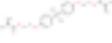
BASIC Search

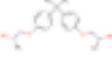
Chemicals Product/Use Categories Assay/Gene

Q Bisphenol

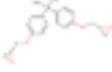
 Bisphenol A
DTXSID7020182

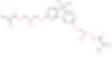
 Bisphenol A bis(2-hydroxyethyl ether) diacrylate
DTXSID6066991

 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

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

Search Results

Searched with 'Synonym Substring': Bisphenol

541 chemicals

Detailed Chemical Pages

The screenshot shows the EPA DSSTox Substance page for Bisphenol A. The page header includes the EPA logo, navigation links (Home, Advanced Search, Batch Search, Lists, Predictions, Downloads), and utility buttons (Copy, Share, Submit Comment, Search all data). The main content area features a sidebar with navigation tabs (DETAILS, EXECUTIVE SUMMARY, PROPERTIES, ENV. FATE/TRANSPORT, HAZARD, ADME, EXPOSURE, BIOACTIVITY, SIMILAR COMPOUNDS, GENRA (BETA), RELATED SUBSTANCES, SYNONYMS, LITERATURE, LINKS, COMMENTS). The central panel displays the chemical name "Bisphenol A", its identifier "80-05-7 | DTXSID7020182", and a note "Searched by DSSTox Substance Id.". Below this is a large chemical structure diagram of Bisphenol A, showing two hydroxyphenyl groups connected by a central carbon atom bonded to two methyl groups (H₃C and CH₃). The right sidebar contains several expandable sections: "Wikipedia" with a snippet about Bisphenol A's chemical formula and properties; "Intrinsic Properties" with fields for Molecular Formula (C₁₅H₁₆O₂), Average Mass (228.291 g/mol), and Monoisotopic Mass (228.11503 g/mol); and "Structural Identifiers", "Linked Substances", "Presence in Lists", "Record Information", and "Quality Control Notes".

- Chemical page: Wikipedia snippet when available, intrinsic properties, structural identifiers, linked substances

“Executive Summary”

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

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, NR113, PPARA, NR112, 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

PHYSICHEM PARAMETERS

ASSAY PLOTS

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)
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Quantitative Hazard Values

- ✓ Minimum oral POD: 3.8 mg/kg-day (reproductive, HPVIS, oral, 6)
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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

- Physchem and Fate & Transport experimental and predicted data
- Data can be downloaded as Excel, TSV and CSV files
- Predictions: multiple algorithms
 - EPI Suite: Estimation Program Interface
 - ACD/Labs (commercial)
 - TEST: **T**oxicity **E**stimation **S**oftware **T**ool
 - OPERA: **O**PEn structure–activity/property **R**elationship **A**pp

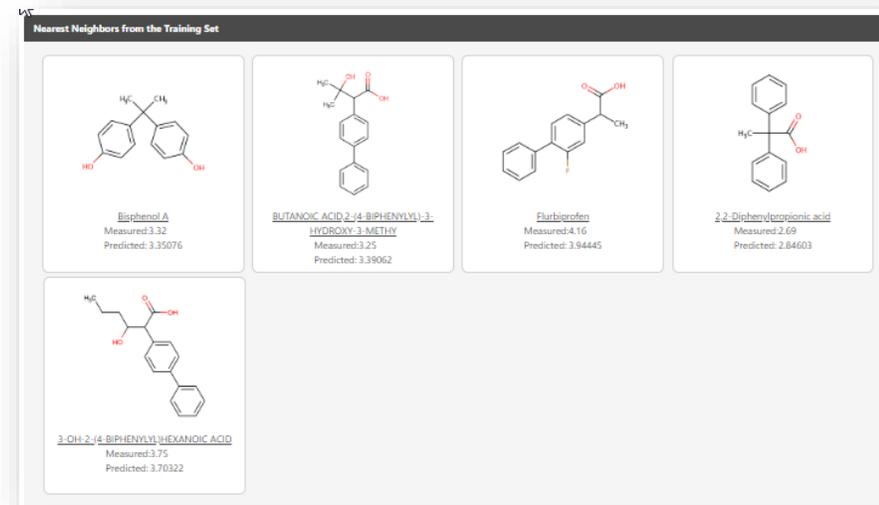
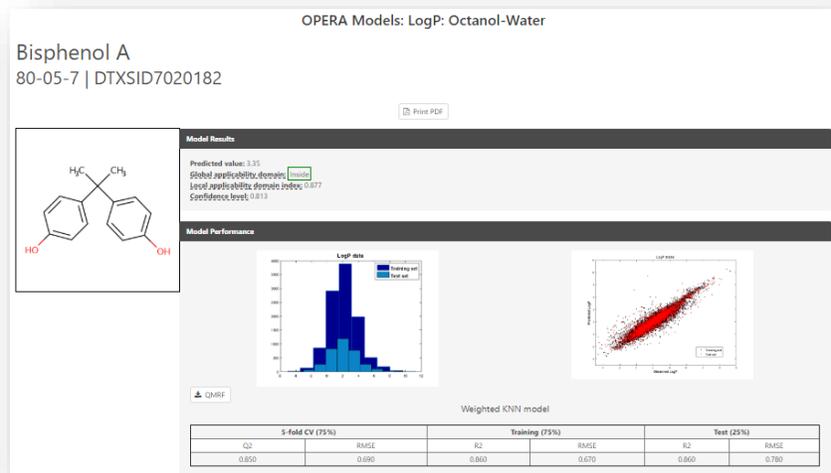
Transparency for prediction models

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

- QMRF – QSAR Model Report Format details
- Applicability Domain
- Plots of expt. vs pred.
- Nearest-neighbors



OPERA Standalone Application

- OPERA predictions available on dashboard
- OPERA application available (from Github)
- Both GUI and command line versions available

Command line

```
OPERA models for physchem and environmental fate properties.
Version 1.5 (September 2017)

OPERA is a command line application developed in Matlab providing QSAR
models predictions as well as applicability domain and accuracy assessment.

Developed by:
Kamel Mansouri
mansourikamel@gmail.com

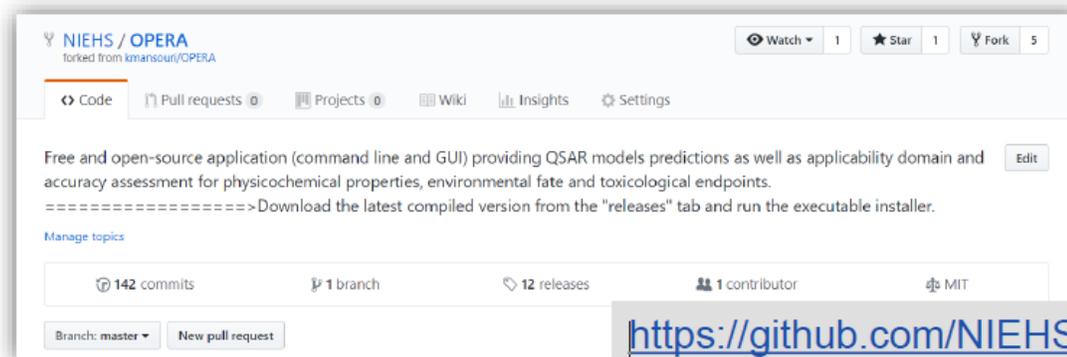
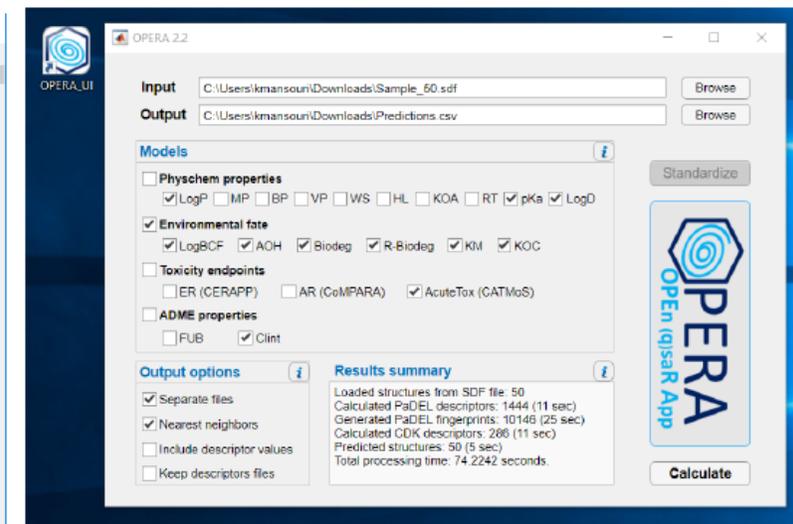
Developed at:
National Center of Computational Toxicology
United States Environmental Protection Agency

Usage: OPERA <argument_list>

Examples:
OPERA -s Sample_50.sdf -o predictions.csv -a -x -v 2
opera -d Sample_50.csv -o predictions.txt -e logP BCF -n -v

Type OPERA -h or OPERA --help for more info.
```

Graphical User Interface



<https://github.com/NIEHS/OPERA>

Chemical Hazard Data

ToxVal Database

- ~30k chemicals
- >770k tox. values
- ~30 sources of data
- ~22k sub-sources
- ~5k journals cited
- ~70k citations

Hazard

DataType
Toxicity Value

Human Eco

Download Columns Search query

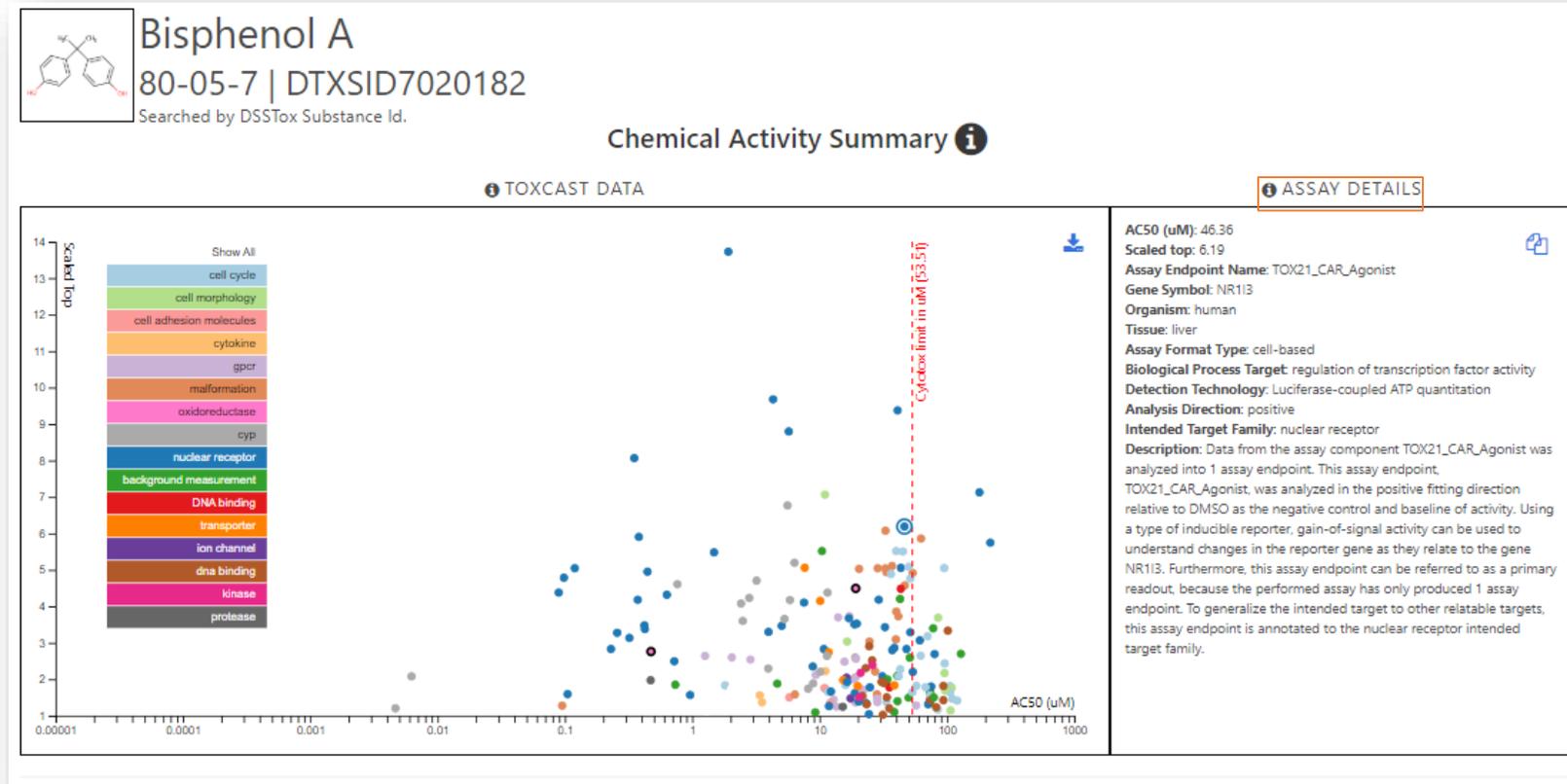
More	Priority	Type	Subtype	Risk assessment class	Value	Units	Study type	Exposure route	Species	Subsource	Source
	7	MEG	Short-term Critical Air	short-term	500	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Short-term Marginal Air	short-term	100	mg/m3	-	inhalation	-	TG 230 Military 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

In Vitro Bioassay Screening

ToxCast and Tox21

In vitro bioactivity

- 4K chemicals (ToxCast)
- 8k chemicals (Tox21)
- ~2k assay endpoints



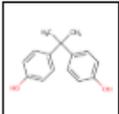
In Vitro Bioassay Screening

ToxCast and Tox21

 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

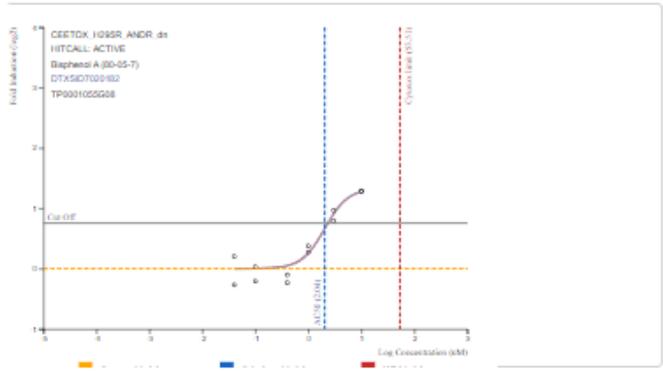
QC Data ID	Grade	Description
Tox21_202992	Pass	Purity>90% and MW confirmed
Tox21_400088	Pass	Purity>90% and MW confirmed

Assay Selection 136 Selected Active Inactive All

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

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)



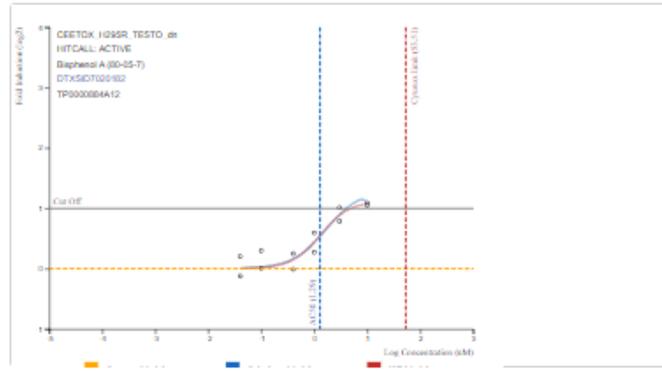
CEETOX_1095R_ANDR dn
HITCALL: ACTIVE
Bisphenol A (80-05-7)
DTXSID7020182
TP9001055208

Y-axis: Fold Induction (log)
X-axis: Log Concentration (nM)

Cur OFF

MTD (100%)

Chemo Line (D50)



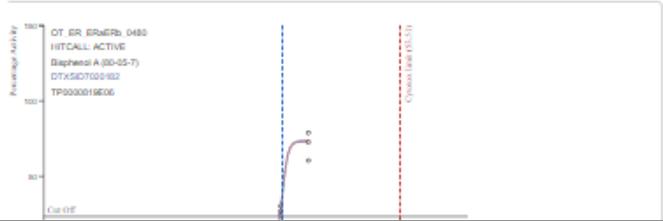
CEETOX_1095R_TESTO dn
HITCALL: ACTIVE
Bisphenol A (80-05-7)
DTXSID7020182
TP9000884412

Y-axis: Fold Induction (log)
X-axis: Log Concentration (nM)

Cur OFF

MTD (100%)

Chemo Line (D50)

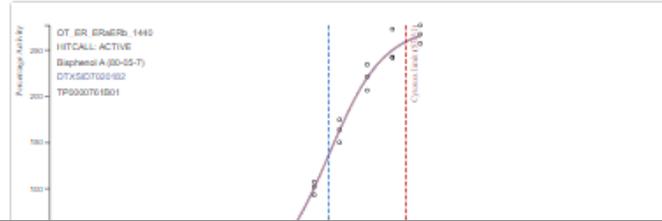


OT_ER_ERaERb_0480
HITCALL: ACTIVE
Bisphenol A (80-05-7)
DTXSID7020182
TP9000019406

Y-axis: Average Activity
X-axis: Log Concentration (nM)

Cur OFF

Chemo Line (D50)



OT_ER_ERaERb_1440
HITCALL: ACTIVE
Bisphenol A (80-05-7)
DTXSID7020182
TP9000761801

Y-axis: Average Activity
X-axis: Log Concentration (nM)

Cur OFF

Chemo Line (D50)

Sources of Exposure to Chemicals

 United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Copy Share Submit Comment Search all data

Bisphenol A

80-05-7 | DTXSID7020182
Searched by DSSTox Substance Id.

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

EXPOSURE

PRODUCT & USE CATEGORIES

CHEMICAL WEIGHT FRACTION

CHEMICAL FUNCTIONAL USE

TOXICS RELEASE INVENTORY

MONITORING DATA

EXPOSURE PREDICTIONS

PRODUCTION VOLUME

BIOACTIVITY

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
paint	CPCat Cassette	16
manufacturing, machines	CPCat Cassette	12
manufacturing, plastics	CPCat Cassette	11
building_material, flooring	CPCat Cassette	8
surface_treatment, metals	CPCat Cassette	8
construction	CPCat Cassette	8
stabilizer	CPCat Cassette	7
manufacturing, chemical	CPCat Cassette	6

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

Identifiers to Support Searches

 United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Copy Share Submit Comment Search all data

Bisphenol A

80-05-7 | DTXSID7020182
Searched by DSSTox Substance Id.

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-diylidiphenol	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

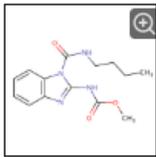
- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
 - ADME
 - EXPOSURE
 - BIOACTIVITY
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS**
- LITERATURE
- LINKS
- COMMENTS

Chemicals Discussed Today

- During talks today we heard about these chemicals. All are on the dashboard.
 - 2,4-dihydroxybenzophenone, 131-56-6 (Mark)
 - 50-00-0, 6898-97-1, 17804-35-2, 1582-09-8, 789-02-6, 50-06-6, 57-30-7, 131-55-5 (Shannon)
 - Argatroban, Lepirudin (Thomas)
 - Arsenic trioxide, chlorpyrifos, cadmium, phorate, butylate, methyl bromide, Diazinon, Fonofos, Atrazine, Dichlorvos, Phorate, Parathion, 2-butenal, pyruvaldehyde, nicotine, formaldehyde, acetaldehyde, acetone, propionaldehyde (Carolyn)

BUILT-IN “MODULES”

Literature Searching

 **Benomyl**
17804-35-2 | DTXSID5023900
Searched by Approved Name.

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

Metabolism/PK/PD  **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

Abstract Sifter

Optionally, edit the query before retrieving.

```
("17804-35-2" OR "Benomyl") AND (metabolism OR metabolite OR tissue distribution OR pharmacokinetics OR pharmacodynamics)
```

- Real-time retrieval of data from PubMed (>29 million abstracts and growing)
- Choose from set of pre-defined queries
- Adjust and fine tune queries based on interests

Literature Searching

- “Sifting” of results using multiple terms
- Frequency counting terms
- Color highlighting of terms
- Download list to Excel
- Send list to PubMed for downloading ref. file
- Direct link via PubMed ID

1) Select PubMed starting point query then 2) click on Retrieve. **Metabolism/PK/PD** Retrieve Articles **714 of 714 articles loaded...**

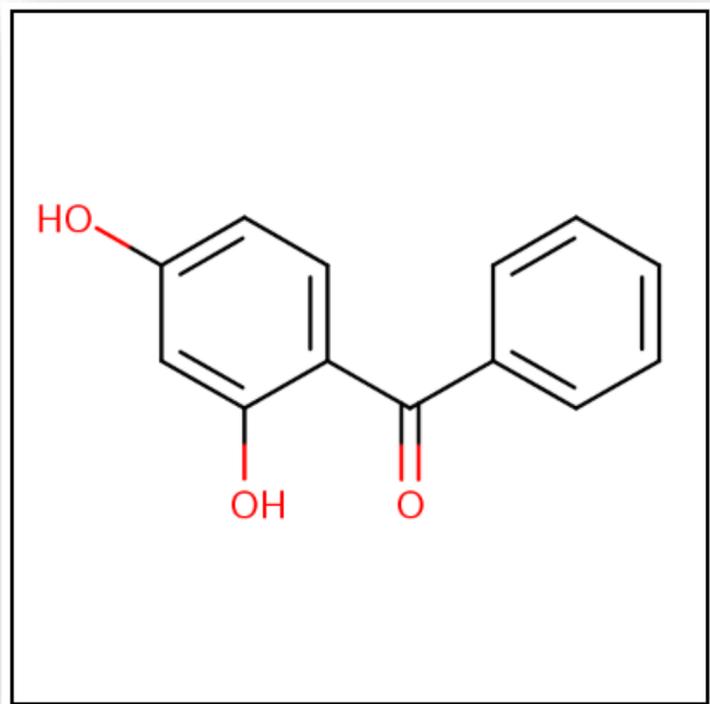
Optionally, edit the query before retrieving.
 ("17804:35-2" OR "Benomyl") AND (metabolism OR metabolite OR tissue distribution OR pharmacokinetics OR pharmacodynamics)

To find articles quickly, enter terms to sift abstracts. **degradation** **benomyl** **N,N'-dibutylurea** Clear Terms Download / Send to... Download Sifter for Excel

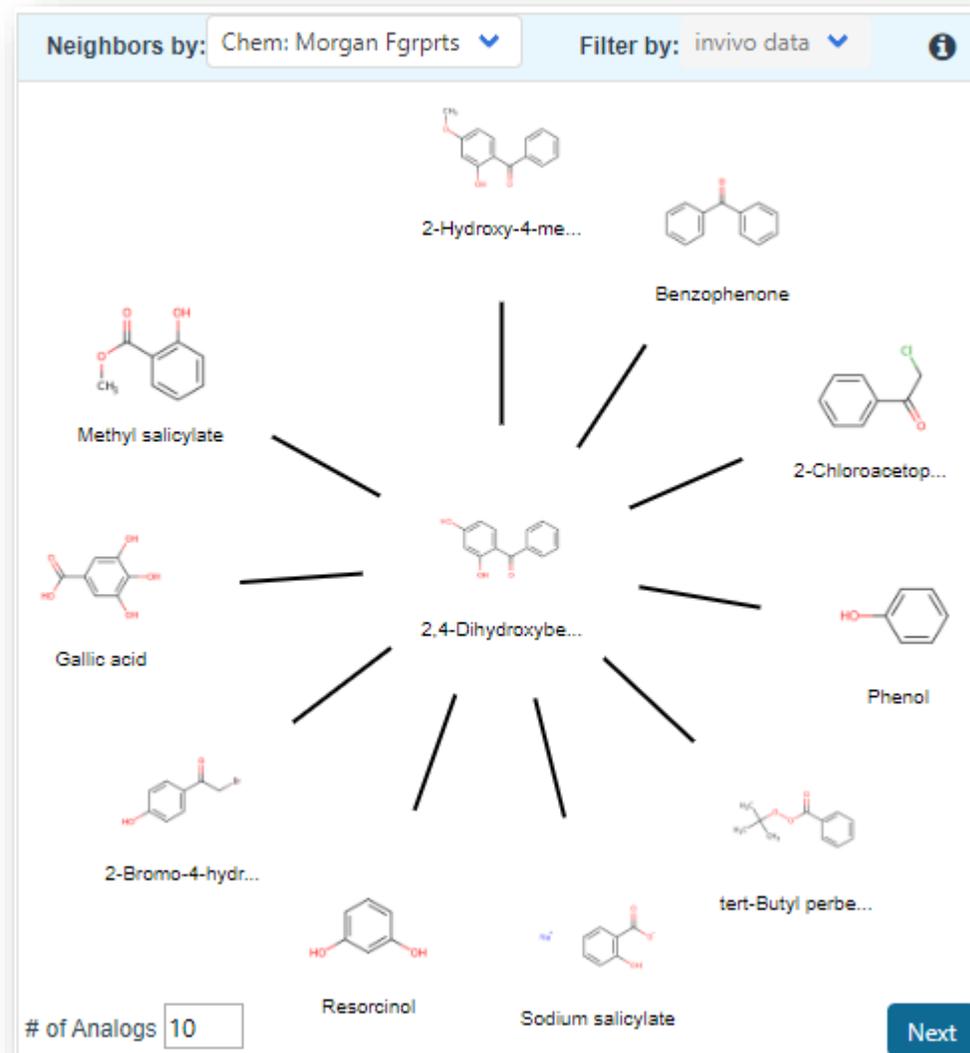
	degradation	benomyl	N,N'-dibutylurea	Total	PMID	Year	Title	Authors	Journal	Rev
<input type="checkbox"/>	1	11	2	14	17493661	2007	Formulation factors that can reduce the formation of the phytotoxic impurity, N,N'-...	Ho; Lin; Wang	Chemosphere	
<input type="checkbox"/>	4	1	2	7	15356237	2004	Degradation of N,N'-dibutylurea (DBU) in soils treated with only DBU and DBU-for...	Lee; Sassman; Bischoff; Turco	Journal of environmental quality	
<input type="checkbox"/>	3	1	1	5	15865150	2005	Accelerated degradation of N, N'-dibutylurea (DBU) upon repeated application.	Bischoff; Lee; Turco	Biodegradation	
<input type="checkbox"/>	1	1	1	3	8854971	1996	Spontaneous N,N'-dibutylurea (DBU) formation in Benlate DF formulation under el...	Tang; Song	Archives of environmental contamination and toxico...	
<input type="checkbox"/>	0	1	0	1	31412509	2019	Arbuscular mycorrhizal fungi alleviate phosphorus limitation by reducing plant N:P ...	Mei; Yang; Zhang; Zhang; Guo	The Science of the total environment	
<input type="checkbox"/>	0	1	0	1	31190279	2019	Two herbicides, two fungicides and spore-associated bacteria affect Funneliformis...	de Novais; Giovannetti; de Faria; Sbrana	Mycorrhiza	
<input type="checkbox"/>	0	1	0	1	31146360	2019	Novel Peptide-Based Inhibitors for Microtubule Polymerization in Phytophthora ca...	Lee; Kim; Hoffmeister; Yoon; Kim	International journal of molecular sciences	
<input type="checkbox"/>	0	6	0	6	31112093	2019	Molecularly imprinted polymers for the detection of benomyl residues in water and...	Guzzella; Casatta; Dahchour; Baggiani; Pozzoni	Journal of environmental science and health. Part. ...	
<input type="checkbox"/>	0	1	0	1	30744902	2019	Benzimidazole- and Qol-resistance in <i>Corynespora cassicola</i> populations from gr...	Duan; Xin; Lu; Li; Li; Wu; Wang; Zhou	Pesticide biochemistry and physiology	
<input type="checkbox"/>	0	1	0	1	30673418	2019	Variation in Fungicide Sensitivity Among <i>Rhizoctonia</i> Isolates Recovered from Pot...	Muzhinji; Woodhall; Truter; van der Waals	Plant disease	
<input type="checkbox"/>	0	1	0	1	30087309	2018	Synthesis and Spectrum of Biological Activities of Novel N-arylcinnamamides.	Pospisilova; Kos; Michnova; Kapustikova; Strharsk...	International journal of molecular sciences	
<input type="checkbox"/>	0	1	0	1	29984740	2018	Occupational Exposure Limits for ethylidene norbornene, ethyleneimine, benomyl,...	Araki; Azuma; Endo; Endo; Fukushima; Hara; Hori; ...	Journal of occupational health	
<input type="checkbox"/>	0	1	0	1	29933012	2018	Bioassay-guided isolation of active substances from <i>Semen Torreyae</i> identifies tw...	Liu; Veyser; Lu; Wenseleers; De Borggraeve; Jian...	Journal of ethnopharmacology	
<input type="checkbox"/>	0	1	0	1	29908479	2018	Incident thyroid disease in female spouses of private pesticide applicators.	Shrestha; Parks; Goldner; Kamet; Umbach; Ward; L...	Environment international	
<input type="checkbox"/>	0	0	0	0	29804677	2018	Purification of kinetochores from the budding yeast <i>Saccharomyces cerevisiae</i> .	Gupta; Evans; Koch; Littleton; Biggins	Methods in cell biology	

Degradation of N,N'-dibutylurea (DBU) in soils treated with only DBU and DBU-fortified benlate fungicides. N,N'-dibutylurea (DBU) is a breakdown product of **benomyl** [methyl 1-(butylcarbamoyl)-2-benzimidazole carbamate], the active ingredient in Benlate fungicides, and has been proposed to cause crop damage after the use of Benlate 50 DF fungicide (DuPont, Wilmington, DE). Our research focused on DBU persistence after application into soil. We assessed DBU persistence on direct application of DBU (carbonyl-(14)C) at two concentrations (0.08 and 0.8 microg DBU kg(-1)) to seven soils and two potting mixes in soil microcosms incubated at various combinations of soil water potential (-0.03 or -0.1 MPa) and temperature (23, 33, 44 degrees C). For two soils at a subset of treatment variables we assessed DBU persistence in the presence of Benlate DF and SP fungicide formulations. Parent compounds, metabolites, and (14)CO(2) were tracked using chromatographic analysis with radioassay and UV detection, liquid scintillation counting, and post-extraction oxidation of the soil. DBU **degradation** was primarily microbial and for most soil-treatment combinations, half-lives were less than 2 wk. DBU **degradation** was retarded at the lower soil water potential and enhanced at 33 degrees C. In the presence of the formulation, DBU **degradation** was slower for one soil type. The longest half-life observed in any case was less than 7 wk; therefore, long-term persistence of DBU applied to soils through a Benlate application is very unlikely.

GenRA in practice – step by step



- Analogue identification: based on Morgan fingerprints and selecting 10 default analogues



GenRA in practice – step by step

- Updated Data matrix view with GenRA predictions for target chemical



- Predictions are binary (yes/no) for toxicity effects
- Predictions summarized on study level basis. Red: “positive” and Blue: “negative”.

Related Publications



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



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



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



Contents lists available at ScienceDirect

Computational Toxicology

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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

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

CHEMICAL LISTS AND CATEGORIES

EPAHFR: Hydraulic Fracturing

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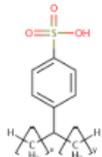
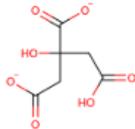
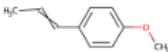
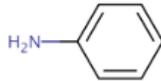
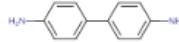
Lists of Chemicals 

List of Assays

WATER|EPA; Chemicals associated with hydraulic fracturing

Identifier substring search

List

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 <p>Anethole DTXSID: DTXSID4020086 PubChem: 59 CPDAT: 33</p>	 <p>Aniline DTXSID: DTXSID8020090 PubChem: 284 CPDAT: 80</p>	 <p>Benzidine DTXSID: DTXSID2020137 PubChem: 112 CPDAT: 15</p>	 <p>Benzo(a)pyrene DTXSID: DTXSID2020139 PubChem: 161 CPDAT: 81</p>

PFAS lists of Chemicals

Select List

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PFAS

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

List of Assays

Assay List

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10 ▾

ATG x OT x NHEERL_PADILLA x ▾

Search query

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Assay Component Endpoint Name	Details	Active Hits	Description	Gene Symbols
ATG_Ahr_CIS_up		573 / 3807	Data from the assay component ATG_Ahr_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 identify potential targets. This assay endpoint can be referred to as a primary target family, where this one serves a reporter targets, this assay endpoint is annotated to the "dna binding" intended target family, where the subfamily is "basic helix-loop-helix protein".	AHR
ATG_AP_1_CIS_up		658 / 3807	Data from the assay component ATG_AP_1_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 identify potential targets. This assay endpoint can be referred to as a primary target family, where this one serves a reporter 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 gain-of-signal activity can be used to identify potential targets. This assay endpoint can be referred to as a primary target family, where this one serves a reporter targets, this assay endpoint is annotated to the "dna binding" intended target family, where the subfamily is "basic leucine zipper".	TFAP2A TFAP2B TFAP2D

- 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

From Assay to Chemicals...



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

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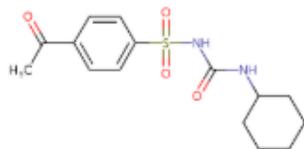
CASRN

TOXCAST

PubMed

Inactive

Filter by Name or CASRN

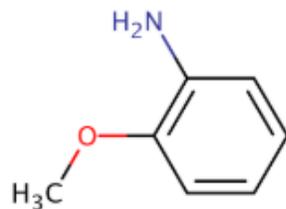


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TOXCAST: 4/376

PubMed: 235



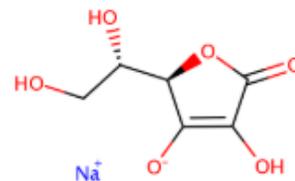
HCl

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

Chemicals

Product/Use Categories

Assay/Gene



Search for chemicals based on product or use categories

Product/Use Categories

Chemicals

Product/Use Categories

Assay/Gene

Q lubricant|

CPDat PRODUCT category: auto products auto lubricant
engine lubricants and belt dressings, not including motor oils (spray or aerosol formulation specified)

CPDat PRODUCT category: auto products auto lubricant
engine lubricants and belt dressings, not including motor oils

CPDat PRODUCT category: home maintenance lubricant
household maintenance lubricants (spray or aerosol formulation specified)

CPDat PRODUCT category: home maintenance lubricant
household maintenance lubricants

CPDat PRODUCT category: personal care clipper lubricant/cleaner
cleaning and lubricating products for hair clippers

CPCat USE category: lubricant
generic lubricants, lubricants for engines, brake fluids, oils, etc (does not include personal care lubricants)

Lubricant

Searched by Product & Use Categories

Results for CPCat Use Category: CPCat term: Lubricant

1738 chemicals

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CPDAT

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DTXSID

PubChem

CPDAT

↓

Hide chemicals that are: ↓

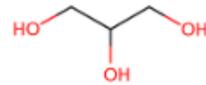
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☰



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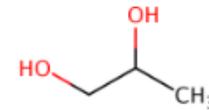
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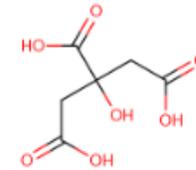
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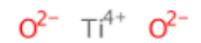
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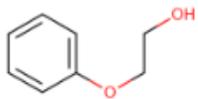
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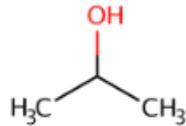
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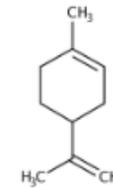
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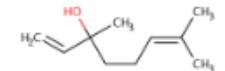
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Limonene

DTXSID: DTXSID2029612
PubChem: 123
CPDAT: 2068



Linalool

DTXSID: DTXSID7025502
PubChem: 118
CPDAT: 1984

Other Searches

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

 Search for assays based on endpoint name or gene symbol

Chemical-Biology

Assay/Gene Search

WS

Chemicals

Product/Use Categories

Assay/Gene

Q 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

Assay List

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ESR1

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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 > >>

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Mass Search 

\pm Min/Max

Adduct

Neutral



All Adducts



Choose adduct from dropdown

191.131

Da

\pm

5

Da

ppm

Search 

Advanced Searches

Mass Search

Search Results

Searched by Mass: 191.131 +/- 5.0 ppm.

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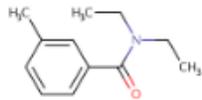
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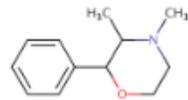
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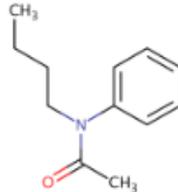
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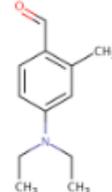
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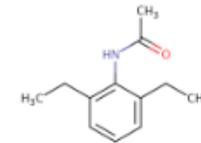
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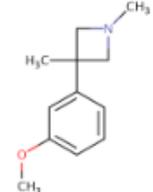
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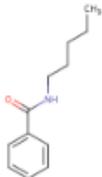
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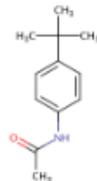
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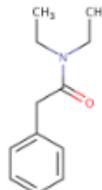
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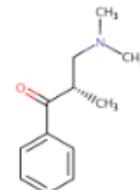
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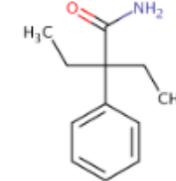
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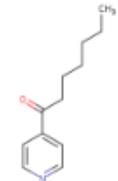
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CASRN: 30568-39-9
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1-Heptanone, 1-(4-pyridyl)-

DTXSID: DTXSID40186594
CASRN: 32941-30-3
TOXCAST: -
Mass Diff: 0.000014

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. Ulrich¹ • Jon R. Sobus¹ • Christopher M. Grulke² • Ann M. Richard² • Seth R. Newton¹ • Mark J. Strynar¹ • Kamel Mansouri^{3,4} • Antony J. Williams²

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

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Mass Spec Focused Applications

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. Sobus¹ · John F. Wambaugh² · Kristin K. Isaacs¹ · Antony J. Williams² · Andrew D. McEachran³ · Ann M. Richard² · Christopher M. Grulke² · Elin M. Ulrich¹ · Julia E. Rager^{3,4} · Mark J. Strynar¹ · Seth R. Newton¹

 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 great but...
- ...we generally want data on LOTS of chemicals!

- Typical questions
 - What are the structures for a set of chemical names? Set of CASRNs?
 - Can I get chemical lists in Excel files? As a list of SMILES strings? Can I get an SDF file?
 - Can I include predicted properties in the download file? OPERA? TEST?
 - Are “these chemicals” screened in Toxcast?
 - I’m a mass spectrometrists and need masses and formulae for a list of chemicals

Chemicals Discussed Today

- During talks today we heard about....
 - 2,4-dihydroxybenzophenone, 131-56-6 (Mark)
 - 50-00-0, 6898-97-1, 17804-35-2, 1582-09-8, 789-02-6, 50-06-6, 57-30-7, 131-55-5 (Shannon)
 - Argatroban, Lepirudin (Thomas)
 - Arsenic trioxide, chlorpyrifos, cadmium, phorate, butylate, methyl bromide, Diazinon, Fonofos, Atrazine, Dichlorvos, Phorate, Parathion, 2-butenal, pyruvaldehyde, nicotine, formaldehyde, acetaldehyde, acetone, propionaldehyde (Carolyn)
- What information can we find and how fast???

Batch Search Identifiers

2,4-dihydroxybenzophenone
50-00-0
6898-97-1
17804-35-2
1582-09-8
789-02-6
50-06-6
57-30-7
131-55-5
Argatroban
Lepirudin
Arsenic trioxide
chlorpyrifos
cadmium
phorate
butylate
methyl bromide
Diazinon
Fonofos
Atrazine
Dichlorvos
Phorate
Parathion
2-butenal
pyruvaldehyde
nicotine
formaldehyde
acetaldehyde
acetone
propionaldehyde

Batch Search

Step 1 Step 2 Step 3 Step 4 Step 5

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

Please enter one identifier per line

Select Input Type(s)

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

Select Output Format:

Excel

Customize Results

- Select All
- Select All in Lists

Chemical Identifiers

- DTXSID 
- Chemical Name 
- DTXCID 

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

2,4-dihydroxybenzophenone
50-00-0
6898-97-1
17804-35-2
1582-09-8
789-02-6
50-06-6
57-30-7
131-55-5
Argatroban

Download

INPUT	FOUND BY	DTXSID	PREFERRED_NAME
2,4-dihydroxyber	Approved Name	DTXSID8022406	2,4-Dihydroxybenzophenone
50-00-0	CAS-RN	DTXSID7020637	Formaldehyde
6898-97-1	CAS-RN	DTXSID3040770	(Z,E)-Diethylstilbestrol
17804-35-2	CAS-RN	DTXSID5023900	Benomyl
1582-09-8	CAS-RN	DTXSID4021395	Trifluralin
789-02-6	CAS-RN	DTXSID6022345	o,p'-DDT
50-06-6	CAS-RN	DTXSID5021122	Phenobarbital
57-30-7	CAS-RN	DTXSID0021123	Phenobarbital sodium
131-55-5	CAS-RN	DTXSID5041306	2,2',4,4'-Tetrahydroxybenzophen
Argatroban	Approved Name	DTXSID7046467	Argatroban
Lepirudin	Approved Name	DTXSID50160461	Lepirudin
Arsenic trioxide	Synonym	DTXSID0074007	Arsenite
chlorpyrifos	Approved Name	DTXSID4020458	Chlorpyrifos
cadmium	Approved Name	DTXSID1023940	Cadmium
phorate	Approved Name	DTXSID4032459	Phorate
butylate	Approved Name	DTXSID7023936	Butylate
methyl bromide	Approved Name	DTXSID8020832	Methyl bromide
Diazinon	Approved Name	DTXSID0020832	Diazinon

Excel Download

Include Data of Interest – then dive deeper...

Chemical Identifiers

- DTXSID **i**
- Chemical Name **i**
- DTXCID **i**
- CAS-RN **i**
- InChIKey **i**
- IUPAC Name **i**

Structures

- Mol File **i**
- SMILES **i**
- InChI String **i**
- MS-Ready SMILES **i**
- QSAR-Ready SMILES **i**

Intrinsic And Predicted Properties

- Molecular Formula **i**
- Average Mass **i**
- Monoisotopic Mass **i**
- TEST Model Predictions **i**
- OPERA Model Predictions **i**

Metadata

- Curation Level Details **i**
- NHANES/Predicted Exposure **i**
- Data Sources **i**
- Include ToxVal Data Availability **i**
- Assay Hit Count **i**
- Number of PubMed Articles **i**
- PubChem Data Sources **i**
- CPDat Product Occurrence Count **i**
- IRIS **i**

DTXSID	PREFERRED_NAME	CASRN	EXPOCAST	EXPOCAST	NHANES	TOXVAL_DATA	TOXCAST_PERCENT	TOXCAST_NUMBER	NUMBER_OF_PUBMED_ARTICLES	IRIS_LINK
DTXSID80	2,4-Dihydroxybenzaldehyde	131-56-6	2.78e-07	Y	-	Y	14.02	92/656	25	-
DTXSID70	Formaldehyde	50-00-0	1.32e-06	Y	-	Y	-	-	19234	Y
DTXSID30	(Z,E)-Diethylstilbestrol	6898-97-1	1.65e-07	Y	-	-	25.1	62/247	8326	-
DTXSID50	Benomyl	17804-35-2	1.11e-07	Y	-	Y	11.23	96/855	476	Y
DTXSID40	Trifluralin	1582-09-8	1.57e-06	Y	-	Y	10.44	87/833	259	Y
DTXSID60	o,p'-DDT	789-02-6	1.16e-07	Y	-	Y	32.87	239/727	125	-
DTXSID50	Phenobarbital	50-06-6	2.57e-08	Y	-	Y	1.7	4/235	18244	-
DTXSID00	Phenobarbital sodium salt	57-30-7	1.66e-07	Y	-	Y	2.15	15/698	17600	-
DTXSID50	2,2',4,4'-Tetrahydroquinazolin-5(1H)-one	131-55-5	2.31e-07	Y	-	Y	18.31	139/759	25	-
DTXSID70	Argatroban	74863-84-6	3.3e-07	Y	-	-	0.43	1/235	868	-
DTXSID50	Lepirudin	138068-37-1	-	-	-	-	-	-	354	-
DTXSID00	Arsenite	15502-74-6	-	-	-	-	-	-	4003	-
DTXSID40	Chlorpyrifos	2921-88-2	2.3e-08	Y	Y	Y	18.73	124/662	2387	Y
DTXSID10	Cadmium	7440-43-9	-	-	-	Y	-	-	29395	Y
DTXSID40	Phorate	298-02-2	1.23e-08	Y	Y	Y	5.26	36/685	113	-
DTXSID70	Butylate	2008-41-5	6.43e-08	Y	-	Y	1.14	9/790	17	Y
DTXSID80	Methyl bromide	74-83-9	-	-	-	Y	-	-	500	Y
DTXSID90	Diazinon	333-41-5	1.02e-07	Y	Y	Y	6.9	59/855	890	-
DTXSID20	Fonofos	944-22-9	7.86e-08	Y	-	Y	2.13	5/235	41	Y
DTXSID90	Atrazine	1912-24-9	6.56e-08	Y	Y	Y	4.62	40/866	14356	Y
DTXSID50	Dichlorvos	62-73-7	1.37e-08	Y	Y	Y	7.13	58/814	1106	Y
DTXSID40	Phorate	298-02-2	1.23e-08	Y	Y	Y	5.26	36/685	113	-
DTXSID70	Parathion	56-38-2	8.86e-08	Y	Y	Y	13.05	116/889	2213	Y
DTXSID80	Crotonaldehyde	4170-30-3	8.64e-07	Y	-	Y	0.0	0/235	172	-
DTXSID00	Methyl glyoxal	78-98-8	-	-	-	Y	0.72	2/277	1553	-
DTXSID10	Nicotine	54-11-5	7.08e-07	Y	-	Y	2.39	17/711	22837	-
DTXSID70	Formaldehyde	50-00-0	1.32e-06	Y	-	Y	-	-	19234	Y
DTXSID50	Acetaldehyde	75-07-0	2.57e-06	Y	-	Y	35.5	142/400	5568	Y
DTXSID80	Acetone	67-64-1	4.72e-05	Y	-	Y	0.43	1/235	7176	Y
DTXSID20	Propanal	123-38-6	2.73e-05	Y	-	Y	0.0	0/235	1219	Y

***Batch collection of data for a
set of pesticides***

Curated List of Pesticides

- Find list of interest

- Select list and send to batch

EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Share Search all data

Select List

PESTICIDES|EPA: Pesticide Chemical Search Database

Search EPAPCS Chemicals

Identifier substring search

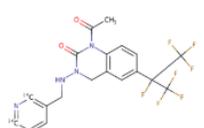
List Details

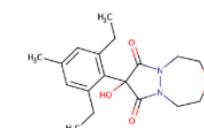
Description: The entries in this list have been classified in the U.S. as pesticidal "active ingredients" (conventional, antimicrobial, or biopesticidal agents), and were sourced from the Pesticide Chemical Search database (<https://iaspub.epa.gov/apex/pesticides/f?p=chemicalsearch:1>) created by EPA's Office of Pesticide Programs. Chemical Search provides a single point of reference for easy access to information previously published in a variety of locations, including various EPA web pages and Regulations.gov. Chemical search contains the following: 1) More than 20,000 regulatory documents; 2) Links to over 800 dockets in Regulations.gov 3) Links to pesticide tolerance (or maximum residue levels) information; 4) A variety of web services providing easy access to other scientific and regulatory information on particular chemicals from other EPA programs and federal government sources.

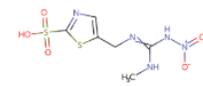
Number of Chemicals: 4012

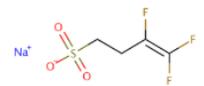
Select all Download **Send to Batch Search** CASRN CASRN DTXSID Mono.Mass 3988 chemicals

Hide chemicals that are: Filter by Name or CASRN


1-Acetyl-6-(1,1,1,2,3,3,3-heptafluoro-2-pyridin-2-yl)pyridin-2(1H)-one
CASRN: NOCAS_920532
DTXSID: DTXSID00920532
Mono.Mass: 468.114807


8-(2,6-Diethyl-4-methylphenyl)-8-hydroxy-2,3,4,5-tetrahydro-1H-benzodioxole
CASRN: NOCAS_920508
DTXSID: DTXSID10920508
Mono.Mass: 332.173607


5-(((Methylamino)(nitroamino)methylene)amino)thiazole
CASRN: NOCAS_912338
DTXSID: DTXSID20912338
Mono.Mass: 295.004511


Sodium 3,4,4-trifluoro-3-butene-1-sulfonate
CASRN: NOCAS_912336
DTXSID: DTXSID00912336
Mono.Mass: 211.973094

Send to batch and select....

- A few seconds to assemble
 - ToxCast data - #actives/#assays and % active
 - # articles in PubMed
 - Links to IRIS or PPRTV reports
 - TEST or OPERA predictions
 - Exposure data: predictions and CPDat

Intrinsic And Predicted Properties

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

Metadata

- Curation Level Details
- NHANES/Predicted Exposure
- Data Sources
- Include ToxVal Data Availability
- Assay Hit Count
- Number of PubMed Articles
- PubChem Data Sources
- CPDat Product Occurrence Count
- IRIS
- PPRTV

A	B	C	D	E	F	G	H	I	J	K	L	M
DTXSID	PREFERRED_NAME	EXPOCAST_MEI	EXPOCAST	NHANES	TOXVAL_DATA	TOXCAST_%_ACT	TOXCAST	#PUBMED	PUBCHEM	CPDAT_COUI	IRIS_LINK	PPRTV_LINK
DTXSID2021105	Pentachloronitrobenzene	1.14e-07	Y	Y	Y	11.8	99/839	69	96	164	Y	-
DTXSID4022527	Propylparaben	1.4e-05	Y	Y	Y	13.77	99/719	201	121	1476	-	-
DTXSID4024064	Dinex	8.29e-08	Y	-	Y	42.13	99/235	-	35	5	Y	-
DTXSID0032493	Triadimenol	1.73e-08	Y	-	Y	10.54	98/930	163	74	83	-	-
DTXSID4032667	Esfenvalerate	1.7e-06	Y	-	Y	11.45	98/856	483	45	198	-	-
DTXSID6020561	Endrin	1.29e-07	Y	-	Y	14.02	98/699	284	16	98	Y	Y
DTXSID6025355	Glutaraldehyde	2.03e-05	Y	-	Y	14.35	98/683	6515	139	1144	-	-
DTXSID8032417	Isofenphos	1.87e-08	Y	-	Y	16.28	98/602	30	42	60	-	-
DTXSID6032352	Chlorpyrifos-methyl	1.07e-07	Y	Y	Y	11.27	97/861	72	50	116	-	-
DTXSID8020620	Fenthion	8.99e-08	Y	Y	Y	11.56	97/839	354	100	99	-	-
DTXSID2020189	FD&C Blue No. 1	0.000178	Y	-	Y	13.72	97/707	174	49	672	-	-
DTXSID7044843	Erythrosin B	6.3e-07	Y	-	-	24.25	97/400	14843	51	7	-	-
DTXSID5041778	Chloropropylate	1.05e-07	Y	-	Y	40.93	97/237	-	36	12	-	-
DTXSID5023900	Benomyl	1.11e-07	Y	-	Y	11.23	96/855	476	91	105	Y	-
DTXSID9020247	Carbaryl	5.61e-08	Y	Y	Y	11.51	96/834	1135	117	245	Y	-
DTXSID8024109	Flutolanil	1.63e-08	Y	-	Y	11.4	95/833	6	59	80	-	-
DTXSID1023998	Cypermethrin	1.62e-06	Y	Y	Y	10.78	94/872	1148	148	246	-	-
DTXSID2024242	Paclitaxel	9.19e-08	Y	-	Y	11.11	94/846	139	-	40	Y	-
DTXSID1020807	2-Mercaptobenzothiazole	4.7e-05	Y	-	Y	12.82	94/733	111	181	86	-	Y

Real-Time Predictions

Input structure
using sketcher

Edit chemical

Select endpoints
for prediction

United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Search all data

Atrazine

100%

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

EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Share Search all data

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/cm ³	1.157 g/cm ³		1.278 g/cm ³	1.197 g/cm ³

- Four individual models plus consensus model with calculation report

Real-Time Predictions with detailed calculation reports

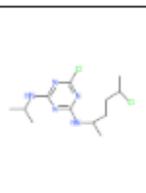
Predicted Vapor pressure at 25°C for C1C=1N=C(N=C(N1)NC(C)CCC(Cl)C)NC(C)C from Consensus method

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

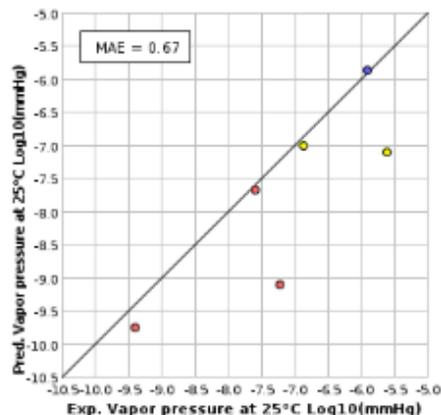
Method	Predicted value Log10(mmHg)
Hierarchical clustering	-6.47
Group contribution	-7.62
Nearest neighbor	-6.46



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

If the predicted value matches the experimental values for similar chemicals in the test set (and the similar chemicals were predicted well), one

Prediction results (colors defined in table below)



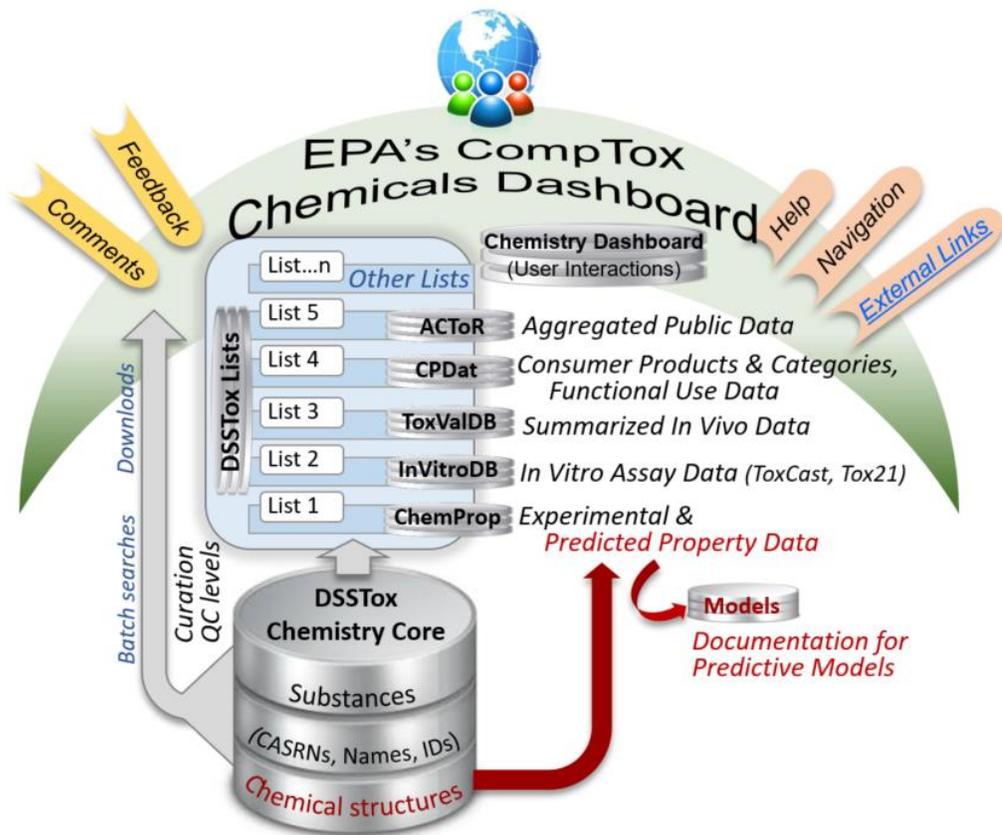
Chemicals	MAE*
Entire set	0.47
Similarity coefficient ≥ 0.5	0.67

*Mean absolute error in Log10(mmHg)

CAS	Structure	Similarity Coefficient	Experimental value Log10(mmHg)	Predicted value Log10(mmHg)
<chem>C1C=1N=C(N=C(N1)NC(C)CCC(Cl)C)NC(C)C</chem> (test chemical)			N/A	-6.85
2287-19-6		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

- Full prediction report
- Shows chemicals used in training set

Summary and Conclusion



- CompTox Chemicals Dashboard - a central hub for environmental data
 - ~875k chemical substances
 - Integrating property data, hazard data, exposure data, *in vitro* bioactivity data
 - Interrogation of bioactivity data -
 - Multiple types of searches
- | | | |
|-----------|------------------------|------------|
| Chemicals | Product/Use Categories | Assay/Gene |
|-----------|------------------------|------------|
- Batch search for thousands of chemicals
 - Real-time property and toxicity predictions
 - Downloadable files – CSV, TSV and Excel

Acknowledgements

EPA-RTP



Credit: the Research Triangle Foundation

- *An enormous team of contributors from Center for Computational Toxicology and Exposure, especially the IT development team*
- *Multiple centers and laboratories across EPA*
- *Special Mentions:*
 - *Dashboard: Jeff Edwards and Chris Grulke*
 - *GenRA: Imran Shah & George Helman*
 - *Abstract Sifter: Nancy Baker*
 - *InvitroDB: Katie Paul-Friedman*

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LIVE DEMO

IF TIME