

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

 United States Environmental Protection Agency

HomeAdvanced SearchBatch SearchLists▼PredictionsDownloads

Share▼



875 Thousand Chemicals

Chemicals

Product/Use Categories

Assay/Gene

☐ Identifier substring search

See what people are saying, read the dashboard [comments!](#)
Cite the Dashboard Publication [click here](#)

Latest News

[Read more news](#)


Journal of Cheminformatics article regarding "MS-Ready structures"

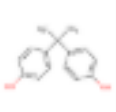
March 9th, 2019 at 1:09:45 PM

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](#).

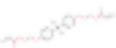
BASIC Search

Chemicals Product/Use Categories Assay/Gene

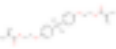
 Bisphenol



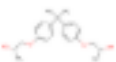
Bisphenol A
DTXSID7020182



Bisphenol A bis(2-hydroxyethyl ether) diacrylate
DTXSID6066991

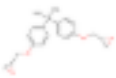


Bisphenol A bis(2-hydroxyethyl ether) dimethacrylate
DTXSID1066992

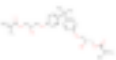


Bisphenol A bis(2-hydroxypropyl) ether
DTXSID8051592

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

EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Copy Share Submit Comment Search all data

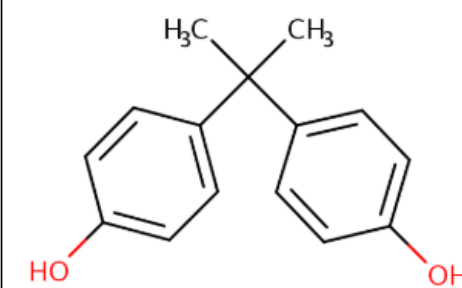
Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

DETAILS

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








Wikipedia


Bisphenol A (BPA) is an organic synthetic compound with the chemical formula $(\text{CH}_3)_2\text{C}(\text{C}_6\text{H}_4\text{OH})_2$ 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:** $\text{C}_{15}\text{H}_{16}\text{O}_2$  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

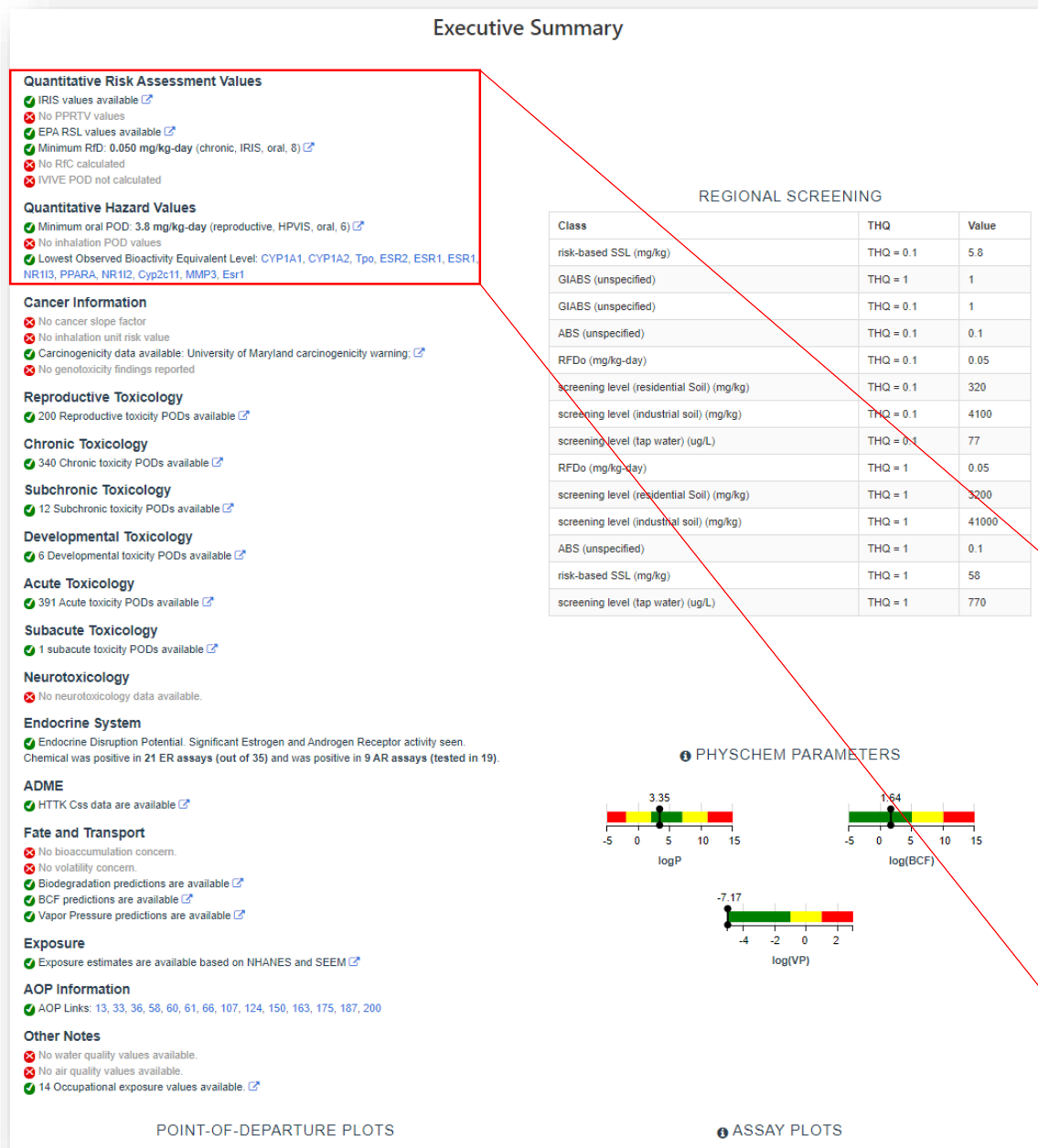
Record Information

Quality Control Notes

- 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



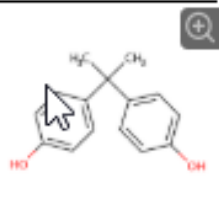
Quantitative Risk Assessment Values

- ✓ 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

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 |

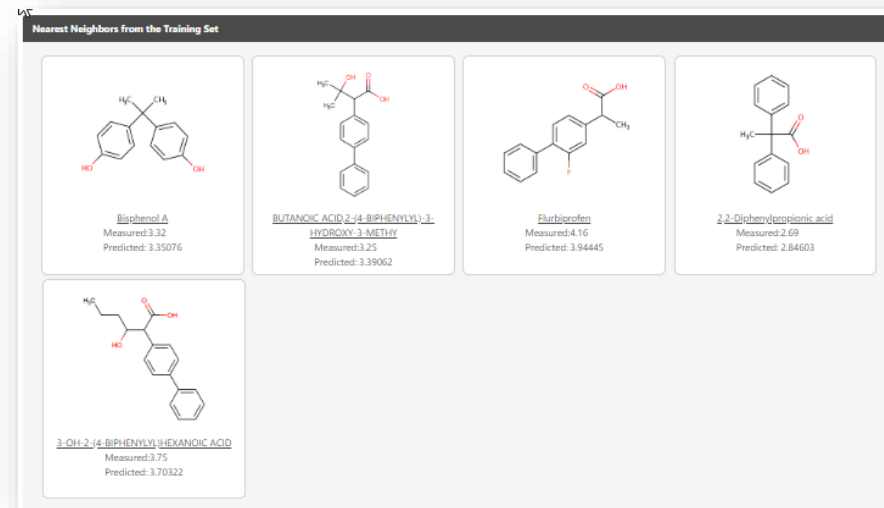
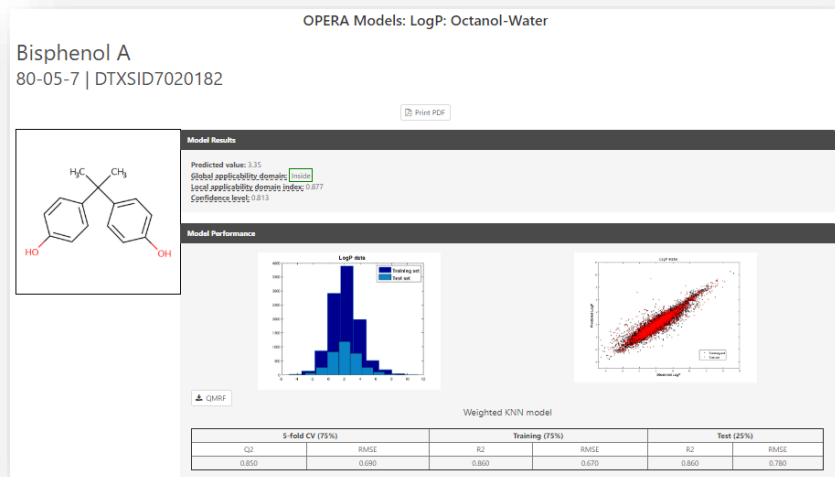
- Physchem and Fate & Transport experimental and predicted data
- Data can be downloaded as Excel, TSV and CSV files
- Predictions: multiple algorithms
 - EPI Suite: Estimation Program Interface
 - ACD/Labs (commercial)
 - TEST: **T**oxicity **E**stimation **S**oftware **T**ool
 - OPERA: **O**PEn structure–activity/property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

Transparency for prediction models

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

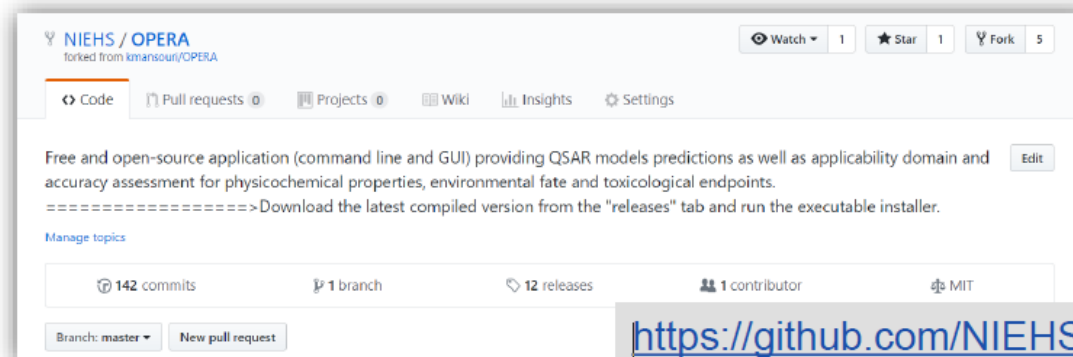
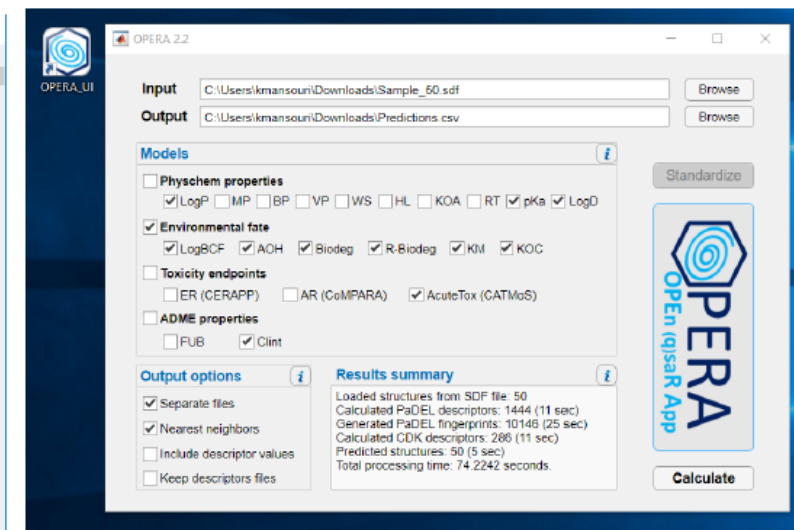
Developed at:
National Center of Computational Toxicology
United States Environmental Protection Agency

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

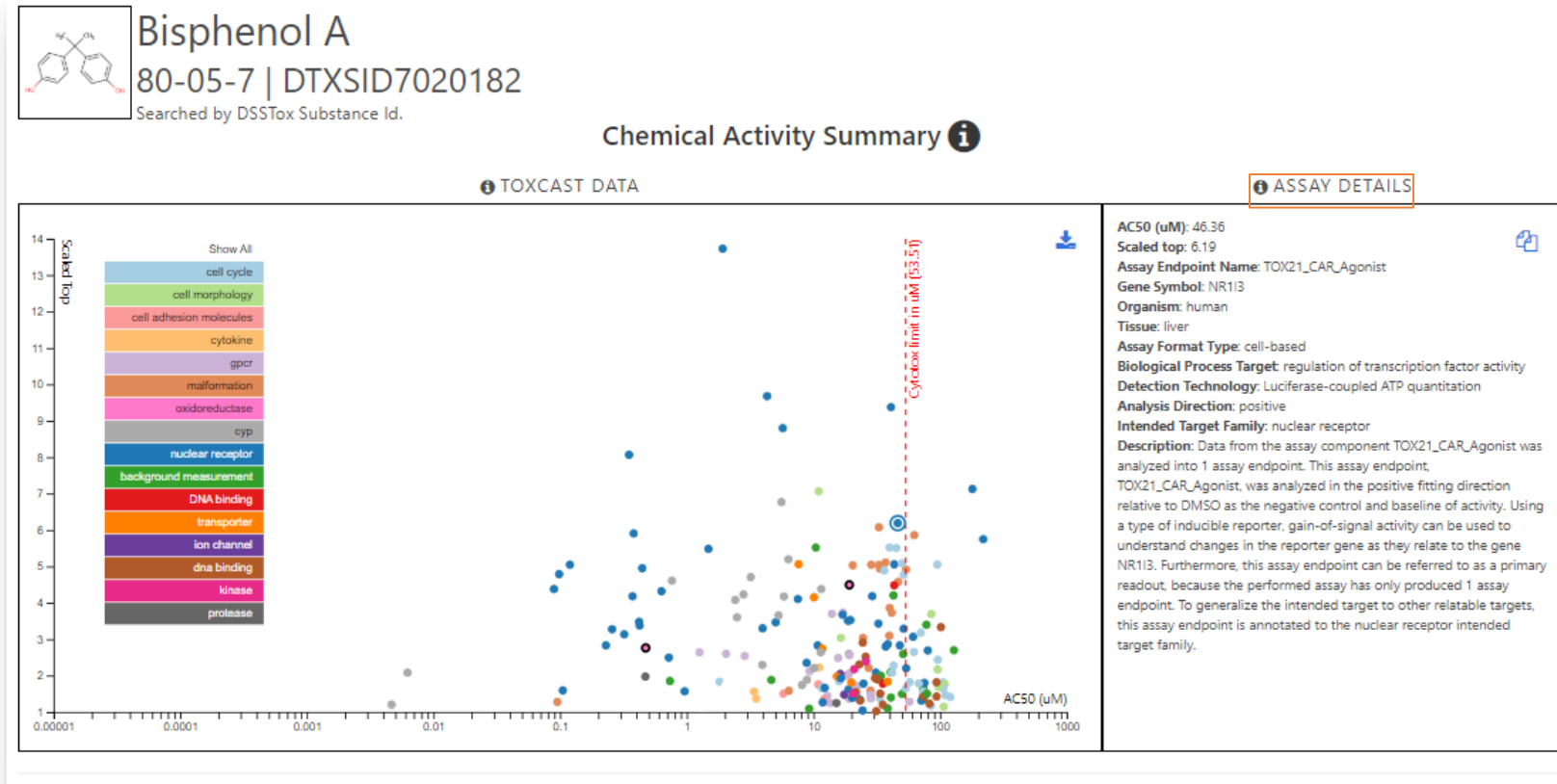
| Hazard | | | | | | | | | | | |
|------------------|----------|------|----------------------------------|-----------------------|--------|-----------|------------|----------------|---------|---|----------------------------|
| DataType | | | | | | | | | | | |
| Toxicity Value | | | | | | | | | | | |
| 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

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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



Bisphenol A
80-05-7 | DTXSID7020182
Searched by Expert Validated Synonym.

Assay Selection 136 Selected

☒ 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)

ToxCast/Tox21

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

A Single Assay Can Have Multiple Charts

☒ Representative Samples Only

Bioactivity Summary▼

Number of Charts: 136

Ceetox, HQSR, ANDR, dn
HITCALL: ACTIVE
Bisphenol A (80-05-7)
DTXSID7020182
TP0001055208



Ceetox, HQSR, TESTO, dn
HITCALL: ACTIVE
Bisphenol A (80-05-7)
DTXSID7020182
TP0003884412




OT, ER, ERGRs, 0480
HITCALL: ACTIVE
Bisphenol A (80-05-7)
DTXSID7020182
TP0000018006



OT, ER, ERGRs, 1440
HITCALL: ACTIVE
Bisphenol A (80-05-7)
DTXSID7020182
TP0003761801




Sources of Exposure to Chemicals



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 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<<<12345678910>>>Last

Identifiers to Support Searches

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DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

▶ ADME

▶ EXPOSURE

▶ BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

▶ LITERATURE

LINKS

COMMENTS

Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

25 ▾

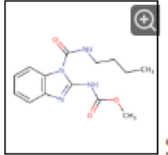
| Synonym | Quality |
|--|-----------|
| Bisphenol A | Valid |
| 4,4'-(Propane-2,2-diyl)diphenol | Valid |
| Phenol, 4,4'-(1-methylethylidene)bis- | Valid |
| 80-05-7 Active CAS-RN | Valid |
| BPA | Valid |
| 4,4'-Propane-2,2-diylidiphenol | Valid |
| Phenol, 4,4'-(1-methylethylidene)bis- | Valid |
| 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 |

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.

Abstract Sifter

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

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.

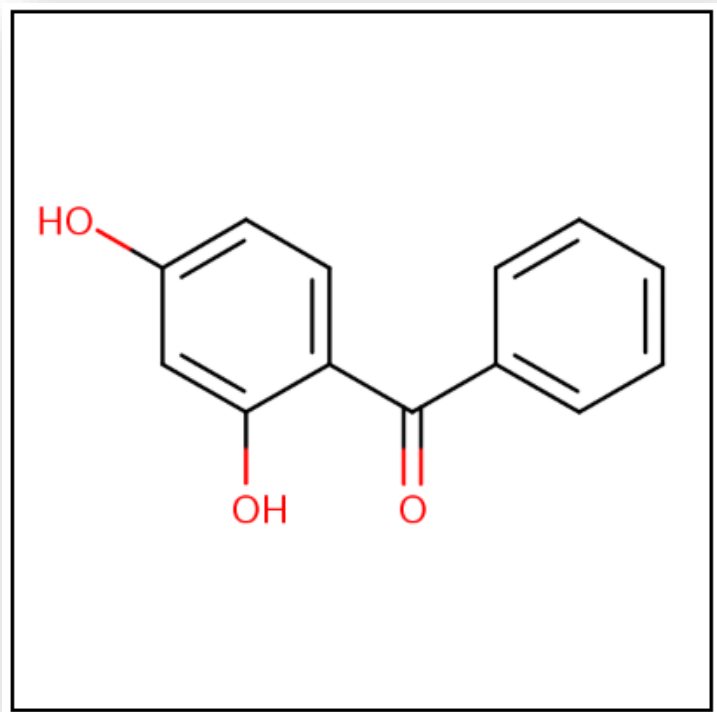
degradation benomyl N,N'-dibutylurea

Download / Send to... [Download Sifter for Excel](#)

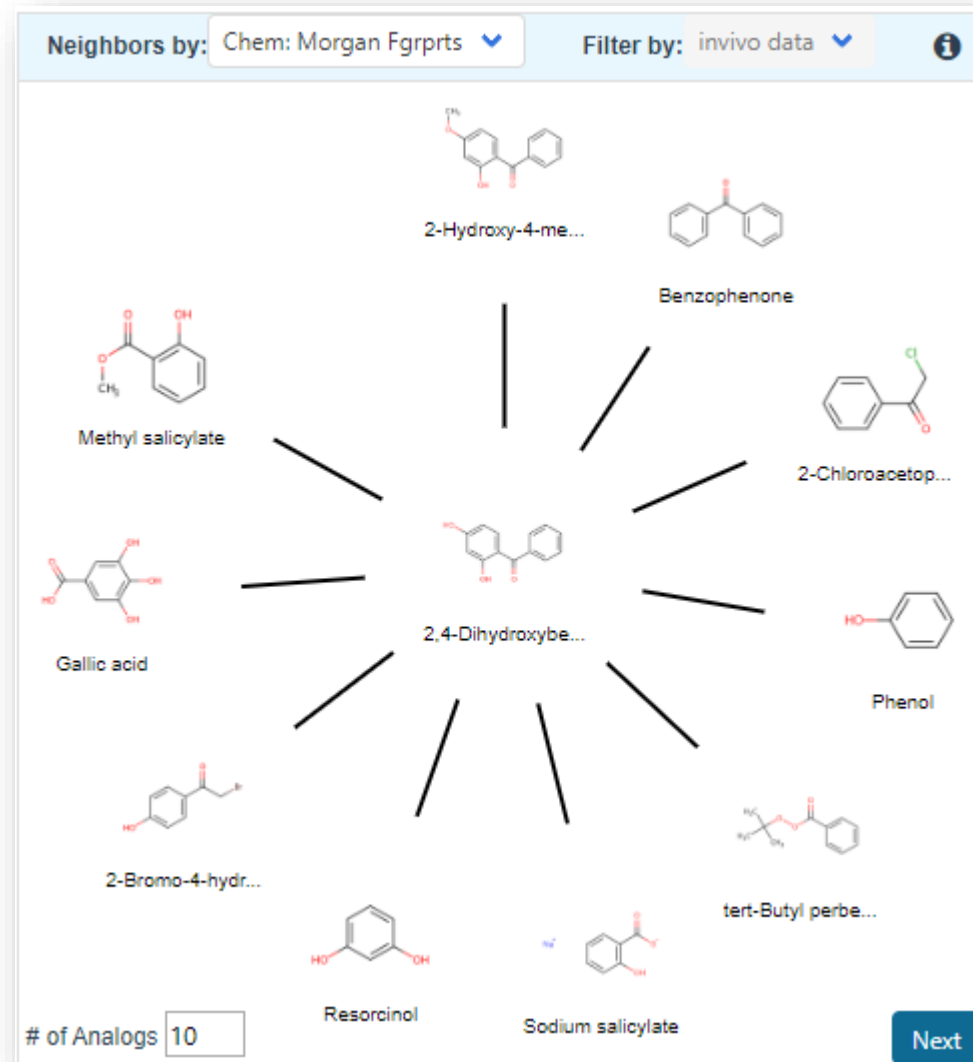
| | degradation | benomyl | N,N'-dibutylurea | Total | PMID | Year | Title | Authors | Journal | Rev |
|--|-------------|---------|------------------|-------|----------|------|--|--|---|-----|
| | 1 | 11 | 2 | 14 | 17493661 | 2007 | Formulation factors that can reduce the formation of the phytotoxic impurity, N,N'-... | Ho; Lin; Wang | Chemosphere | |
| | 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 | |
| | 3 | 1 | 1 | 5 | 15865150 | 2005 | Accelerated degradation of N, N'-dibutylurea (DBU) upon repeated application. | Bischoff; Lee; Turco | Biodegradation | |
| | 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... | |
| | 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 | |
| | 0 | 1 | 0 | 1 | 31190279 | 2019 | Two herbicides, two fungicides and spore-associated bacteria affect Funneliformis... | de Novais; Giovannetti; de Faria; Sbrana | Mycorrhiza | |
| | 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 | |
| | 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 ... | |
| | 0 | 1 | 0 | 1 | 30744902 | 2019 | Benzimidazole- and Qol-resistance in <i>Corynespora cassicola</i> populations from gr... | Duan; Xin; Lu; Li; Wu; Wang; Zhou | Pesticide biochemistry and physiology | |
| | 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 | |
| | 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 | |
| | 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 | |
| | 0 | 1 | 0 | 1 | 29933012 | 2018 | Bioassay-guided isolation of active substances from <i>Semen Torreyae</i> identifies tw... | Liu; Veyerer; Lu; Wenseleers; De Borggraeve; Jian... | Journal of ethnopharmacology | |
| | 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 | |
| | 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

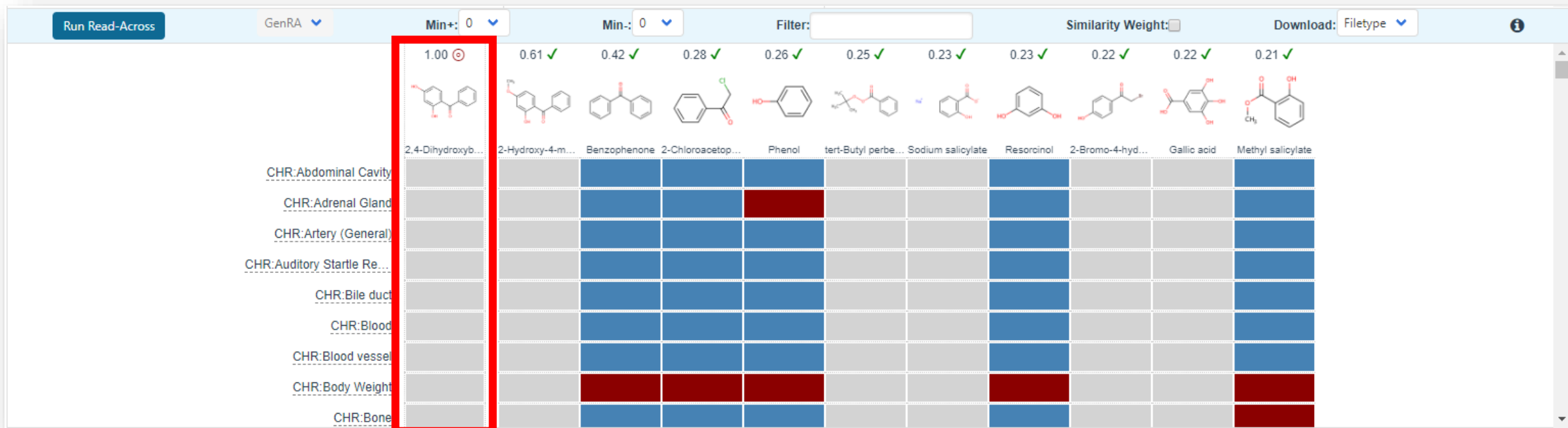


- Analogue identification: based on Morgan fingerprints and selecting 10 default analogues



GenRA in practice – step by step

- Data matrix view of source analogues relative to target chemical



GenRA in practice – step by step

- Updated Data matrix view with GenRA predictions for target chemical

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

| | 1.00 | 0.61 | 0.42 | 0.28 | 0.26 | 0.25 | 0.23 | 0.23 | 0.22 | 0.22 | 0.21 |
|----------------------------|-------------------|------------------|--------------|-------------------|--------|---------------------|-------------------|------------|------------------|-------------|-------------------|
| | | | | | | | | | | | |
| | 2,4-Dihydroxyb... | 2-Hydroxy-4-m... | Benzophenone | 2-Chloroacetop... | Phenol | tert-Butyl perbe... | Sodium salicylate | Resorcinol | 2-Bromo-4-hyd... | Gallic acid | Methyl salicylate |
| CHR:Abdominal Cavity | Blue | Grey | Blue | Blue | Blue | Grey | Grey | Blue | Grey | Grey | Blue |
| CHR:Adrenal Gland | Blue | Grey | Blue | Blue | Red | Grey | Grey | Blue | Grey | Grey | Blue |
| CHR:Artery (General) | Blue | Grey | Blue | Blue | Blue | Grey | Grey | Blue | Grey | Grey | Blue |
| CHR:Auditory Startle Re... | Blue | Grey | Blue | Blue | Blue | Grey | Grey | Blue | Grey | Grey | Blue |
| CHR:Bile duct | Blue | Grey | Blue | Blue | Blue | Grey | Grey | Blue | Grey | Grey | Blue |
| CHR:Blood | Blue | Grey | Blue | Blue | Blue | Grey | Grey | Blue | Grey | Grey | Blue |
| CHR:Blood vessel | Blue | Grey | Blue | Blue | Blue | Grey | Grey | Blue | Grey | Grey | Blue |
| CHR:Body Weight | Red | Grey | Red | Red | Red | Grey | Grey | Red | Grey | Grey | Red |
| CHR:Bone | Blue | Grey | Blue | Blue | Blue | Grey | Grey | Blue | Grey | Grey | Red |

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

Related Publications



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, b, c}, Jie Liu^{b, c}, Richard S. Judson^a, Russell S. Thomas^a, Grace Patlewicz^a



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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

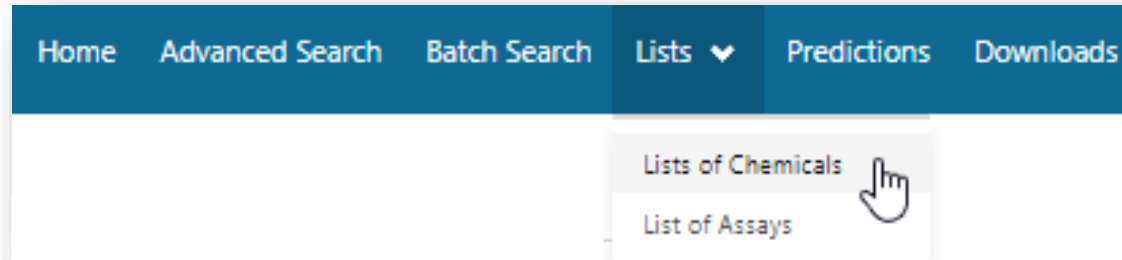
^b School of Pharmacy and Biomolecular Sciences, Liverpool John Moores University, Byrom Street, Liverpool L3 3AF, UK

^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

CHEMICAL LISTS AND CATEGORIES

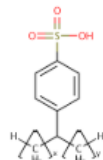

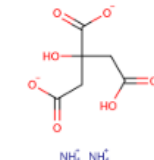

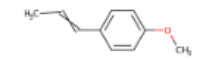
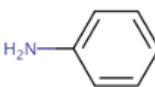
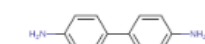
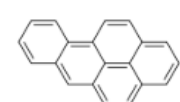
EPAHFR: Hydraulic Fracturing



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

 Download ▼

Columns ▼

PFAS

 Copy Filtered Lists URL

| 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

Download

10

ATG

OT

NHEERL_PADILLA

Search query

Copy page URL

| 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 determine if a target gene is upregulated. They relate to the gene AHR. Furthermore, this assay endpoint can be referred to as a primary readout, because this assay has produced a reporter gene function. To generalize the 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 determine if a target gene is upregulated. They relate to the gene FOS and JUN. Furthermore, this assay endpoint can be referred to as a primary readout, because this assay has produced a reporter gene function. To generalize the 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 determine if a target gene is upregulated. They relate to the gene TFAP2A, TFAP2B, and TFAP2D. Furthermore, this assay endpoint can be referred to as a primary readout, because this assay has produced a reporter gene function. To generalize the intended target family, where the subfamily is "basic leucine zipper". | TFAP2A TFAP2B TFAP2D |

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

Select all

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Send to Batch Search

Default



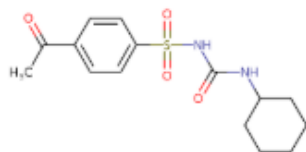
CASRN

TOXCAST

PubMed

Inactive

Filter by Name or CASRN

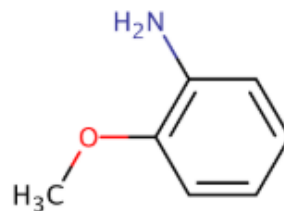


Acetohexamide

CASRN: 968-81-0

TOXCAST: 4/376

PubMed: 235



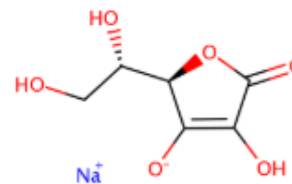
HCl

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

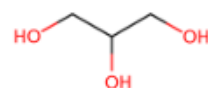
Results for CPCat Use Category: CPCat term: Lubricant

1738 chemicals

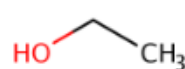
Select all Download Send to Batch Search CPDAT DTXSID PubChem CPDAT Hide chemicals that are: Filter by Name or CASR



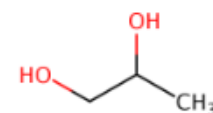
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PubChem: 637
CPDAT: 8270



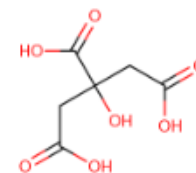
Glycerol
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PubChem: 13028
CPDAT: 4249



Ethanol
DTXSID: DTXSID9020584
PubChem: 1591
CPDAT: 3635



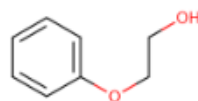
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Citric acid
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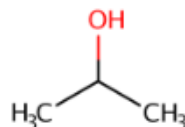
Titanium dioxide
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PubChem: 103
CPDAT: 2519



2-Phenoxyethanol
DTXSID: DTXSID9021976
PubChem: 140
CPDAT: 2314



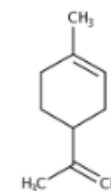
Sodium chloride
DTXSID: DTXSID3021271
PubChem: 203
CPDAT: 2197



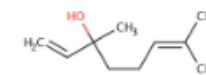
Isopropanol
DTXSID: DTXSID7020762
PubChem: 1267
CPDAT: 2176



Sodium hydroxide
DTXSID: DTXSID0029634
PubChem: 203
CPDAT: 2085



Limonene
DTXSID: DTXSID2029612
PubChem: 123
CPDAT: 2068



Linalool
DTXSID: DTXSID7025502
PubChem: 118
CPDAT: 1984

Other Searches

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

 Search for assays based on endpoint name or gene symbol

Chemical-Biology

Assay/Gene Search

W

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



 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

Advanced Searches

Mass Search

Mass Search 

± Min/Max

Adduct

Neutral



All Adducts



Choose adduct from dropdown

191.131

Da

±

5

Da

ppm

Search



Advanced Searches

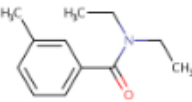
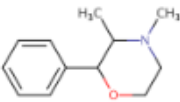
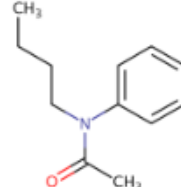
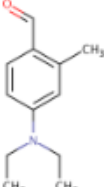
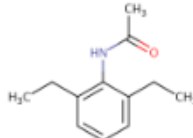
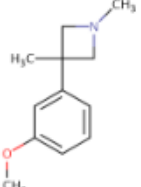
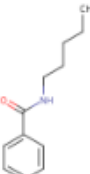
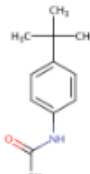
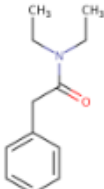
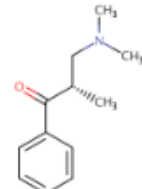
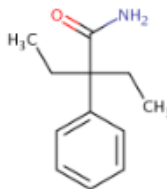
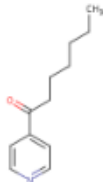
Mass Search

Search Results

Searched by Mass: 191.131 +/- 5.0 ppm.

329 of 329 chemicals visible

[Select all](#) [Download](#) [Send to Batch Search](#) [Mass Difference](#) [DTXSID](#) [CASRN](#) [TOXCAST](#) [Mass Diff](#) [Multicomponent Chemicals](#) [Filter by Name or CASRN](#)

| | | | | | |
|---|---|--|--|--|--|
|  <p>DEET DTXSID: DTXSID2021995 CASRN: 134-62-3 TOXCAST: 12/768 Mass Diff: 0.000014</p> |  <p>Phendimetrazine DTXSID: DTXSID1023447 CASRN: 634-03-7 TOXCAST: - Mass Diff: 0.000014</p> |  <p>N-Butylacetanilide DTXSID: DTXSID2042197 CASRN: 91-49-6 TOXCAST: - Mass Diff: 0.000014</p> |  <p>Benzaldehyde, 4-(diethylamino)-2-methoxy- DTXSID: DTXSID4059041 CASRN: 92-14-8 TOXCAST: - Mass Diff: 0.000014</p> |  <p>Acetanilide, 2',6'-diethyl- DTXSID: DTXSID90168148 CASRN: 16665-89-7 TOXCAST: - Mass Diff: 0.000014</p> |  <p>Azetidine, 1,3-dimethyl-3-(m-methoxyphenyl)- DTXSID: DTXSID40173560 CASRN: 19832-26-9 TOXCAST: - Mass Diff: 0.000014</p> |
|  <p>Benzamide, N-pentyl- DTXSID: DTXSID20174196 CASRN: 20308-43-4 TOXCAST: - Mass Diff: 0.000014</p> |  <p>p-t-Butylacetanilide DTXSID: DTXSID80174238 CASRN: 20330-45-4 TOXCAST: - Mass Diff: 0.000014</p> |  <p>N,N-Diethylphenylacetamide DTXSID: DTXSID00179048 CASRN: 2431-96-1 TOXCAST: - Mass Diff: 0.000014</p> |  <p>3-(Dimethylamino)-2-methylpropionophenone DTXSID: DTXSID60180796 CASRN: 26171-50-6 TOXCAST: - Mass Diff: 0.000014</p> |  <p>Butyramide, 2-ethyl-2-phenyl- DTXSID: DTXSID60184653 CASRN: 30568-39-9 TOXCAST: - Mass Diff: 0.000014</p> |  <p>1-Heptanone, 1-(4-pyridyl)- DTXSID: DTXSID40186594 CASRN: 32941-30-3 TOXCAST: - Mass Diff: 0.000014</p> |

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

Jon R. Sobus¹  • Jarod N. Grossman^{2,3} • Alex Chao² • Randolph Singh⁴ • Antony J. Williams⁵ • Christopher M. Grulke⁵ • Ann M. Richard⁵ • Seth R. Newton¹ • Andrew D. McEachran⁴ • Elin M. Ulrich¹

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

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Article

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

Display All Chemicals Download Chemical Data

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

Excel Download

| INPUT | FOUND BY | DTXSID | PREFERRED NAME |
|---------------------------|---------------|----------------|------------------------------------|
| 2,4-dihydroxybenzophenone | 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'-Tetrahydroxybenzophenone |
| 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 | DTXSID0020637 | Diazinon |

Include Data of Interest – then dive deeper...

Chemical Identifiers

- ☒ DTXSID ⓘ
- ☒ Chemical Name ⓘ
- ☐ DTXCID ⓘ
- ☒ CAS-RN ⓘ
- ☐ InChIKey ⓘ
- ☐ IUPAC Name ⓘ

Structures

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

Intrinsic And Predicted Properties

- ☐ Molecular Formula ⓘ
- ☐ Average Mass ⓘ
- ☐ Monoisotopic Mass ⓘ
- ☐ TEST Model Predictions ⓘ
- ☒ OPERA Model Predictions ⓘ

Metadata


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

| 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)-Diethylstilbene | 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 | 57-30-7 | 1.66e-07 | Y | - | Y | 2.15 | 15/698 | 17600 | - |
| DTXSID50 | 2,2',4,4'-Tetrahydroxydiphenyl ether | 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

- Select list and send to batch



United States
Environmental Protection
Agency

Home
Advanced Search
Batch Search
Lists
Predictions
Downloads

Share

Select List

PESTICIDES|EPA: Pesticide Chemical Search Database

☐ 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://aspub.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

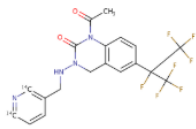
DTXSID

Mono.Mass

3988 chemicals

Hide chemicals that are:

Filter by Name or CASRN

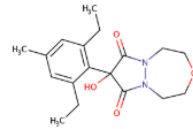


1-Acetyl-6-(1,1,1,2,3,3,3-heptafluoro-2-p...

CASRN: NOCAS_920532

DTXSID: DTXSID00920532

Mono.Mass: 468.114807

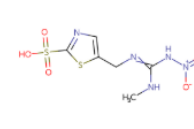


8-(2,6-Diethyl-4-methylphenyl)-8-hydro...

CASRN: NOCAS_920508

DTXSID: DTXSID10920508

Mono.Mass: 332.173607

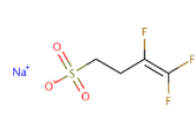


5-(((Methylamino)(nitroamino)methylen...

CASRN: NOCAS_912338

DTXSID: DTXSID20912338

Mono.Mass: 295.004511



Sodium 3,4,4-trifluoro-3-butene-1-sulfo...

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_ME | EXPOCAST | NHANES | TOXVAL_DATA | TOXCAST_%_ACT | TOXCAST | #PUBMED | PUBCHEM | CPDAT_COU | 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 | Paclobutrazol | 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

The screenshot shows the EPA's Real-Time Predictions web application. The header includes the EPA logo, "United States Environmental Protection Agency", and navigation links: Home, Advanced Search, Batch Search, Lists, Predictions, and Downloads. A search bar contains the text "Atrazine". Below the header is a toolbar with various icons for file operations and editing. The main workspace displays the chemical structure of Atrazine, a triazine derivative with two isopropylamino groups and a 4-chlorophenyl group. To the right of the workspace is a panel titled "Select properties to predict". It lists two categories: "T.E.S.T." and "Physical properties". Under "T.E.S.T.", there are seven checked items: "Toxicological properties", "96 hour fathead minnow LC50", "48 hour D. magna LC50", "48 hour T. pyriformis IGC50", "Oral rat LD50", "Bioaccumulation factor", and "Developmental toxicity". Under "Physical properties", there are eight checked items: "Ames mutagenicity", "Estrogen Receptor RBA", "Estrogen Receptor Binding", "Normal boiling point", "Melting point", "Flash point", "Vapor pressure", and "Density". A "Calculate" button is located at the bottom right of the panel. The bottom of the interface shows a row of geometric shapes for selection and a "Chiral" checkbox.

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

Physical properties

- ☒ Ames mutagenicity
- ☒ Estrogen Receptor RBA
- ☒ Estrogen Receptor Binding
- ☒ 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

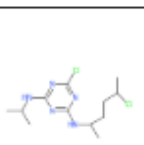
Predicted Vapor pressure at 25°C for ClC=1N=C(N=C(N)NC(C)CCC(Cl)C)NC(C)C from Consensus method

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

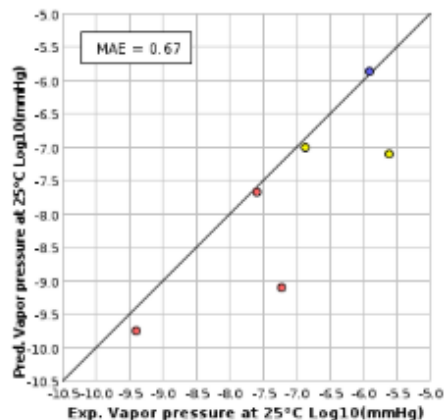
| Method | Predicted value Log10(mmHg) |
|-------------------------|-----------------------------|
| Hierarchical clustering | -6.47 |
| Group contribution | -7.62 |
| Nearest neighbor | -6.46 |



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

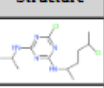
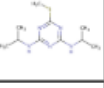
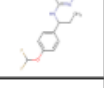
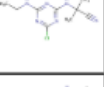
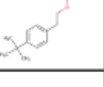
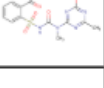

If the predicted value matches the experimental values for similar chemicals in the test set (and the similar chemicals were predicted well), one

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>ClC=1N=C(N=C(N)NC(C)CCC(Cl)C)NC(C)C</chem> (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 |

- 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

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LIVE DEMO

IF TIME