

US-EPA CompTox chemicals dashboard: A web-based data integration hub for environmental chemistry data

***Antony Williams, Chris Grulke, Richard Judson,
John Wambaugh, Jeremy Dunne and Jeff Edwards***

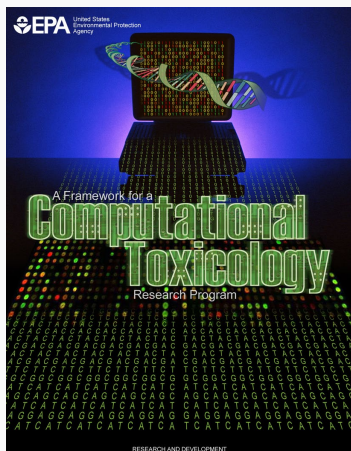
National Center for Computational Toxicology, U.S. Environmental Protection Agency, RTP, NC

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

*Spring 2019
ACS Spring Meeting, Orlando*

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

National Center for Computational Toxicology




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



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EDSP Dashboard

Endocrine Disruption Screening Program for the 21st Century

Chemical Summary

Public Information

Bioactivity Summary

Bioactivity

High Throughput Exposure

Assay Definitions

Tools

EDSP Dashboard Overview

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

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

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



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

ToxCast Data Use Considerations

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

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

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



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

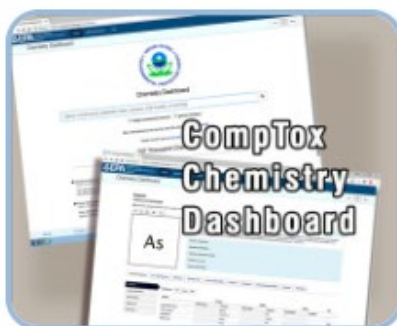
CompTox Portal

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CompTox Dashboard

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

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762 Thousand Chemicals

Chemicals Product/Use Categories Assay/Gene

Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey

Identifier substring search

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

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[Read more news](#)

YouTube video regarding using the Dashboard for Non-Targeted Analysis

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

Ar
Mar

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




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CompTox Dashboard Chemicals


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
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762 Thousand Chemicals


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




Bisphenol A
DTXSID7020182



Bisphenol A bis(2-hydroxyethyl ether) diacrylate
DTXSID6066991




Bisphenol A bis(2-hydroxyethyl ether) dimethacrylate
DTXSID1066992




Bisphenol A bis(2-hydroxypropyl) ether
DTXSID8051592


Bisphenol A carbonate polymer
DTXSID6027840




Bisphenol A diglycidyl ether
DTXSID6024624



Bisphenol A glycidyl methacrylate
DTXSID7044841




Bisphenol A propoxylate diglycidyl ether
DTXSID10399098



Bisphenol A propoxylate glycerolate diacrylate
DTXSID40400126

comptox-prod.epa.gov/dashboard


CompTox Dashboard Products and Use Categories



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762 Thousand Chemicals

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

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

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


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

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

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

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

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



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CompTox Dashboard Assays and Genes



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762 Thousand Chemicals

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

GENE: ESR1
estrogen receptor 1


GENE: ESR2
estrogen receptor 2 (ER beta)

GENE: ESRRB
estrogen-related receptor alpha

GENE: ESRRA
estrogen-related receptor beta

GENE: ESRRG
estrogen-related receptor gamma

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



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Detailed Chemical Pages

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

► ADME

► EXPOSURE

► BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

► LITERATURE

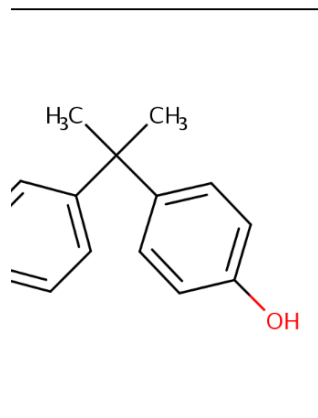
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COMMENTS

Bisphenol A

DTXSID7020182

3STox Substance Id.



Batch Search Lists Predictions Downloads

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Search all data

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. It has been in commercial use since 1957.

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

[Read more](#)

Intrinsic Properties

Structural Identifiers

Linked Substances

Presence in Lists

Record Information

Quality Control Notes

Physicochemical properties

Property



Summary



Summary

LogP: Octanol-Water

Melting Point

Boiling Point

Water Solubility

Vapor Pressure

Flash Point

Surface Tension

Index of Refraction

Molar Refractivity

Polarizability

Density

Molar Volume

Thermal Conductivity

Viscosity

Henry's Law

LogKoa: Octanol-Air

Summary

Search query

Average	Experimental median	Predicted median	Experimental range	Predicted range	Unit
		3.43	3.32	2.40 to 3.64	
	156	138	153 to 156	125 to 157	°C
		360	200	343 to 401	°C
		1.00e-3	5.26e-4	5.44e-4 to 1.31e-3	mol/L
		3.43e-7	-	6.83e-8 to 2.59e-6	mmHg
		190	-	188 to 192	°C
			-	46.0	dyn/cm
			-	1.60	
			-	68.2	cm ³
			-	27.0	Å ³
		1.17	-	1.14 to 1.20	g/cm ³
			-	200	cm ³
			-	150	mW/(m ² K)

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

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

To cite this article: K. Mansouri, C. M. Grulke, A. M. Richard, R. S. Judson & A. J. Williams (2016)

An automate
datasets use
DOI: [10.1081](https://doi.org/10.1081)

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

 Journal of Cheminformatics

To link to th

RESEARCH ARTICLE

Open Access



OPERA models for predicting physicochemical properties and environmental fate endpoints

Kamel Mansouri^{1,2,3*} , Chris M. Grulke¹, Richard S. Judson¹ and Antony J. Williams¹

Detailed OPERA Prediction Reports

Source

Result

Calculation Details

Experimental Values

PhysPropNCCT

Predicted Values

EPISUITE

NICEATM

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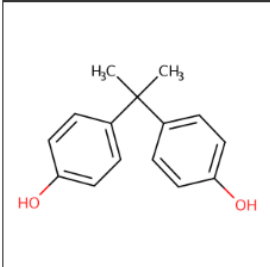
ACD/Labs

OPERA

OPERA Models: LogP: Octanol-Water

Bisphenol A

80-05-7 | DTXSID7020182



Model Results

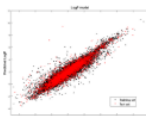
Predicted value: 3.35

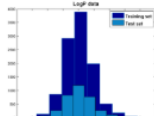
Global applicability domain: Inside

Local applicability domain index: 0.88

Confidence level: 0.75

Model Performance



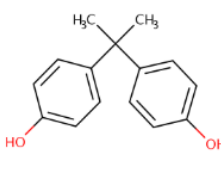


Weighted KNN model

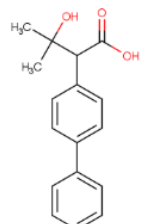
QMRP

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.89	0.85	0.87	0.88	0.78

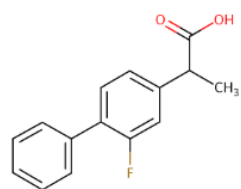
Nearest Neighbors from the Training Set



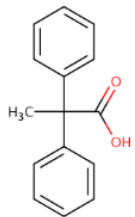
Bisphenol A
Measured: 3.32
Predicted: 3.35



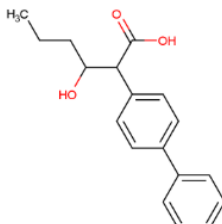
BUTANOIC ACID,2-(4-BIPHENYL)-3-HYDROXY-
Measured: 3.25
Predicted: 3.45



Flurbiprofen
Measured: 4.18
Predicted: 3.83




2,2-Diphenylpropionic acid
Measured: 2.89
Predicted: 2.93



3-OH-2-(4-BIPHENYL)HEXANOIC ACID
Measured: 3.75
Predicted: 3.88

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Access to Chemical Hazard Data

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DETAILS

EXECUTIVE SUMMARY

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ENV. FATE/TRANSPORT

HAZARD

▶ ADME

▶ EXPOSURE

▶ BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES


SYNONYMS

▶ LITERATURE

LINKS

COMMENTS

Data Type











 Point of Departure ▼


Download ▼

Human

Eco

Columns ▼ 10 ▼

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



- ToxVal Database contains following data:
 - 30,050 chemicals
 - 772,721 toxicity values
 - 29 sources of data
 - 21,507 sub-sources
 - 4585 journals cited
 - 69,833 literature citations

In Vitro Bioassay Screening

ToxCast and Tox21

Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

DETAILS

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TOXCAST: SUMMARY

PUBCHEM

TOXCAST: DATA

TOXCAST: MODELS

SIMILAR COMPOUNDS

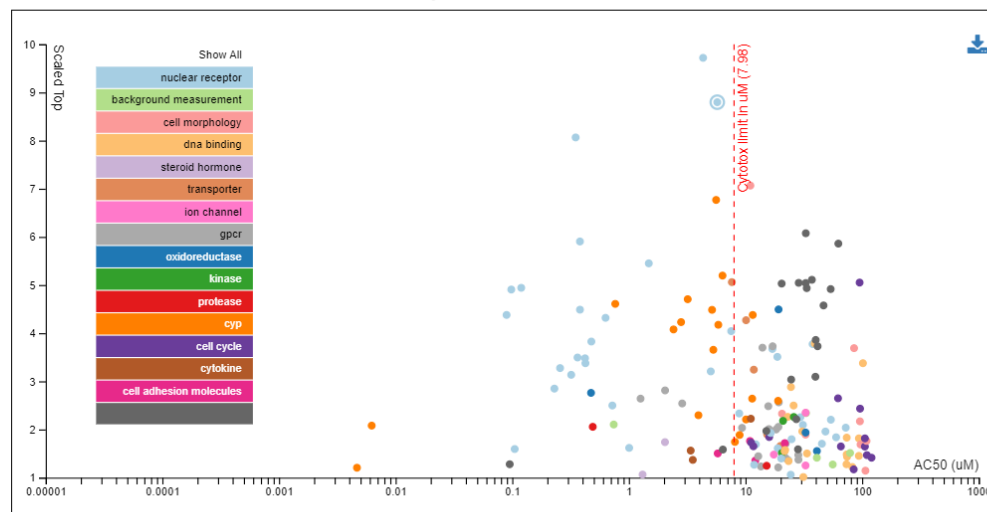
GENRA (BETA)

RELATED SUBSTANCES

Chemical Activity Summary

TOXCAST DATA

ASSAY DETAILS



AC50 (uM): 5.73
Scaled top: 8.80
Assay Endpoint Name: OT_ER_ERaEra_0480
Assay Description: [742](#)
Gene Symbol: ESR1
Organism: human
Tissue: kidney
Assay Format Type: cell-based
Biological Process Target: protein stabilization
Detection Technology: Protein-fragment Complementation
Analysis Direction: positive
Intended Target Family: nuclear receptor
Description: Data from the assay component OT_ER_ERaEra_0480 was analyzed into 1 assay endpoint. This assay endpoint, OT_ER_ERaEra_0480, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of binding reporter, measures of receptor for gain-of-signal activity can be used to understand the binding at the pathway-level as they relate to the gene ESR1. Furthermore, this assay endpoint can be referred to as a primary readout, because the performed assay has only produced 1 assay endpoint. To generalize the intended target to other relatable targets, this assay endpoint is annotated to the 'nuclear receptor' intended target family, where the subfamily is 'steroidal'.

In Vitro Bioassay Screening

ToxCast and Tox21

RELATED SUBSTANCES

SYNONYMS

► LITERATURE

LINKS

COMMENTS

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Search query

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

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Showing 1 to 10 of 161 records

In Vitro Bioassay Screening

ToxCast and Tox21

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TOXCAST: SUMMARY

PUBCHEM

TOXCAST: DATA

TOXCAST: MODELS

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

LITERATURE

LINKS

COMMENTS

Assay Selection 1 Selected

☒ Active
 ☐ Inactive
 ☐ All

Filter

Filter assays

Assay Set: ER (1 of 18 Selected)

- ☒ ACEA_T47D_80hr_Positive
- ☐ ATG_ERE_CIS_up
- ☐ ATG_ERa_TRANS_up
- ☐ NVS_NR_bER
- ☐ NVS_NR_hER
- ☐ NVS_NR_mERa
- ☐ OT_ER_ERaERa_0480
- ☐ OT_ER_ERaERa_1440
- ☐ OT_ER_ERaERb_0480
- ☐ OT_ER_ERaERb_1440
- ☐ OT_ER_ERbERb_0480
- ☐ OT_ER_ERbERb_1440
- ☐ OT_ERa_EREGFP_0120
- ☐ OT_ERa_EREGFP_0480

A Single Assay Can Have Multiple Charts

Number of Charts: 6

ACEA_T47D_80hr_Positive
HITCALL: ACTIVE
Bisphenol A (80-05-7)
DTXSID7020182

Percent Activity

Log Concentration (uM)

Cut Off

1.00

50

0

TX000158

TX011529

TX100158

TX111529



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Searched by DSSTox Substance Id.

- DETAILS
 - EXECUTIVE SUMMARY
 - PROPERTIES
 - ENV. FATE/TRANSPORT
 - HAZARD
 - ▶ ADME

Product and Use Categories (PUCs)

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Columns 10

Product or Use Categorization		↕	Categorization type	↕	Number of Unique Products
manufacturing, metals			CPCat Cassette		17
adhesive			CPCat Cassette		17
CATEGORIES			CPCat Cassette		16
			CPCat Cassette		12
			CPCat Cassette		11
			CPCat Cassette		8
			CPCat Cassette		8
			CPCat Cassette		8
			CPCat Cassette		7
			CPCat Cassette		6
LIGHT FRACTION					
ADDITIONAL USE					

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

PRODUCT & USE CATEGORIES

CHEMICAL WEIGHT FRACTION

CHEMICAL FUNCTIONAL USE

TOXICS RELEASE INVENTORY

MONITORING DATA

EXPOSURE PREDICTIONS

PRODUCTION VOLUME

Sources of Exposure to Chemicals

Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

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PRODUCT & USE CATEGORIES

CHEMICAL WEIGHT FRACTION

CHEMICAL FUNCTIONAL USE

TOXICS RELEASE INVENTORY

MONITORING DATA

EXPOSURE PREDICTIONS

PRODUCTION VOLUME

▼ BIOACTIVITY

Toxics Release Inventory

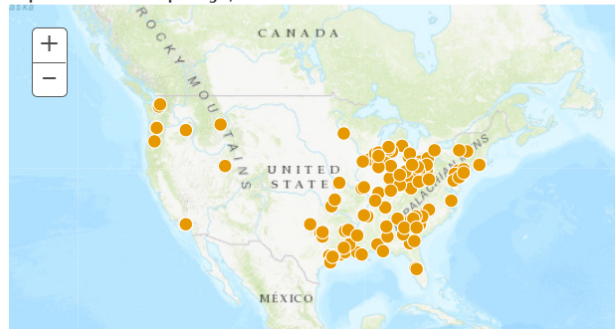
Print Page

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

Data Source: 2016 Dataset (released March 2018)

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

Map of TRI Facilities Reporting 4,4'-ISOPROPYLIDENEDIPHENOL



Quick Facts for 2015

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




United States
Environmental Protection
Agency

Searched by Expert Validated Synonym.

COMMENTS

[illegible]

Identifiers to Support Searches



United States
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Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

DETAILS

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PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

▶ ADME

▶ EXPOSURE

▶ BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

▶ LITERATURE

LINKS

COMMENTS

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

Literature Searches and Links



United States
Environmental Protection
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Bisphenol A

80-05-7 | DTXSID7020182

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▼ LITERATURE

[GOOGLE SCHOLAR](#)[PUBMED ABSTRACT SIFTER](#)[PUBCHEM ARTICLES](#)[PUBCHEM PATENTS](#)[PPRTV](#)[IRIS](#)

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

[Retrieve Articles](#)[Select a Query Term](#)

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

Optionally, edit the query before retrieving.

Abstract Sifter – PubMed Integration

Bisphenol A

80-05-7 | DTXSID7020182

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GOOGLE SCHOLAR

PUBMED ABSTRACT SIFTER

PUBCHEM ARTICLES

PUBCHEM PATENTS

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Hazard

Retrieve Articles

118 of 118 articles loaded...

To find articles quickly, enter terms to sift abstracts.

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

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

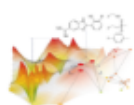


SOFTWARE TOOL ARTICLE

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

✉ Nancy Baker ¹, Thomas Knudsen², Antony Williams ²


 [Author details](#)



This article is included in the [Chemical Information Science](#) gateway.

Abstract


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



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Bisphenol A

80-05-7 | DTXSID7020182

Searched by Approved Name.

DETAILS

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PROPERTIES

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HAZARD

ADME

EXPOSURE

BIOACTIVITY

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES
























SYNONYMS

LITERATURE

LINKS

COMMENTS

General

-  EPA Substance Registry Service
-  Household Products Database
-  Chemical Entities of Biological Interest (ChEBI)
-  PubChem
-  Chemsplider
-  CPCat
-  DrugBank
-  HMDB
-  Wikipedia
-  MSDS Lookup
-  ChEMBL
-  Chemical Vendors
-  CalEPA Office of Environmental Health Hazard Assessment
-  NIOSH Chemical Safety Cards
-  ToxPlanet
-  ACS Reagent Chemicals
-  Wikidata
-  ChemHat: Hazards and Alternatives Toolbox
-  Wolfram Alpha
-  ScrubChem
-  ECHA Brief Profile
-  ECHA Infocard
-  ChemAgora

Toxicology

ACToR

OH₂ DrugPortal

CCRIS

ChemView





CTD

eChemPortal

Gene-Tox

HSDB

Analytical

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

Prediction

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

Integrated Linkouts

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



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

[NIOSH Chemical Safety ...](#)

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



Integrated Linkouts

Comparative Toxicogenomics DB

Comparative Toxicogenomics Database

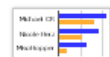
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Propylene Glycol

Basics Gene Interactions Genes **Diseases** Phenotypes Comps Pathways GO Exposure Studies Exposure Details References

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

Disease categories [\[Show chart\]](#)



Filter by

Disease category

ALL

Association type

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Filter

1-50 of 240 results.

First

Previous

1

2

3

4

5

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

Not just chemical “structures”

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

(C10-C16) Alkylbenzenesulfonic acid

68584-22-5 | DTXSID2028723

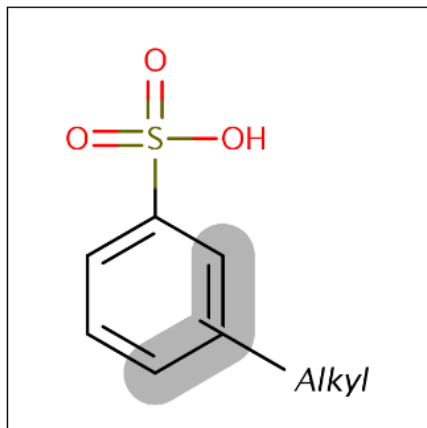
Searched by DSSTox Substance Id.

DETAILS

RELATED SUBSTANCES

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Intrinsic Properties

Presence in Lists

Federal

Safer Choice Chemical List

TOX21SL: Tox21 Screening Library

TSCA Workplan Step 2 Chemicals

EPAHFR - EPA Chemicals associated with hydraulic fracturing

US State

None.

International

OLEM RapidTox Chemicals

REACH Dossier Chemicals

Other

Surfactant List Screened in Swiss Wastewater (2014)

EDSP Universe

TSCAACTIVE

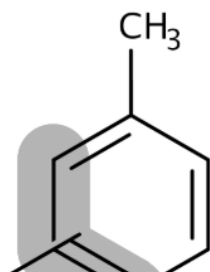
EPA Chemicals associated with hydraulic fracturing

Markush Structures

Xylenes

1330-20-7 | DTXSID2021446

Searched by DSSTox Substance Id.



Wikipedia

Xylene (from Greek ξύλο, *xýlo*, "wood"), **xylo**l or **dimethylbenzene** is any one of three isomers of dimethylbenzene, or a combination thereof. With the formula $(\text{CH}_3)_2\text{C}_6\text{H}_4$, each of the three compounds has a central benzene ring with two methyl groups attached at substituents. They are all colorless, flammable liquids, some of which are of great industrial value. The mixture is referred to as both xylene and, more precisely, xylenes

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Intrinsic Properties

Presence in Lists

Record Information

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8 chemicals

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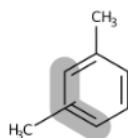
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Searched Chemical



Xylenes

DTXSID: DTXSID2021446
CASRN: 1330-20-7

Predecessor: Component

4 related chemical
structures with this
substance

Xylenes; defined mixture 1
DTXSID: DTXSID0021421
CASRN: NOCAS_21421

Predecessor: Component

4 related chemical
structures with this
substance

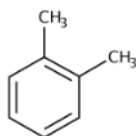
Xylenes; defined mixture 2
DTXSID: DTXSID7021447
CASRN: NOCAS_21447

Predecessor: Component

5 related chemical
structures with this
substance

Total Petroleum Hydrocarbons (TPH)
DTXSID: DTXSID30801529
CASRN: NOCAS_801529

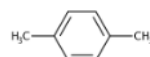
Markush Child



o-Xylene

DTXSID: DTXSID3021807
CASRN: 95-47-6

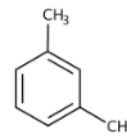
Markush Child



p-Xylene

DTXSID: DTXSID2021888
CASRN: 106-42-3

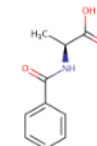
Markush Child



m-Xylene

DTXSID: DTXSID6026298
CASRN: 106-38-3

Transformation Product



N-Benzoylalanine

DTXSID: DTXSID40176394
CASRN: 2198-84-3

Transformation Products

Chlorothalonil

1897-45-6 | DTXSID0020319

Searched by DSSTox Substance Id.

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8 chemicals

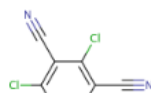
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Show info: DTXSID CASRN Select all

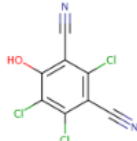
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Searched Chemical



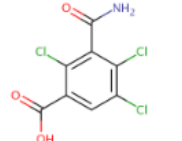
Chlorothalonil
DTXSID: DTXSID0020319
CASRN: 1897-45-6

Transformation Product



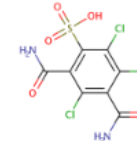
4-Hydroxy-2,5,6-trichloroisophthalonitrile
DTXSID: DTXSID00182588
CASRN: 28343-81-5

Transformation Product



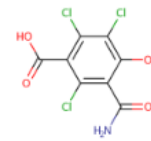
3-Carbamoyl-2,4,5-trichlorobenzoic acid
DTXSID: DTXSID10597537
CASRN: 142733-37-7

Transformation Product



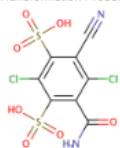
2,4-dicarbamoyl-3,5,6-trichlorobenzene-1-sulfonic acid
DTXSID: DTXSID30891327
CASRN: NOCAS_891327

Transformation Product



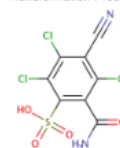
3-carbamoyl-2,5,6-trichloro-4-hydroxybenzoic acid
DTXSID: DTXSID00891328
CASRN: NOCAS_891328

Transformation Product



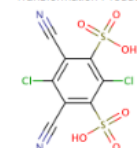
4-carbamoyl-2,5-dichloro-6-cyanobenzene-1-sulfonic acid
DTXSID: DTXSID00891329
CASRN: NOCAS_891329

Transformation Product



2-carbamoyl-3,5,6-trichloro-4-cyanobenzene-1-sulfonic acid
DTXSID: DTXSID00891330
CASRN: NOCAS_891330

Transformation Product



2,5-dichloro-4,6-dicyanobenzene-1,3-disulfonic acid
DTXSID: DTXSID20891331
CASRN: NOCAS_891331

Not just chemical “structures”

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

List of Chemicals

Lists of Chemicals

List of Assays

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List Acronym	List Name	Last Updated	Number of Chemicals	List Description
40CFR355	40CFR355	2018-01-05	354	Extremely Hazardous Substance List and Threshold Planning Quantities; Emergency Planning and Release Notification Requirements; Final Rule. (52 FR 13378)
AEGLVALUES	Acute exposure guideline levels	2018-04-20	174	Acute exposure guideline levels (AEGLs) describe the human health effects from once-in-a-lifetime, or rare, exposure to airborne chemicals.
ALGALTOX	Algal Toxins	2017-11-21	54	A set of algal toxins of interest
APCRA_PRO	APCRA Chemicals for Prospective Analysis	2018-02-14	204	The APCRA prospective case study list of approximately 200 chemicals as of January 2018, developed by ECHA in consultation with EPA and other partners
APCRA_RETRO	APCRA Chemicals for Retrospective Analysis	2018-02-14	380	The APCRA retrospective case study list of 380 chemicals that have ToxCast/Tox21 data, httk, and point-of-departure values that meet case study criteria in ToxValDB.
APCRAAPPLIST	APCRA Chemicals for Retrospective Analysis_App_List_448_Chemicals	2018-05-23	447	The APCRA retrospective case study list of 380 chemicals that have ToxCast/Tox21 data, httk, and point-of-departure values that meet case study criteria in ToxValDB. This is the EDITABLE app list
ARCHEMICALS	Androgen Receptor Chemicals	2018-05-01	110	The list of chemicals used to identify references with in vitro AR binding . From Kleinstreuer et al http://pubs.acs.org/doi/abs/10.1021/acs.chemrestox.6b00347
ATHENSSUS	University of Athens Surfactant and Suspect List	2017-07-14	60	ATHENSSUS is a compilation of suspects, predicted transformation products and surfactants screened in wastewater by University of Athens, as described in Gago-Ferrero et al 2015, DOI: 10.1021/acs.est.5b03454
comptox-prod.epa.gov/dashboard/chemical_lists	ATSDR List	2017-03-11	200	The Agency for Toxic Substances and Disease Registry (ATSDR) is a federal public health

Algal Toxins



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54 chemicals

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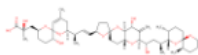
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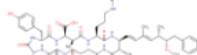
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Dinophysistoxin 1

DTXSID: DTXSID00880001

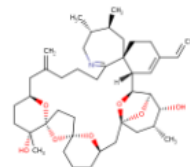
CASRN: 81720-10-7



Microcystin YR

DTXSID: DTXSID00880086

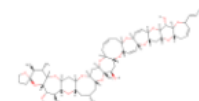
CASRN: 101064-48-6



Pinnatoxin G

DTXSID: DTXSID00880102

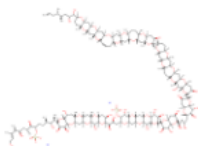
CASRN: NOCAS_880102



CTX 4B

DTXSID: DTXSID00880107

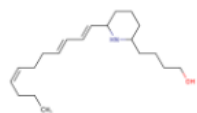
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Maitotoxin

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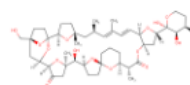
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Euglenophycin

DTXSID: DTXSID10880017

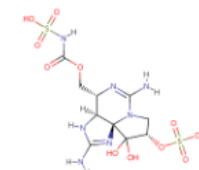
CASRN: 1219817-69-2



Pectenotoxin-1

DTXSID: DTXSID10880092

CASRN: 97564-90-4



Gonyautoxin

DTXSID: DTXSID10880097

CASRN: 80226-62-6

Mass and Formula Searches

Supporting Mass Spectrometry

Advanced Search?

Mass Search?

Select Adduct: ▼

Da \pm

Molecular Formula Search?

☒ **MS Ready Formula?** ☐ **Exact Formula?**

Generate Molecular Formula(e)?

Da \pm

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

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

Advanced Searches

Mass Based Search

Mass Search

±

Min/Max

M

191.131


Da

±

5

Da


ppm

Search 

Search Results

Searched by Mass: 191.131 +/- 5.0 ppm.

298 of 298 chemicals visible


Download / Send 

Show info:

DTXSID 

CASRN 

TOXCAST 

Mass Diff 


Select all

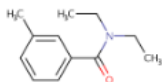


Sort by: Mass Difference 



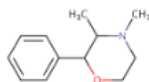
Filter by: Name or CASRN

Multicomponent Chemicals 



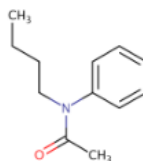
DEET

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



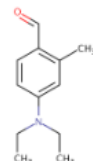
Phendimetrazine

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



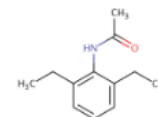
N-Butylacetanilide

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



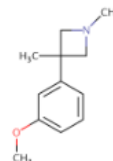
Benzaldehyde, 4-(diethylamino)-2-methyl-

DTXSID: DTXSID4059041
CASRN: 92-14-8
TOXCAST: 0
Mass Diff: 0.000014



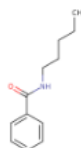
Acetanilide, 2',6'-diethyl-

DTXSID: DTXSID90168148
CASRN: 16665-89-7
TOXCAST: 0
Mass Diff: 0.000014



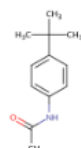
Azetidine, 1,3-dimethyl-3-(m-methoxyphenyl)-

DTXSID: DTXSID40173560
CASRN: 19832-26-8
TOXCAST: 0
Mass Diff: 0.000014



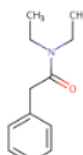
Benzamide, N-pentyl-

DTXSID: DTXSID20174198
CASRN: 20308-43-4



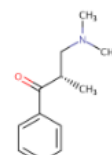
p-t-Butylacetanilide

DTXSID: DTXSID80174238
CASRN: 20330-45-4



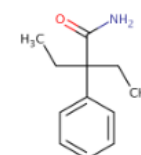
N,N-Diethylphenylacetamide

DTXSID: DTXSID00179048
CASRN: 2431-98-1



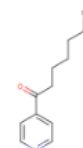
3-(Dimethylamino)-2-methylpropiphen-

DTXSID: DTXSID60180798
CASRN: 26171-60-6



Butyramide, 2-ethyl-2-phenyl-

DTXSID: DTXSID60184653
CASRN: 30568-39-9



1-Heptanone, 1-(4-pyridyl)-

DTXSID: DTXSID40188594
CASRN: 32841-30-3

Advanced Searches

Mass Based Search

Search Results

Searched by Mass: 191.131 +/- 5.0 ppm.

296 of 296 chemicals visible

Download / Send

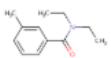
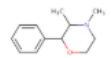
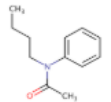
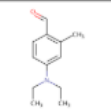
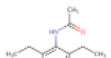
Select all

Sort by: Mass Difference



Filter by: Name or CASRN

Multicomponent Chemicals

Structure	DTXSID	Preferred Name	CASRN	QC Level	CPDat Count	Number of Sources	PubChem Data Sources	PubMed Ref. Counts	Monoisotopic Mass	Mass Difference
	DTXSID2021995 ToxCast™	DEET	134-82-3	Level 1	111	111	155	753	191.131014	0.000014
	DTXSID1023447	Phendimetrazine	634-03-7	Level 2	12	28	35	50	191.131014	0.000014
	DTXSID2042197	N-Butylacetanilide	91-49-6	Level 2	1	26	50	1	191.131014	0.000014
	DTXSID4059041	Benzaldehyde, 4-(diethylamino)-2-methyl-	92-14-8	Level 3	0	7	51	0	191.131014	0.000014
	DTXSID90168148	Acetanilide, 2',6'-diethyl-	16665-89-7	Level 4	0	4	33	0	191.131014	0.000014

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








Batch Search?



Step Three: Select Download Data or Display Chemicals

Please enter one identifier per line

Select Input Type(s)

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



Chemical Data


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

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

Batch Searching

Select Output Format:






 Excel 

 Download






Customize Results

- ☐ Select All
- ☐ Select All in Lists






Chemical Identifiers

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

Structures

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

Intrinsic And Predicted Properties

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

Presence in Lists:

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

Excel Output

INPUT	FOUND_BY	DTXCID_IN	DATA_SOURCE	TOXVAL_D	TOXCAST	TOXCAST	NUMBER_C	PUBCHEM	STO
C6H12O3	MS Ready	DTXCID701	51	Y	0.36	2/562	24	83	Y
C6H12O3	MS Ready	DTXCID003	67	Y	0.36	1/276	376	80	Y
C6H12O3	MS Ready	DTXCID106	65	Y	4.42	5/113	6	77	Y
C6H12O3	MS Ready	DTXCID105	45	Y	0.0	0/163	3	94	-
C6H12O3	MS Ready	DTXCID901	38	Y	-	-	14	110	Y
C6H12O3	MS Ready	DTXCID402	34	Y	0.0	0/113	-	53	Y
C6H12O3	MS Ready	DTXCID202	31	Y	-	-	-	36	Y
C6H12O3	MS Ready	DTXCID202	30	-	2.54	7/276	-	54	-
C6H12O3	MS Ready	DTXCID109	26	Y	-	-	-	46	-
C6H12O3	MS Ready	DTXCID202	24	Y	0.0	0/113	-	47	-
C6H12O3	MS Ready	DTXCID303	22	Y	-	-	-	89	-
C6H12O3	MS Ready	DTXCID302	20	Y	-	-	2	25	Y
C6H12O3	MS Ready	DTXCID407	19	Y	-	-	12	62	-
C6H12O3	MS Ready	DTXCID704	17	Y	-	-	-	64	-
C6H12O3	MS Ready	DTXCID704	16	Y	-	-	3	49	-



United States
Environmental Protection
Agency

43

Real-Time Predictions

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

Our support for FAIR Data

F_{indable}



A_{ccessible}



I_{nteroperable}



R_{eusable}



Downloadable Data



[DSSTox Identifier to PubChem Identifier Mapping File](#)

Posted: 11/14/2016

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

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

[DSSTox identifiers mapped to CAS Numbers and Names File](#)

Posted: 11/14/2016

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

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

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

Prototype Development

AADashboard

atrazine Search

100%

Select properties to predict
H T.E.S.T. 18 OPERA Search
C
N ☐ Exact
O ☒ Substructure

Search result 2540 Show ☐ Isotopically Labeled ☐ Charged ☐ Salts or Mixtures Sort Similarity

 1	 0.62	 0.57	 0.57	 0.57	 0.53	 0.53	 0.53	 0.5	 0.5	 0.5
 0.5	 0.5	 0.5	 0.47	 0.44	 0.44	 0.44	 0.42	 0.42	 0.42	 0.42
 0.42	 0.42	 0.42	 0.42	 0.42	 0.4	 0.4	 0.4	 0.4	 0.4	 0.4
 0.4	 0.4	 0.4	 0.4	 0.4	 0.4	 0.4	 0.4	 0.4	 0.38	 0.38
 0.38	 0.38	 0.38	 0.38	 0.38	 0.38	 0.38	 0.38	 0.38	 0.38	 0.38

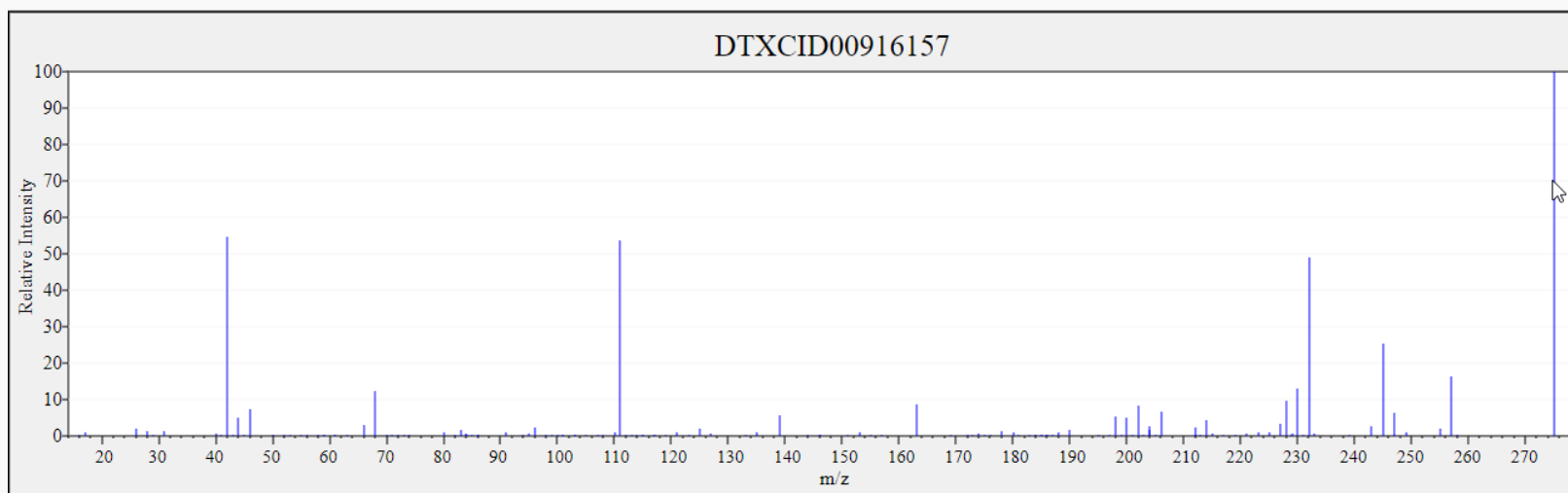
Search result 2540 Show ☐ Isotopically Labeled

Predicted Mass Spectra

<http://cfmid.wishartlab.com/>



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



- The EPA CompTox Dashboard provides access to data for ~875,000 chemicals, ToxCast assays and associated product use categories
- High quality data from ongoing curation efforts
- An integration hub for multiple “modules”
 - Experimental and predicted properties
 - Human and Ecological Hazard data
 - Exposure data – products, data in the environment
 - *In vitro* bioassay data – ToxCast/Tox21
 - Literature searching – Google Scholar and PubMed
 - Specialized searches – mass/formula for analytical support
 - Batch searching and Real Time Predictions
- Data and functionality increases with every release

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

Antony Williams

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National Center for Computational Toxicology (NCCT)

Williams.Antony@epa.gov

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