

The CompTox Chemistry Dashboard v3.0 – New Searches and Support for Bioactivity Data

Antony Williams

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

*September 27th 2018
Communities of Practice*

Outline – what's new in v3.0?

- Welcome the CompTox Portal
- New name for the dashboard
- User interface overhaul – easier navigation
- New search capabilities
- Enhanced support for bioactivity data
- New data and new lists added
- Work in progress

The CompTox Portal

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



Watch for our news

https://comptox.epa.gov/dashboard/news_info



 United States Environmental Protection Agency [Home](#) [Advanced Search](#) [Batch Search](#) [Lists](#) [Predictions](#) [Downloads](#) [Share](#)

765 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](#)

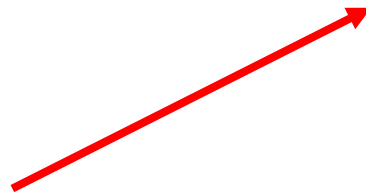
Latest News

[Read more news](#)

Full list of release notes for Version 3.0 now available

September 26th, 2018 at 9:42:43 AM

In August 2018 we released version 3.0 of the CompTox Chemicals Dashboard and we hope you are enjoying our latest release and we welcome your feedback. We can now point you to the release notes [here](#).



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- A detailed list of new functionality and fixes

**** New Functionality**

- [ICD-2992] - Allow Display of Sets of Chemicals based on Product or Use Categories
- [ICD-3045] - Improve Submit Comment capability
- [ICD-3157] - Add Assay/Gene Search based on assays available for ToxCast
- [ICD-3174] – On-hover Zoom on structure general solution across the dashboard
- [ICD-3182] - Build Assay Chart display window for displaying one or more assay charts
- [ICD-3183] - Build multiple chart display mode
- [ICD-3242] - Include image to depict presence of isotopes
- [ICD-3324] - Add on hover display of AOP title associated with AOP Link and AOP Event
- [ICD-3339] - Create MultiStep Navigation Workflow for GenRA
- [ICD-3340] - Create GenRA layout Block 1
- [ICD-3341] - Create GenRA layout Block 2
- [ICD-3342] - Create GenRA layout Block 3
- [ICD-3355] - Create GenRA layout Block 4
- [ICD-3361] - DSSTox relationships controlled vocab table
- [ICD-3362] - Provide list of all assays that chemicals have been measured in
- [ICD-3363] - Add More Columns to Lists Page
- [ICD-3369] - Add Data Picker to Tile Mode
- [ICD-3373] - Add additional Functionality to the Assay Selection Tab
- [ICD-3374] - Create Dedicated Chemical Lists Pages associated with individual assays

Staying up with the Dashboard

https://comptox.epa.gov/dashboard/news_info

New list of pesticides added

September 19th, 2018 at 10:22:58 AM

A list of pesticides associated with the EPA Pesticide Chemical Search Database has been added to the list page. The PC codes (pesticide codes) have also been added as searchable synonyms to the chemical search page. The list is available [here](#)

Video describing how to use the "Generalized Read-Across (GenRA) module" now on YouTube

August 31st, 2018 at 12:22:02 PM

A new module describing Generalized Read-Across (GenRA) is now available [here on YouTube](#). The video runs through the basic science behind GenRA and how to use the module in the dashboard.

New publication released: "'MS-Ready" structures for non-targeted high-resolution mass spectrometry screening studies"

August 31st, 2018 at 12:07:25 PM

"MS-Ready" structures are the basis of many of the searches to support mass spectrometry that are supported on the dashboard. Our recent publication "MS-Ready" structures for non-targeted high-resolution mass spectrometry screening studies" explains the concept and production of MS-Ready structures in detail. Read the paper [here](#) .

Version 3 of the Dashboard released August 10th 2018

August 12th, 2018 at 2:46:01 PM

A new version of the CompTox Dashboard has been released to the community. Other than just searching for chemicals, this version includes new searches for product and use categories and assays and genes associated with ToxCast and Tox21 assays. Bioactivity curves are now viewable for assays associated with the Endocrine Disruptor Screening Program (EDSP21). A detailed list of new functionality will be forthcoming.

A Major Update to the Dashboard Releases on March 7th 2018

March 8th, 2018 at 3:49:25 PM

A major update to the dashboard has been released prior to the Society of Toxicology and American Chemical Society Spring meetings. This release brings together six months of effort in adding 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.

A YouTube video regarding using the Dashboard for Non-Targeted Analysis

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

A 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 of the dashboard in terms of data quality and focused data set for environmental non-targeted analysis. [View it here on Youtube](#).

An article regarding an Excel Version of the Abstract Sifter is published.

March 7th, 2018 at 9:24:37 AM

CompTox Chemicals Dashboard

https://comptox.epa.gov/dashboard



United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Share



Chemicals Product/Use Categories Assay/Gene

762 Thousand Chemicals

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](#)

Latest News

[Read more news](#)

YouTube video regarding using the Dashboard for Non-Targeted Analysis

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

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








CompTox Dashboard Chemicals

762 Thousand Chemicals



Chemicals Product/Use Categories Assay/Gene

Q Bisphenol A

-  Bisphenol A
DTXSID7020182
-  Bisphenol A bis(2-hydroxyethyl ether) diacrylate
DTXSID6066991
-  Bisphenol A bis(2-hydroxyethyl ether) dimethacrylate
DTXSID1066992
-  Bisphenol A bis(2-hydroxypropyl) ether
DTXSID8051592
-  Bisphenol A carbonate polymer
DTXSID6027840
-  Bisphenol A diglycidyl ether
DTXSID6024624
-  Bisphenol A glycidyl methacrylate
DTXSID7044841
-  Bisphenol A propoxylate diglycidyl ether
DTXSID10399098
-  Bisphenol A propoxylate glycerolate diacrylate
DTXSID40400126

CompTox Dashboard Products and Use Categories



762 Thousand Chemicals



[Chemicals](#) [Product/Use Categories](#) [Assay/Gene](#)

hair color

- CPDat PRODUCT category: personal care hair color
hair colors and dyes characterized as permanent
- CPDat PRODUCT category: personal care hair color
hair colors and dyes characterized as for professional use
- CPDat PRODUCT category: personal care hair color
hair colors and dyes characterized as temporary
- CPDat PRODUCT category: personal care hair color
hair coloring products not otherwise categorized
- CPDat PRODUCT category: personal care hair color activator
chemical activators for hair coloring products
- CPDat PRODUCT category: personal care hair color developer
chemical developers for hair coloring products
- CPDat PRODUCT category: personal care hair color toner
chemical toners for hair coloring products



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CompTox Dashboard Assays and Genes



762 Thousand Chemicals



Chemicals Product/Use Categories Assay/Gene

estrogen

GENE: ESR1
estrogen receptor 1

GENE: ESR2
estrogen receptor 2 (ER beta)

GENE: ESRA
estrogen-related receptor alpha

GENE: ESRRB
estrogen-related receptor beta

GENE: ESRRG
estrogen-related receptor gamma

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



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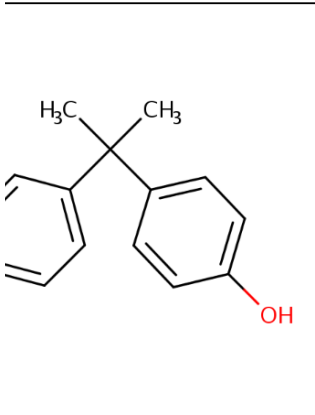
Detailed Chemical Pages New User Interface Design

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

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

Bisphenol A

DTXSID7020182
EPA Substance Id.



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

Access to Chemical Hazard Data

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

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

Search query

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

Hazard Data from “ToxVal_DB”

Lots of new data added - ECOTOX

- 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

Sources of Exposure to Chemicals

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

Download

Columns 10

Search query

Product and Use Categories (PUCs) i

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


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

What chemicals in what product and use categories?

Methylparaben

99-76-3 | DTXSID4022529

Searched by Synonym from Valid Source.

 Download ▾

Columns ▾

10 ▾

Product or Use Categorization

[personal care: eye liner](#)

[personal care: body wash](#)

[personal care: sunscreen](#)

[personal care: hair conditioning treatment](#)

[personal care: lip color](#)

What chemicals in what product and use categories?

Searched by Product & Use Categories

Results for CPDat Product Category: Personal Care: Eye Liner

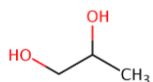
182 chemicals

Download / Send

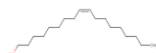
Show info: DTXSID CASRN TOXCAST Select all

Sort by: DTXSID

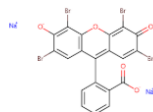
Filter by: Name or CASRN Hide



1,2-Propylene glycol
DTXSID: DTXSID0021206
CASRN: 57-55-6
TOXCAST: 11/539



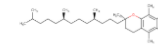
cis-Oleyl alcohol
DTXSID: DTXSID0022010
CASRN: 143-28-2
TOXCAST: 0



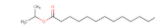
Eosin
DTXSID: DTXSID0025234
CASRN: 17372-87-1
TOXCAST: 45/302

1 related chemical structure with this substance

Polyvinylpyrrolidone
DTXSID: DTXSID0025941
CASRN: 9003-39-8
TOXCAST: 0



alpha-Vitamin E
DTXSID: DTXSID0026339
CASRN: 59-02-9
TOXCAST: 0



Isopropyl tetradecanoate
DTXSID: DTXSID0026838
CASRN: 110-27-0
TOXCAST: 1/299

0 related chemical structures with this substance

Paraffin waxes and Hydrocarbon waxes...
DTXSID: DTXSID0028115
CASRN: 63231-60-7
TOXCAST: 0

1 related chemical structure with this substance

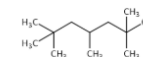
Alcohols, C16-18
DTXSID: DTXSID0028323
CASRN: 67762-27-0
TOXCAST: 1/163

0 related chemical structures with this substance

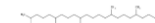
Fats and Glyceric oils, vegetable, hyd...
DTXSID: DTXSID0028454
CASRN: 68334-28-1
TOXCAST: 0



Iron(III) oxide
DTXSID: DTXSID0029632
CASRN: 1309-37-1
TOXCAST: 0



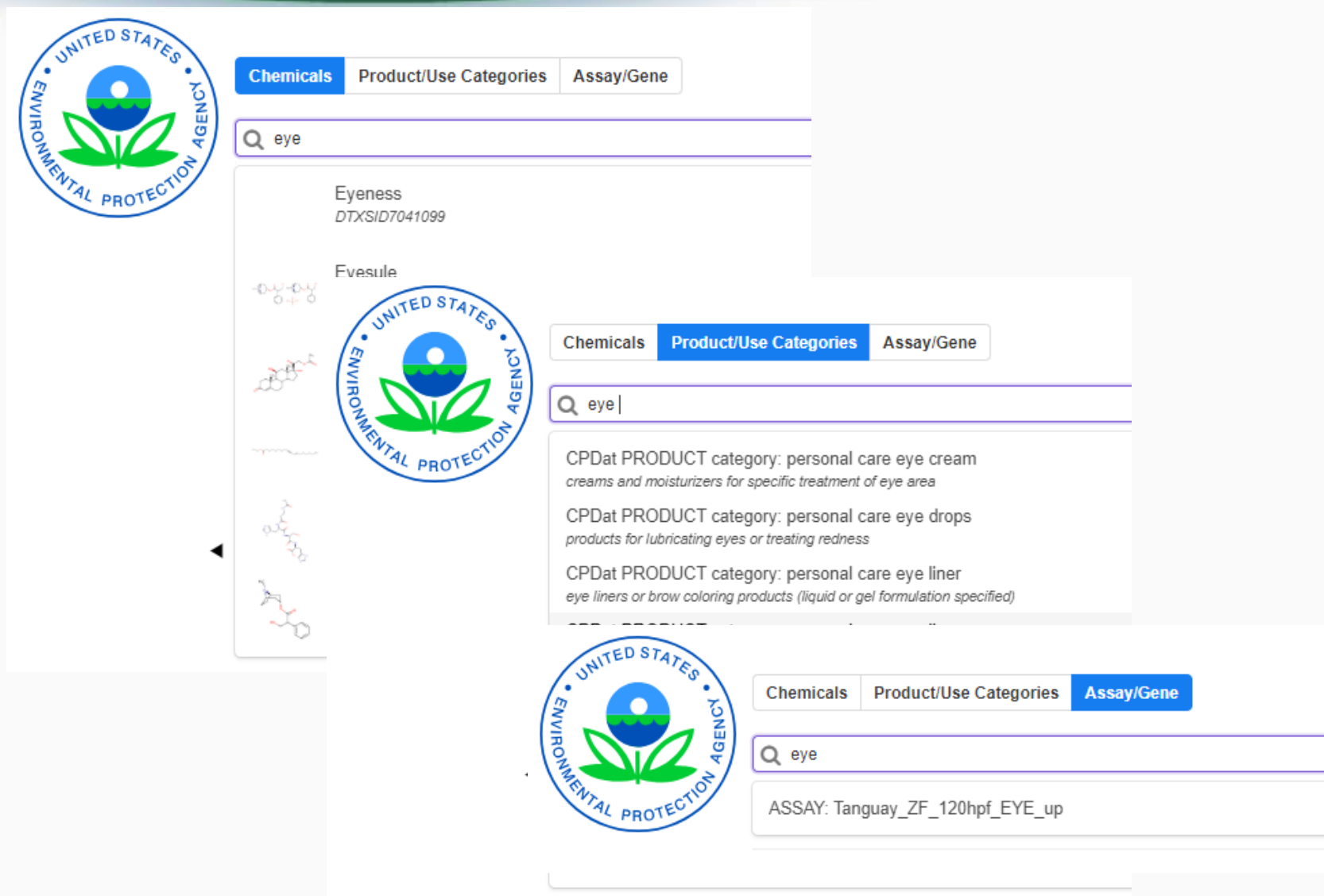
2,2,4,6,6-Pentamethylheptane
DTXSID: DTXSID0042034
CASRN: 13475-82-6
TOXCAST: 0



Squalane
DTXSID: DTXSID0046513
CASRN: 111-01-3
TOXCAST: 2/109

Remember home page searches

Searching for “eye” ...



The image displays three screenshots of the EPA's search interface. Each screenshot features the EPA logo on the left and a search bar at the top with tabs for 'Chemicals', 'Product/Use Categories', and 'Assay/Gene'. The search term 'eye' is entered in the search bar.

Top Screenshot: Shows search results for 'eye'. The first result is 'Eyeness' with DTSID7041099. Below it is 'Evesule' with a chemical structure icon. A vertical list of chemical structures is visible on the left side of the results area.

Middle Screenshot: Shows the search results for 'eye' under the 'Product/Use Categories' tab. The results list CPDat product categories: 'personal care eye cream', 'personal care eye drops', and 'personal care eye liner', each with a brief description of the products.

Bottom Screenshot: Shows the search results for 'eye' under the 'Assay/Gene' tab. The result is 'ASSAY: Tanguay_ZF_120hpf_EYE_up'.

In Vitro Bioassay Screening

ToxCast and Tox21

Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

▶ ADME

▶ EXPOSURE

▼ BIOACTIVITY

TOXCAST SUMMARY

PUBCHEM

TOXCAST DATA

TOXCAST MODELS

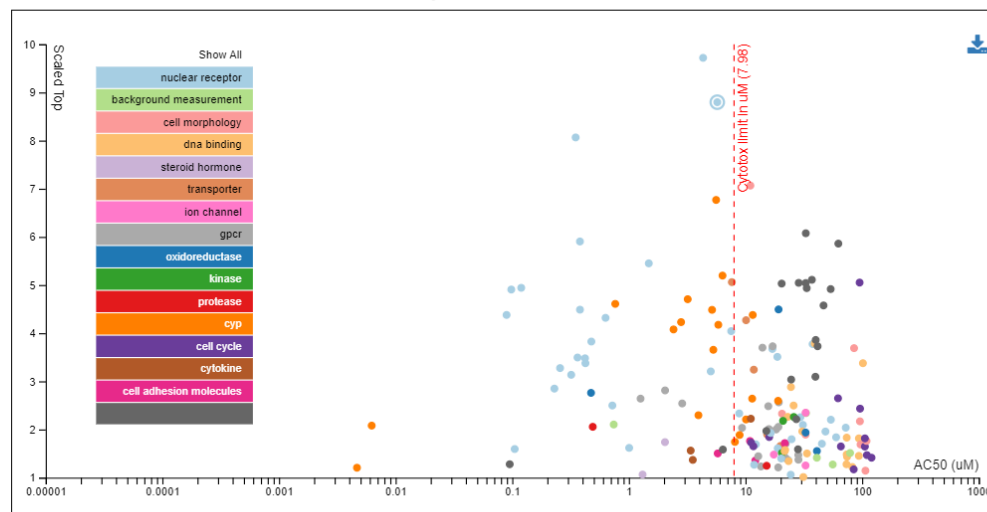
SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

Chemical Activity Summary

 TOXCAST DATA



 ASSAY DETAILS

AC50 (uM): 5.73
Scaled top: 8.80
Assay Endpoint Name: OT_ER_ERaEa_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_ERaEa_0480 was analyzed into 1 assay endpoint. This assay endpoint, OT_ER_ERaEa_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 relateable 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

Download

Search query

Show Inactive Show Background

Columns 10

- Name
- Modal
- Description
- SeqPASS
- Gene Name
- AOP
- Event
- Hit Call
- Top
- Scaled Top
- AC50
- logAC50
- Intended Target Family

	Description	SeqPASS	Gene Name	AOP	Event	Hit Call	Top	Scaled Top	AC50	logAC50	Intended Target Family
	-	-	-	-	-	ACTIVE	35.5	1.65	65.8	1.82	cell cycle
2		NP_000116.2	ESR1	200	1181	ACTIVE	109	4.49	0.381	-0.419	nuclear receptor
	-	-	-	-	-	ACTIVE	1.20	1.81	106	2.02	cell cycle
	-	-	-	-	-	ACTIVE	0.874	1.76	109	2.04	cell morphology
	-	-	-	-	-	ACTIVE	5.92	7.07	11.0	1.04	cell morphology
	-	-	-	-	-	ACTIVE	1.20	1.47	110	2.04	cell cycle
4h_dr	-	-	-	-	-	ACTIVE	4.49	5.05	95.2	1.98	cell cycle
	-	-	-	-	-	ACTIVE	2.71	3.69	85.3	1.93	cell morphology
24h_d	-	-	-	-	-	ACTIVE	1.66	1.17	84.7	1.93	cell cycle
pot_24	-	-	-	-	-	ACTIVE	1.80	1.65	106	2.02	cell cycle

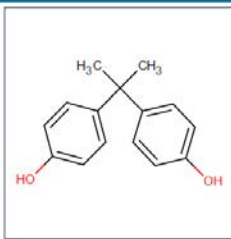
First << < 1 2 3 4 5 6 7 8 9 10 > >> Last

Showing 1 to 10 of 161 records

Earlier Dashboard Applications



ACToR Home Data Collections Search Assays Chemical Download Apps



Bisphenol A
80-05-7; DTXSID7029192

INCHEM: InChI=1S/C15H16O2=C1=C5C=C(C)C=C1C2=C(C)C=CC=C2
 InChI Key: HSBACLPANRBTUJHFFKQYSAH
 SMILES: CC(C)(C1=CC=C(O)C=C1)C2=CC=C(O)C=C2
 Molecular Formula: C15H16O2
 Molecular Weight: 228.291 g/mol

Synonyms

Hazard

More Data: [HMS Data](#)

- Chemicals known to be listed by California to Cause Cancer or Reproductive Toxicity (Reg 67) (2014)
- Chemical Contaminator of 2 Year from PRC Program 188
- Chemical Contaminator of Food from EU Research 188
- Chemical Contaminator of Food from National Academies Group
- EU REACH Registration Category 1 (Prep. 10, 10/16, 10/20)
- EU REACH Registration Category 2 (Prep. 10, 10/16, 10/20)
- EU REACH Registration Category 3 (Prep. 10, 10/16, 10/20)
- EU REACH Registration Category 4 (Prep. 10, 10/16, 10/20)
- EU REACH Registration Category 5 (Prep. 10, 10/16, 10/20)
- EU REACH Registration Category 6 (Prep. 10, 10/16, 10/20)
- EU REACH Registration Category 7 (Prep. 10, 10/16, 10/20)
- EU REACH Registration Category 8 (Prep. 10, 10/16, 10/20)
- EU REACH Registration Category 9 (Prep. 10, 10/16, 10/20)
- EU REACH Registration Category 10 (Prep. 10, 10/16, 10/20)
- EU REACH Registration Category 11 (Prep. 10, 10/16, 10/20)
- EU REACH Registration Category 12 (Prep. 10, 10/16, 10/20)
- EU REACH Registration Category 13 (Prep. 10, 10/16, 10/20)
- EU REACH Registration Category 14 (Prep. 10, 10/16, 10/20)
- EU REACH Registration Category 15 (Prep. 10, 10/16, 10/20)
- EU REACH Registration Category 16 (Prep. 10, 10/16, 10/20)
- EU REACH Registration Category 17 (Prep. 10, 10/16, 10/20)
- EU REACH Registration Category 18 (Prep. 10, 10/16, 10/20)
- EU REACH Registration Category 19 (Prep. 10, 10/16, 10/20)
- EU REACH Registration Category 20 (Prep. 10, 10/16, 10/20)

EPA iCSS ToxCast Dashboard Home Export

Choose a view: Assays Chemicals Database: prot_dashboard_v2 Dashboard: v2

Chemicals - 1

ID-05-7	Chemical Name
80-05-7	Bisphenol A

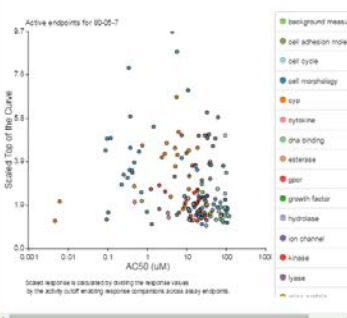
Assays - 1091

Active: MG Only All Tested

Assay Component	Endpoint Name
ACEA_T4TD_02H_Negative	
ACEA_T4TD_02H_Positive	
APR_HepG2_CellCycleArrest_Tx_Th	
APR_HepG2_CellCycleArrest_Tx_Up	
APR_HepG2_CellTox_Tx_Th	
APR_HepG2_CellTox_Tx_Up	
APR_HepG2_MicrotubuleDisrupt_Tx_Th	
APR_HepG2_MicrotubuleDisrupt_Tx_Up	
APR_HepG2_Mitochondria_Tx_Th	
APR_HepG2_Mitochondria_Tx_Up	
APR_HepG2_Mitochondria_Pul_Tx_Th	
APR_HepG2_Mitochondria_Pul_Tx_Up	
APR_HepG2_Mitochondria_Pul_Tx_Th	
APR_HepG2_Mitochondria_Pul_Tx_Up	

Chemical Activity Summary

Active endpoints for 80-05-7



Sorted response is calculated by using the response values by the activity cutoff enabling response comparison across assay endpoints.

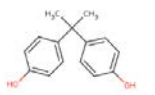
EPA United States Environmental Protection Agency

CPCat: Chemical and Product Categories [Contact Us](#)

You are here: [EPA Home](#) > [Computational Toxicology Research](#) > [Chemical Use](#)

[Home](#) [Search](#) [Results](#) [Dictionary](#) [Download](#) [Help](#)

Chemical: **BISPHENOL A** CASRN: 80-05-7



[Export Use Data](#) [Export Product Data](#)

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

EPA United States Environmental Protection Agency

EDSP21 Dashboard Endocrine Disruption Screening Program for the 21st Century

[Chemical Summary](#) [Public Information](#) [Bioactivity Summary](#) [Bioactivity](#) [High-Throughput Exposure](#) [Assay Definitions](#) [Toxicology](#)

EDSP Dashboard Overview

EDSP Dashboard Overview

Congress requires EPA's [Endocrine Disruptor Screening Program](#) to evaluate chemicals for potential endocrine disruption, and there are thousands of chemicals of interest to the program. EPA researchers developed the Endocrine Disruption Screening Program for the 21st Century Dashboard (EDSP21 Dashboard) to provide access to raw chemical data on over 1,500 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 situ 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 (E-PECaDB).
- High quality chemical structures and annotations (CASTox).
- Physiomechanism Properties Database (PhysToxDB).

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.



In Vitro Bioassay Screening

ToxCast and Tox21

Download 10 Show Inactive Show Background

Name	Modal	Description	SeqPASS	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			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

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

Showing 1 to 10 of 161 records

Assay Modal Details

All Chemicals in Assay Endpoint: ACEA_T47D_80hr_Negative

Annotations Citations tcpl Processing Reagents AOPs

Aeid 1

Entrez Gene Id 0

Gene Name All Chemicals in Assay Endpoint: ACEA_T47D_80hr_Negative

Gene Symb Annotations Citations tcpl Processing Reagents AOPs

Assay Sourc

Assay Sourc

Assay Name

Assay Desc

Timepoint H

Organism

Tissue

Cell Format

Cell Free Component Source

Cell Short Name

Cell Growth Mode

Assay Footprint

Assay Run Type	Level Applied	Method Name	Description
1 MULTI	level2	none	apply no level 2 method
2 MULTI	level3	bval.apid.nwlslowconc.med	Take the median cval of the n wells and the first two concentrations, by apid
3 MULTI	level3	pval.apid.mednbyconc.min	plate-wise meidan based on negative control, (min)

All Chemicals in Assay Endpoint: ACEA_T47D_80hr_Negative

Annotations Citations tcpl Processing Reagents AOPs

	Reagent Type	Reagent Value	Culture or Assay
1	media_base	RPMI-1640	culture
2	media_serum	10% FBS	culture
3	media_temp_celcius	37	culture
4	media_time_hr_min	24	culture
5	media_cell_aliquot	20000	culture
6	media_base	RPMI-1640	assay
7	media_serum	10% charcoal-stripped FBS	assay
8	media_temp_celcius_min	37	assay
9	media_time_hr	80	assay

In Vitro Bioassay Screening

ToxCast and Tox21

Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

EXPOSURE

BIOACTIVITY

TOXCAST: SUMMARY

PUBCHEM

TOXCAST: DATA

TOXCAST: MODELS

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

LITERATURE

LINKS

COMMENTS

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

Assay Selection 1 Selected

A Single Assay Can Have Multiple Charts

Number of Charts: 6

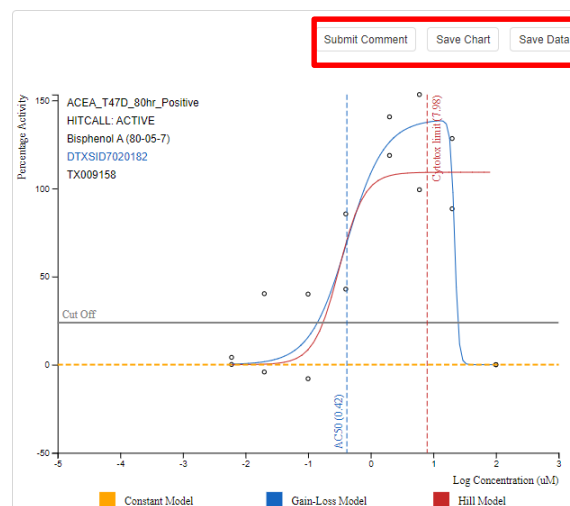
Active Inactive All

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



In Vitro Bioassay Screening

Multi-chart Display

EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

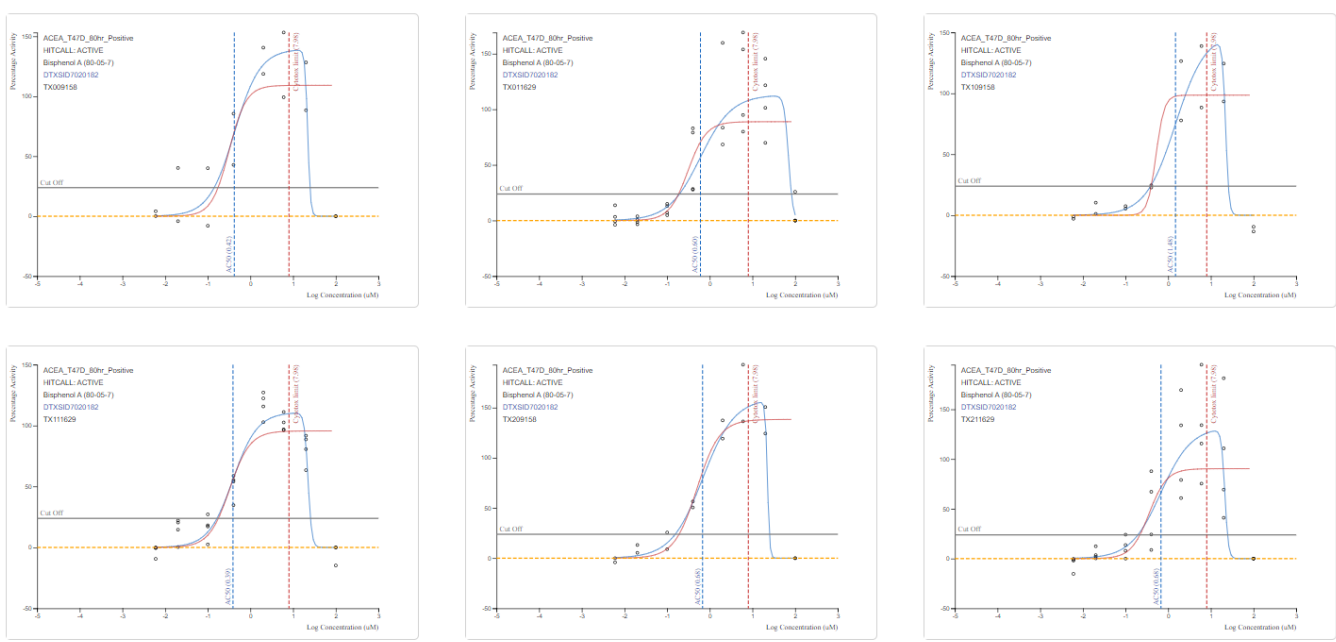
Copy Share Submit Comment Search all data

Tox21_400088 Pass Purity>90% and MW confirmed

A Single Assay Can Have Multiple Charts Number of Charts: 6

Filter

- ADME
- EXPOSURE
- BIOACTIVITY
 - TOXCAST: SUMMARY
 - PUBCHEM
 - TOXCAST: DATA**
 - TOXCAST: MODELS
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE
- LINKS
- COMMENTS



ACEA_T4TD_80hr_Positive
HITCALL: ACTIVE
Bisphenol A (B0-05-7)
DTXSID1021162
TX09158

ACEA_T4TD_80hr_Positive
HITCALL: ACTIVE
Bisphenol A (B0-05-7)
DTXSID1021162
TX11629

ACEA_T4TD_80hr_Positive
HITCALL: ACTIVE
Bisphenol A (B0-05-7)
DTXSID1021162
TX209158

ACEA_T4TD_80hr_Positive
HITCALL: ACTIVE
Bisphenol A (B0-05-7)
DTXSID1021162
TX211629

In Vitro Bioassay Screening

ToxCast and Tox21

Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

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

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

Assay Selection 1 Selected

A Single Assay Can Have Multiple Charts

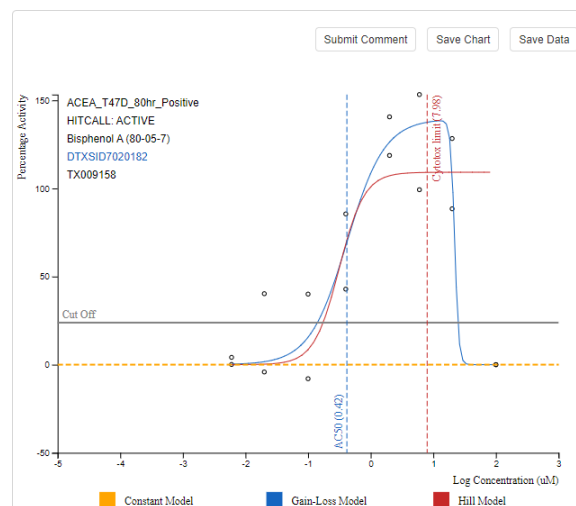
Number of Charts: 6

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



Assay Modal Details

All Chemicals in Assay Endpoint: ACEA_T47D_80hr_Negative

Annotations Citations tcpl Processing Reagents AOPs

Aeid 1

Entrez Gene Id 0

Gene Name All Chemicals in Assay Endpoint: ACEA_T47D_80hr_Negative

Gene Symb Annotations Citations tcpl Processing Reagents AOPs

Assay Sourc

Assay Sourc

Assay Name

Assay Desc

Timepoint H

Organism

Tissue

Cell Format

Cell Free Component Source

Cell Short Name

Cell Growth Mode

Assay Footprint

PMID	url	Title	Author	Citation	doi
1 16481145	PubMed URL	Microelectronic cell sensor assay for detection of cytotoxicity and prediction of acute toxicity	Xing JZ, Zhu L, Gabos S, Xie L	Xing JZ, Zhu L, Gabos S, Xie L. Microelectronic cell sensor assay for detection of cytotoxicity and prediction of acute toxicity. Toxicol In Vitro. 2006 Sep;20(6):995-1004. Epub 2006 Feb 14. PubMed PMID: 16481145.	

2 23682706 All Chemicals in Assay Endpoint: ACEA_T47D_80hr_Negative

Annotations Citations tcpl Processing Reagents AOPs

Assay Run Type	Level Applied	Method Name	Description
1 MULTI	level2	none	apply no level 2 method
2 MULTI	level3	bval.apid.nwslowconc.med	Take the median cval of the n wells and the first two concentrations, by apid
3 MULTI	level3	pval.apid.mednbyconc.min	plate-wise median based on negative control, (min)

4 MULTI All Chemicals in Assay Endpoint: ACEA_T47D_80hr_Negative


5 MULTI Annotations Citations tcpl Processing Reagents AOPs

	Reagent Type	Reagent Value	Culture or Assay
1	media_base	RPMI-1640	culture
2	media_serum	10% FBS	culture
3	media_temp_celcius	37	culture
4	media_time_hr_min	24	culture
5	media_cell_aliquot	20000	culture
6	media_base	RPMI-1640	assay
7	media_serum	10% charcoal-stripped FBS	assay
8	media_temp_celcius_min	37	assay
9	media_time_hr	80	assay

List of Chemicals for an Assay

Assay Endpoint Name: ACEA_T47D_80hr_Negative

Assay Details



Assay Endpoint Name: ACEA_T47D_80hr_Negative 


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.

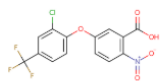
1813 chemicals

Download / Send 

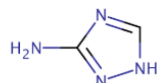
Show info: DTXSID CASRN TOXCAST  Select all 

Sort by: DTXSID  

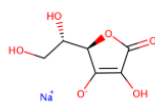
Filter by: Name or CASRN Hide 



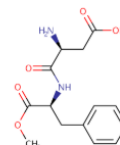
Acifluorfen
DTXSID: DTXSID0020022
CASRN: 50594-66-6
TOXCAST: 23/694



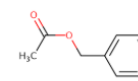
Amitrole
DTXSID: DTXSID0020076
CASRN: 61-82-5
TOXCAST: 1/303



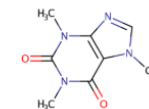
Sodium L-ascorbate
DTXSID: DTXSID0020105
CASRN: 134-03-2
TOXCAST: 19/561



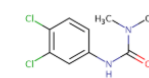
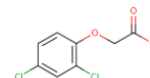
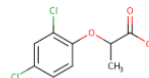
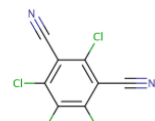
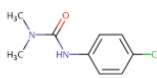
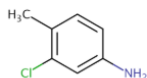
Aspartame
DTXSID: DTXSID0020107
CASRN: 22839-47-0
TOXCAST: 1/296



Benzyl acetate
DTXSID: DTXSID0020151
CASRN: 140-11-4
TOXCAST: 1/298



Caffeine
DTXSID: DTXSID0020232
CASRN: 58-08-2
TOXCAST: 21/546

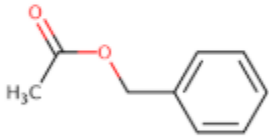


Choose Display Details

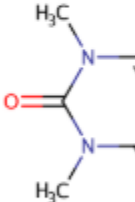
Show info: DTXSID x CASRN x TOXCAST x Select all ☰

Filter by: Hide

107



Benzyl acetate
DTXSID: DTXSID0020151
CASRN: 140-11-4
TOXCAST: 1/298



Caffeine
DTXSID: DTXSID0020151
CASRN: 58-08-3
TOXCAST: 21/546

- Unselected
- Isotopes
- Multicomponent Chemicals
- No Structures
- Inactive
- Active

Tile/Table Mode

More flexibility in table display

Assay Endpoint Name: ACEA_T47D_80hr_Negative

Assay Details

Assay Endpoint Name: ACEA_T47D_80hr_Negative

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.

466 of 1813 chemicals visible





Download / Send

Select all

Sort by: log AC50

Filter by: Name or CASRN

Inactive

Structure	PubMed	Preferred Name	# ToxCast Active	% ToxCast Active	Hit Call	Top	Scaled Top	AC50 (uM)	logAC50 (uM)
	069	2-Amino-5-azotoluene	166/602	28%	Active	78.4	3.64	316	2.50
	339	SR144190	62/614	10%	Active	102	4.72	285	2.45
	261	Tris(1,3-dichloro-2-propyl) phosphate	131/583	22%	Active	86.8	4.03	220	2.34
	DTXSID1026081 ToxCast™	3,3',5,5'-Tetrabromobisphenol A	197/574	34%	Active	117	5.42	128	2.11

In Vitro Bioassay Screening

ToxCast and Tox21

Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

ADME

EXPOSURE

BIOACTIVITY

TOXCAST: SUMMARY

PUBCHEM

TOXCAST: DATA

TOXCAST: MODELS

SIMILAR COMPOUNDS

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

LITERATURE

LINKS

COMMENTS

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

Assay Selection 1 Selected

A Single Assay Can Have Multiple Charts

Number of Charts: 6

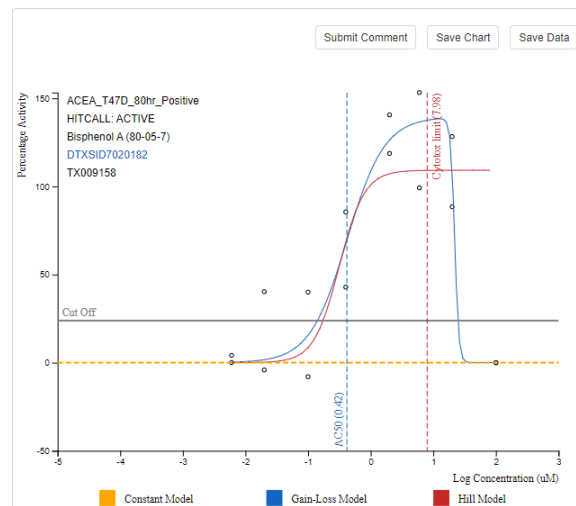
Active Inactive All

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
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- OT_ER_ERBERb_1440





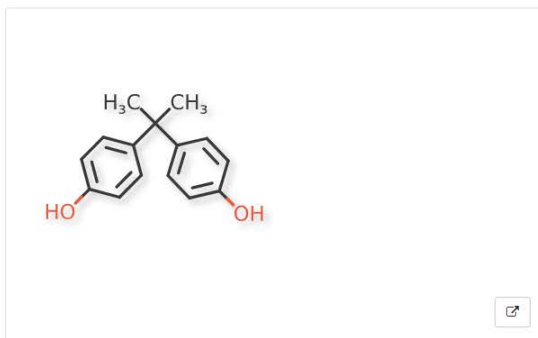
Structure Search

Search...



[Home](#) / [Tox21 Samples](#) / [Tox21_202992](#)

Bisphenol A



QC Grade

T0	A	MW Confirmed, Purity > 90%
T4	A	MW Confirmed, Purity > 90%

Identifiers

Tox21	Tox21_202992
NCATS	NCGC00260537-01
CAS	80-05-7
PubChem	144210190

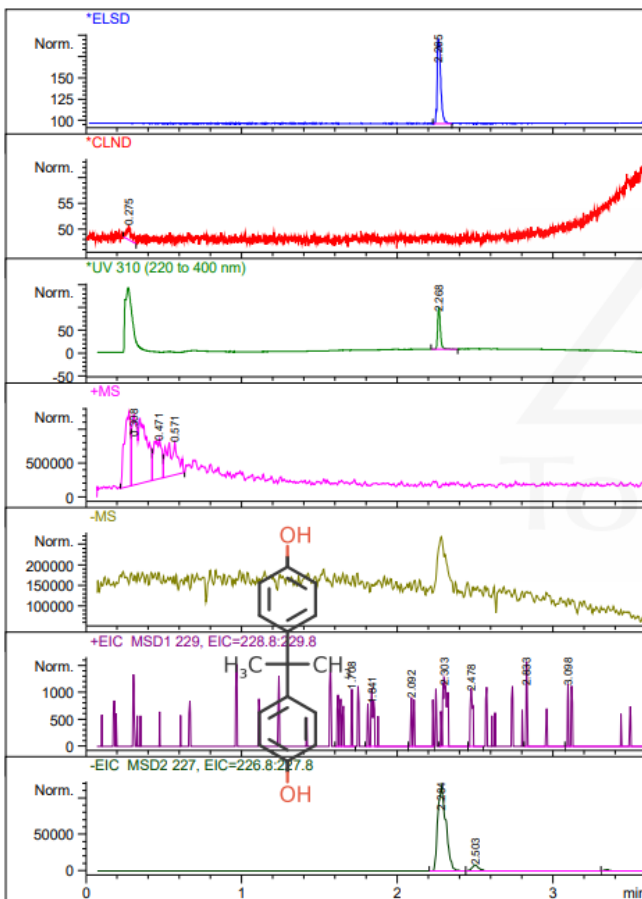
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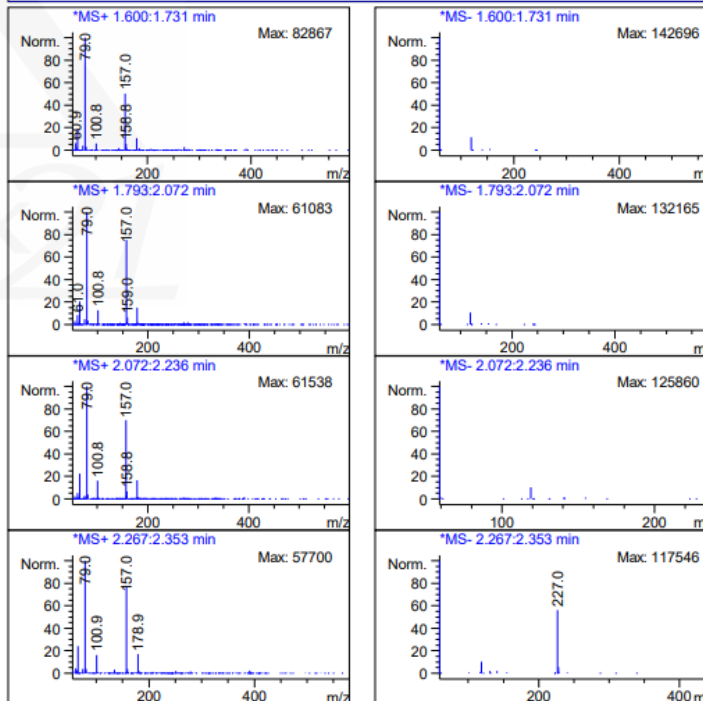
Access to Analytical QC Data

ID Tox21_202992 Plate Batch3-SP115973 Well P1-D-09 File SP115973_D009.D Inj Date: 5 May 12 1:33 am - MF C15H16O2 MW 228.1 Expected Conc: 2.97 mM



RT	Found	ELS%	UV %	ELS [mg/mL]	Adj [ELS]	[N mM]	Adj [CLN]	#N
1.71		0.0	0.0					0.0
1.84		0.0	0.0					0.0
2.09		0.0	0.0					0.0
2.27	Yes	100.0	100.0	1.76	7.73 mM			0.0

Comment: Passed



PubChem MW Confirmed, Purity > 90%
OpAns_Process.MAC Version A.01.10 - Dec 9, 2010

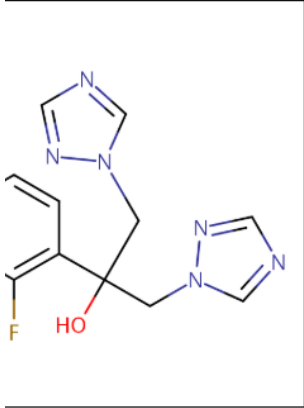
GenRA (Generalised Read-Across)

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

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

azole

-4 | DTXSID3020627
STox Substance Id.



Wikipedia

Fluconazole is an antifungal medication used for a number of fungal infections. This includes candidiasis, blastomycosis, coccidioidomycosis, cryptococcosis, histoplasmosis, dermatophytosis, and pityriasis versicolor. It is also used to prevent candidiasis in those who are at high risk such as following organ transplantation, low birth weight babies, and those with low blood neutrophil counts. It is given either by mouth or by injection into a vein. Common side effects include vomiting

...
[Read more](#)

Intrinsic Properties

Molecular Formula: C₁₃H₁₂F₂N₆O [Mol File](#) [Find All Chemicals](#)

Average Mass: 306.277 g/mol [Isotope Mass Distribution](#)

Monoisotopic Mass: 306.104065 g/mol

Structural Identifiers

Linked Substances

Presence in Lists

Record Information

Quality Control Notes

GenRA (Generalised Read-Across)

Fluconazole

86386-73-4 | DTXSID3020627

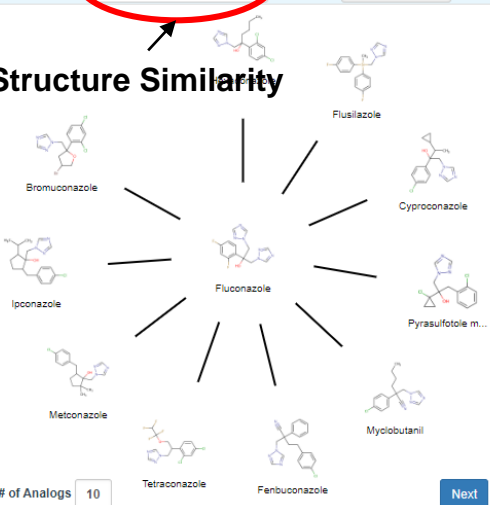
Searched by DSSTox Substance Id.

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

Step One: Analog Identification and Evaluation

Neighbors by: **Chem: Morgan Fgrprts** Filter by: invivo data

Structure Similarity



of Analogs: 10

Next

Select and Review Analogs

GenRA (Generalised Read-Across)

GenRA

Step Two: Data Gap Analysis & Generate Data Matrix

Neighbors by: Chem: Morgan Fgrpts

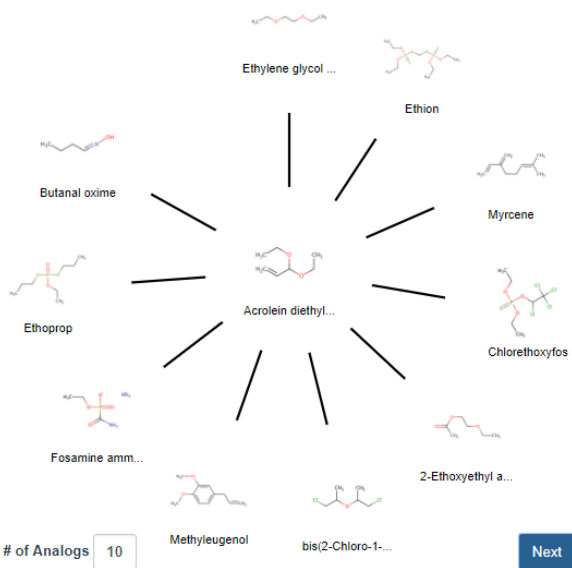
Filter by: invivo data

Summary Data Gap Analysis

Group: ToxRef

By: Tox Fingerprint

Generate Data Matrix



	bio_hx21	bio_hxct	chm_ct	tox_brf
Fluconazole	3	714	15	0
Hexaconazole	43	819	18	345
Flusilazole	28	819	9	345
Cyproconazole	14	819	16	408
Pyrasulfotole metabolite ...	0	0	18	234
Myclobutanil	15	818	15	345
Fenbuconazole	34	819	17	345
Tetraconazole	35	819	20	345
Metconazole	35	215	15	82
Ipconazole	46	232	16	180
Bromuconazole	24	277	13	345

	Fluconazole	Hexaconazole	Flusilazole	Cyproconazole	Pyrasulfotole metab...	Myclobutanil	Fenbuconazole	Tetraconazole	Metconazole	Ipconazole	Bromuconazole
CHR:Abdominal Cavity	Black	Black	Black	Black	Black	Black	Black	Black	Black	Black	Black
CHR:Adrenal Gland	Black	Black	Black	Black	Black	Black	Black	Black	Black	Black	Black
CHR:Artery (General)	Black	Black	Black	Black	Black	Black	Black	Black	Black	Black	Black
CHR:Auditory Startle Re...	Black	Black	Black	Black	Black	Black	Black	Black	Black	Black	Black
CHR:Bile duct	Black	Black	Black	Black	Black	Black	Black	Black	Black	Black	Black
CHR:Blood	Black	Black	Black	Black	Black	Black	Black	Black	Black	Black	Black
CHR:Blood vessel	Black	Black	Black	Black	Black	Black	Black	Black	Black	Black	Black
CHR:Body Weight	Black	Black	Black	Black	Black	Black	Black	Black	Black	Black	Black
CHR:Bone	Black	Black	Black	Black	Black	Black	Black	Black	Black	Black	Black
CHR:Bone Marrow	Black	Black	Black	Black	Black	Black	Black	Black	Black	Black	Black
CHR:Brain	Black	Black	Black	Black	Black	Black	Black	Black	Black	Black	Black
CHR:Tracheus	Black	Black	Black	Black	Black	Black	Black	Black	Black	Black	Black

Select and Review Analogs

Review Available Data

Fingerprint indicating available data

GenRA (Generalised Read-Across)

GenRA

Step Three: Run GenRA Prediction

Neighbors by: Chem: Morgan Fgrprts | Filter by: invivo data | Summary Data Gap Analysis | Group: ToxRef | By: Tox Fingerprint | Run Read-Across

Chemicals shown: Ethylene glycol..., Ethion, Butanal oxime, Myrcene, Acrolein diethylacetal, Ethylene glycol diethyl e...

Similarity Weight: 0.39 ✓, 0.31 ✓, 0.29 ✓, 0.29 ✓, 0.26 ✓, 0.24 ✓, 0.22 ✓, 0.21 ✓, 0.21 ✓, 0.20 ✓

Source analogues

Target

Run GenRA

Organ	Fluconazole	Hexaconazole	Flusilazole	Cyproconazole	Pyrasulfotole m...	Myclobutanil	Fenbuconazole	Tetraconazole	Metconazole	Ipconazole	Bromuconazole
CHR:Abdominal Cavity	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue
CHR:Adrenal Gland	Red	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Red
CHR:Artery (General)	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue
CHR:Auditory Startle Re...	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue
CHR:Bile duct	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue
CHR:Blood	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue
CHR:Blood vessel	Red	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue
CHR:Body Weight	Red	Blue	Blue	Blue	Blue	Blue	Red	Blue	Blue	Blue	Red
CHR:Bone	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue

Red : Toxicity effects.
 Blue: No Toxicity effects
 Grey : Absence of data

Related Substances

e.g. Transformation Products

Chlorothalonil

1897-45-6 | DTXSID0020319

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

8 chemicals

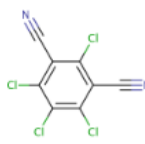
Download / Send

Show info: [DTXSID](#) [CASRN](#) [Select all](#)

Sort by: Relationship

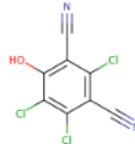
Filter by: Name or CASRN [Hide](#)

Searched Chemical



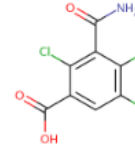
Chlorothalonil
DTXSID: DTXSID0020319
CASRN: 1897-45-6

Transformation Product



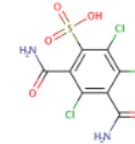
4-Hydroxy-2,5,6-trichloroisophthalonitrile
DTXSID: DTXSID00182588
CASRN: 28343-81-6

Transformation Product



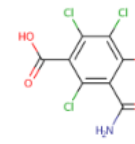
3-Carbamoyl-2,4,5-trichlorobenzoic acid
DTXSID: DTXSID10597537
CASRN: 142733-37-7

Transformation Product



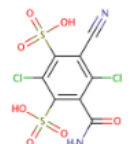
2,4-dicarbamoyl-3,5,6-trichlorobenzene
DTXSID: DTXSID30891327
CASRN: NOCAS_891327

Transformation Product



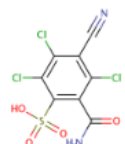
3-carbamoyl-2,5,6-trichloro-4-hydroxybenzoic acid
DTXSID: DTXSID00891328
CASRN: NOCAS_891328

Transformation Product



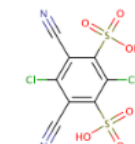
4-carbamoyl-2,5-dichloro-6-cyanobenzene
DTXSID: DTXSID00891329
CASRN: NOCAS_891329

Transformation Product



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

Transformation Product



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

(C10-C16) Alkylbenzenesulfonic acid

68584-22-5 | DTXSID2028723

Searched by CAS-RN.

DETAILS

[RELATED SUBSTANCES](#)

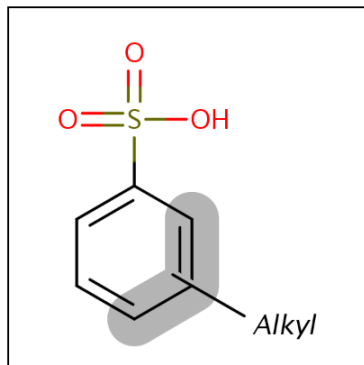
[PROPERTIES](#)

[ENV. FATE/TRANSPORT](#)

[BIOACTIVITY](#)

[SYNONYMS](#)

[COMMENTS](#)



Intrinsic Properties

Molecular Formula: Not Found [Mol File](#) [Find All Chemicals](#)

Average Mass: 0 g/mol [Isotope Mass Distribution](#)

Monoisotopic Mass: 0 g/mol

Presence in Lists

Federal

[Endocrine Disruptor Screening Program \(EDSP\) Universe of Chemicals](#) [EPAHFR Table H-2 - Chemicals in hydraulic fracturing fluids from 2005-2013](#)
[TSCA Inventory, active non-confidential portion](#) [ECOTOXology knowledgebase \(ECOTOX\)](#) [TOX21SL: Tox21 Screening Library](#)
[EPAHFR - EPA Chemicals associated with hydraulic fracturing](#)

US State

None.


International

None.

Other

[SUSDAT: The NORMAN Network Suspect Screening List](#) [TSCA Workplan Step 2 Chemicals](#) [Surfactant List Screened in Swiss Wastewater \(2014\)](#)

Related Substances for Markush

 United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Copy Share Submit Comment Search all data

27 chemicals

Download / Send

Show info: DTXSID CASRN TOXCAST Select all

Sort by: Relationship Filter by: Name or CASRN Hide

Chemical Name	DTXSID	CASRN	TOXCAST
(C10-C16) Alkylbenzenesulfonic acid	DTXSID2028723	68584-22-5	15/113
Alkylbenzenesulfonate, linear	DTXSID3020041	42615-29-2	0
C10-linear alkylbenzenesulfonate	DTXSID70891689	NOCAS_891689	0
C12-linear alkyl benzene sulfonate	DTXSID90891641	NOCAS_891641	0
4-(decan-4-yl)benzenesulfonic acid	DTXSID40891333	NOCAS_891333	0
4-(decan-5-yl)benzene-1-sulfonic acid	DTXSID70881146	NOCAS_881146	0
4-(undecan-5-yl)benzene-1-sulfonic acid	DTXSID40881097	NOCAS_881097	0
4-Tetradecylbenzenesulfonic acid	DTXSID1068489	47377-16-2	0
4-(dodecan-4-yl)benzene-1-sulfonic acid	DTXSID30862870	NOCAS_862870	0
4-(Dodecan-6-yl)benzene-1-sulfonic acid	DTXSID30860093	NOCAS_23003-92-1	0

Identifiers to Support Searches

Bisphenol A

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

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

25

Synonym	Quality
Bisphenol A	Valid
4,4'-(Propane-2,2-diyldiphenol	Valid
Phenol, 4,4'-(1-methylethylidene)bis-	Valid
80-05-7 Active CAS-RM	Valid
BPA	Valid
4,4'-Propane-2,2-diyldiphenol	Valid
Phenol, 4,4'-(1-methylethylidene)bis-	Valid
4-06-00-06717 Beilstein Registry Number	Bellstein
(4,4'-Dihydroxydiphenyl)dimethylmethane	Good
2,2-Bis(4'-hydroxyphenyl) propane	Good
2,2'-Bis(4-hydroxyphenyl)propane	Good
2,2-BIS-(4-HYDROXY-PHENYL)-PROPANE	Good
2,2-Bis(4-hydroxyphenyl)propane	Good
2,2-Bis(p-hydroxyphenyl)propane	Good
2,2-Di(4-Hydroxyphenyl) Propane	Good

Literature Searches and Links

Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

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

Select a Query Term

Retrieve Articles

Select a Query Term

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

Optionally, edit the query before retrieving.

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

LITERATURE

GOOGLE SCHOLAR

PUBMED ABSTRACT SIFTER

PUBCHEM ARTICLES

PUBCHEM PATENTS

PPRTV

IRIS

Abstract Sifter – PubMed Integration

searching >28 million abstracts

Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

▶ ADME

▶ EXPOSURE

▶ BIOACTIVITY

GENRA (BETA)

SIMILAR COMPOUNDS

RELATED SUBSTANCES

SYNONYMS

▼ LITERATURE

GOOGLE SCHOLAR

PUBMED ABSTRACT SIFTER

PUBCHEM ARTICLES

PUBCHEM PATENTS

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

Hazard

Retrieve Articles

118 of 118 articles loaded...

To find articles quickly, enter terms to sift abstracts.

Optionally, edit the query before retrieving.

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

Download / Send to...

Download Sifter for Excel

<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	▼

External Links to ~80 websites

Growing list of out links -

Bisphenol A

80-05-7 | DTXSID7020182
Searched by Approved Name.

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

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
- Chempidier
- CPCat
- DrugBank
- HMDB
- Wikipedia
- MSDS Lookup
- ChEMBL
- Chemical Vendors
- CalEPA Office of Environmental Health Hazard Assessment
- NIOSH Chemical Safety Cards
- ToxPlanet
- ACS Reagent Chemicals
- Wikidata
- ChemHat: Hazards and Alternatives Toolbox
- Wolfram Alpha
- ScrubChem
- ECHA Brief Profile
- ECHA Infocard
- ChemAgora

Toxicology

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

Publications

- Toxline
- Environmental Health Perspectives
- NIEHS
- National Toxicology Program
- Google Books
- Google Scholar
- Google Patents
- PPRTVWEB
- PubMed
- IRIS Assessments
- EPA HERO
- NIOSH Skin Notation Profiles
- NIOSH Pocket Guide
- RSC Publications
- BioCaddie DataMed
- Springer Materials
- Federal Register
- Regulations.gov
- Bielefeld Academic Search Engine
- CORE Literature Search

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

Mass and Formula Searches Supporting Mass Spectrometry

Advanced Search

Mass Search

 ± Min/Max

Select Adduct: ▼


 Da

±

 Da ppm

Search Q

Molecular Formula Search

MS Ready Formula 

Exact Formula 

Search Q

Generate Molecular Formula(e)

 ± Min/Max Da

±

 Da ppm

Search Q

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


Da Da

Search Results

Searched by Mass: 191.131 +/- 5.0 ppm.

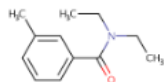
298 of 298 chemicals visible

Download / Send 

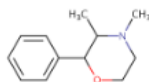
Show info: 

Sort by: 

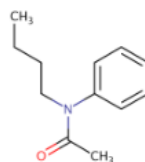
Filter by:



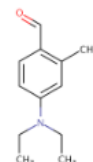
DEET
DTXSID: DTXSID2021995
CASRN: 134-62-3
TOXCAST: 14/663
Mass Diff: 0.000014



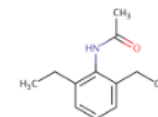
Phendimetrazine
DTXSID: DTXSID1023447
CASRN: 634-03-7
TOXCAST: 0
Mass Diff: 0.000014



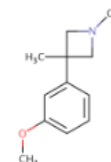
N-Butylacetanilide
DTXSID: DTXSID2042197
CASRN: 91-49-6
TOXCAST: 0
Mass Diff: 0.000014



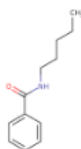
Benzaldehyde, 4-(diethylamino)-2-methyl-
DTXSID: DTXSID4059041
CASRN: 92-14-8
TOXCAST: 0
Mass Diff: 0.000014



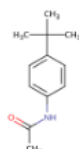
Acetanilide, 2',6'-diethyl-
DTXSID: DTXSID90168148
CASRN: 16665-89-7
TOXCAST: 0
Mass Diff: 0.000014



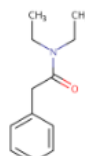
Azetidine, 1,3-dimethyl-3-(m-methoxyphenyl)-
DTXSID: DTXSID40173560
CASRN: 19832-26-9
TOXCAST: 0
Mass Diff: 0.000014



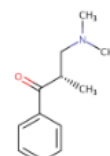
Benzamide, N-pentyl-
DTXSID: DTXSID20174198
CASRN: 20308-43-4



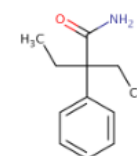
p-t-Butylacetanilide
DTXSID: DTXSID80174238
CASRN: 20330-45-4



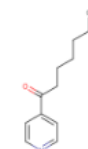
N,N-Diethylphenylacetamide
DTXSID: DTXSID00179048
CASRN: 2431-98-1



3-(Dimethylamino)-2-methylpropiofenone
DTXSID: DTXSID80180796
CASRN: 26171-60-6



Butyramide, 2-ethyl-2-phenyl-
DTXSID: DTXSID60184653
CASRN: 30568-39-0



1-Heptanone, 1-(4-pyridyl)-
DTXSID: DTXSID40188594
CASRN: 32941-30-3

Advanced Searches

Mass Based Search

Search Results

Searched by Mass: 191.131 +/- 5.0 ppm.

298 of 298 chemicals visible

Download / Send

Select all

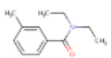
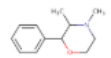
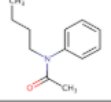
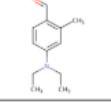
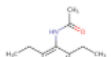


Sort by: Mass Difference



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

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[Background](#)

[Methods](#)

[Results and discussion](#)

[Conclusions](#)

[Declarations](#)

[References](#)

Methodology | [Open Access](#)

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

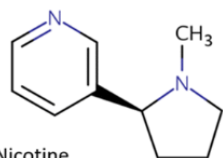
[Andrew D. McEachran](#) , [Kamel Mansouri](#), [Chris Grulke](#), [Emma L. Schymanski](#), [Christoph Ruttkies](#) and [Antony J. Williams](#) 

Journal of Cheminformatics 2018 **10**:45

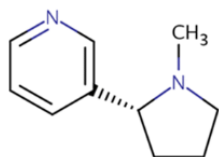
<https://doi.org/10.1186/s13321-018-0299-2> | © The Author(s) 2018

Received: 16 May 2018 | **Accepted:** 21 August 2018 | **Published:** 30 August 2018

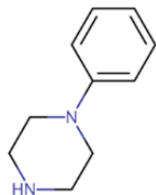
Exact Formula Match and MS-Ready Match



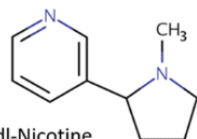
Nicotine
DTXSID1020930 | DTXCID9028128
Tox: yes | Expo: yes | Bioassay: yes
 $C_{10}H_{14}N_2$ | 54-11-5 | 87



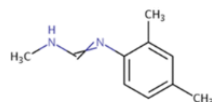
D-Nicotine
DTXSID0046351 | DTXCID9028128
Tox: no | Expo: yes | Bioassay: yes
 $C_{10}H_{14}N_2$ | 25162-00-9 | 21



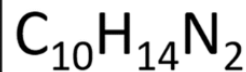
Phenylpiperazine
DTXSID8057855 | DTXCID9031644
Tox: no | Expo: no | Bioassay: yes
 $C_{10}H_{14}N_2$ | 25162-00-9 | 32



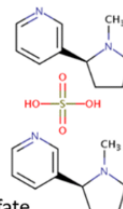
dl-Nicotine
DTXSID3048154 | DTXCID9028128
Tox: yes | Expo: no | Bioassay: yes
 $C_{10}H_{14}N_2$ | 22083-74-5 | 16



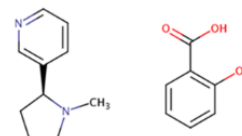
N'-(2,4-Dimethylphenyl)-N-methylformamide
DTXSID1037696 | DTXCID9017696
Tox: no | Expo: Yes | Bioassay: yes
 $C_{10}H_{14}N_2$ | 33089-74-6 | 27



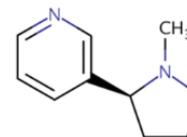
MS-Ready Match Only



Nicotine sulfate
DTXSID8021725 | DTXCID9028128
Tox: yes | Expo: yes | Bioassay: yes
 $C_{10}H_{14}N_2 \cdot C_{10}H_{14}N_2 \cdot SH_2O_4$ | 65-30-5 | 28



Benzoic acid, 2-hydroxy-, compd. with 3-[(2S)-1-methyl-2-pyrrolidinyl]pyridine (1:1)
DTXSID5075319 | DTXCID9028128 | DTXCID206368
Tox: no | Expo: yes | Bioassay: no
 $C_{10}H_{14}N_2 \cdot C_7H_6O_3$ | 29790-52-1 | 7



HCl
Nicotine hydrochloride
DTXSID6020931 | DTXCID9028128
Tox: no | Expo: yes | Bioassay: yes
 $C_{10}H_{14}N_2 \cdot HCl$ | 2820-51-1 | 10

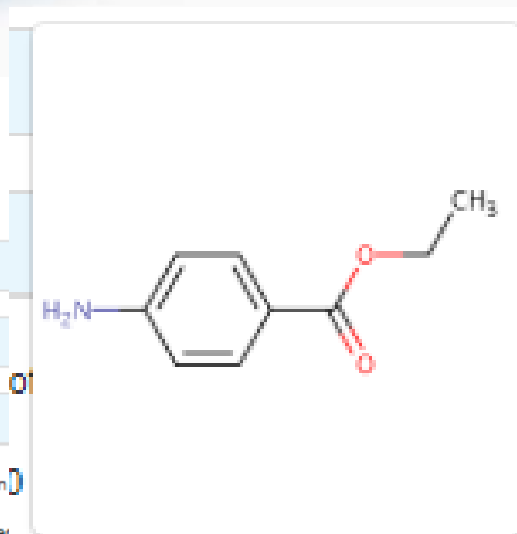
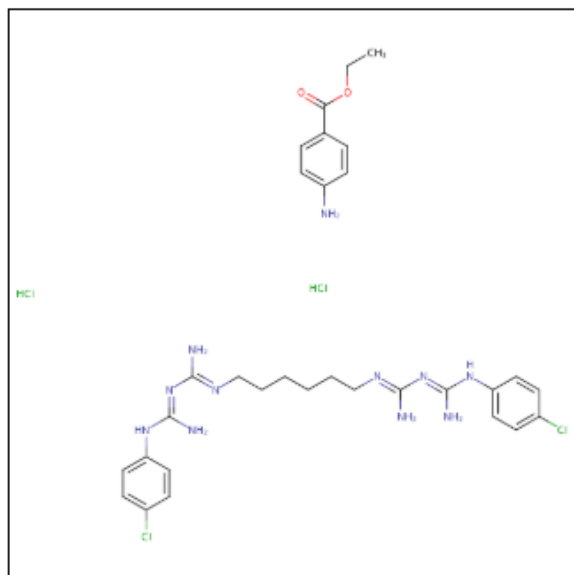
LEGEND: Preferred Name
DTXSID | MS-ready DTXCID
Avail. Data: Toxicity | Exposure | Bioassay
Formula | CAS | Data Sources

MS-Ready Mappings

Progaron

108532-15-6 | DTXSID20148579

Searched by DSSTox Substance Id.



Intrinsic Properties

Structural Identifiers

Linked Substances

Same Connectivity: [1 record](#) (based on)

Mixtures, Components and Neutralizer:

MS-Ready Mappings: [DTXCID0013314](#); [DTXCID301804](#): **11 records**; [D](#)

Similar Compounds: 0 records

Presence in Lists

Record Information

Quality Control Notes

MS-Ready Mappings Set

MS-Ready Mappings of Benzocaine (Isotopes pre-filtered)

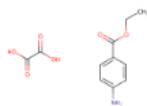
9 of 11 chemicals visible

Download / Send

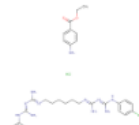
Show info: DTXSID CASRN Select all

Sort by: DTXSID

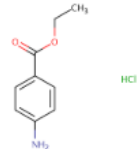
Filter by: Name or CASRN Isotopes



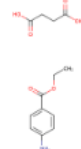
Anesthesine oxalate
DTXSID: DTXSID20148337
CASRN: 107948-47-0



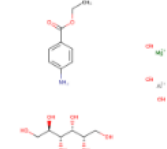
Progaron
DTXSID: DTXSID20148679
CASRN: 108532-15-8



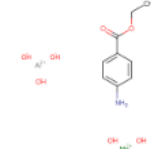
Benzocaine hydrochloride
DTXSID: DTXSID50177812
CASRN: 23239-88-5



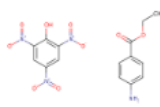
Anesthesine succinate
DTXSID: DTXSID60148336
CASRN: 107948-46-9



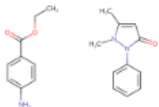
Almagel A-neo
DTXSID: DTXSID80227559
CASRN: 76741-92-9



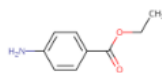
Almagel
DTXSID: DTXSID70227560
CASRN: 76741-95-2



Ethyl 4-aminobenzoate-2,4,6-trinitrophenol
DTXSID: DTXSID70787033
CASRN: 5982-70-7



Antipyrine mixture with benzocaine
DTXSID: DTXSID80212886
CASRN: 63448-01-1



Benzocaine
DTXSID: DTXSID8021804
CASRN: 94-09-7


- Singleton searches are useful but we work with thousands of chemicals!
- Typical questions
 - What chemicals can I get for 5000 CAS Numbers?
 - Can I get predicted properties for 1000 chemicals?
 - What is the list of chemicals for the formula $C_xH_yO_z$?
 - What is the list of chemicals for a mass +/- error ?
 - Can I get chemical lists in Excel files? In SDF files?

Batch Searching








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



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

Chemical Data

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

	A	B	C	D	E	F	G	H
1	INPUT	FOUND_BY	DTXSID	PREFERRED_NAME	EXPOCAST	EXPOCAST	NHANES	TOXVAL_D
2	1445-75-6	CAS-RN	DTXSID5024051	Diisopropyl methylpho	2.09e-08	Y	-	Y
3	50-00-0	CAS-RN	DTXSID7020637	Formaldehyde	1.32e-06	Y	-	Y
4	107-06-2	CAS-RN	DTXSID6020438	1,2-Dichloroethane	4.9e-06	Y	-	Y
5	57-12-5	CAS-RN	DTXSID6023991	Cyanide	-	-	-	Y
6	7550-45-0	CAS-RN	DTXSID8042476	Titanium tetrachloride	-	-	-	Y
7	79-01-6	CAS-RN	DTXSID0021383	Trichloroethylene	7.27e-06	Y	-	Y
8	121-82-4	CAS-RN	DTXSID9024142	Cyclonite	6.72e-08	Y	-	Y
9	108-05-4	CAS-RN	DTXSID3021431	Vinyl acetate	8.3e-05	Y	-	Y
10	7803-51-2	CAS-RN	DTXSID2021157	Phosphine	-	-	-	Y
11	122-66-7	CAS-RN	DTXSID7020710	1,2-Diphenylhydrazine	1.49e-07	Y	-	Y
12	101-77-9	CAS-RN	DTXSID6022422	4,4'-Methylenedianiline	6.08e-06	Y	-	Y
13	14017-34-6	CAS-RN	DTXSID90161250	Selenium difluoride	-	-	-	-
14	75-44-5	CAS-RN	DTXSID0024260	Phosgene	-	-	-	Y
15	621-64-7	CAS-RN	DTXSID6021032	N-Nitrosodipropylamine	4.55e-07	Y	-	Y
16	75-09-2	CAS-RN	DTXSID0020868	Dichloromethane	2.02e-06	Y	-	Y
17	100-41-4	CAS-RN	DTXSID3020596	Ethylbenzene	8.32e-05	Y	-	Y
18	7440-28-0	CAS-RN	DTXSID2036035	Thallium	-	-	-	Y
19	108-88-3	CAS-RN	DTXSID7021360	Toluene	8.61e-05	Y	-	Y
20	111-44-4	CAS-RN	DTXSID9020168	Bis(2-chloroethyl) ethe	2.82e-07	Y	-	Y
21	7440-42-8	CAS-RN	DTXSID3023922	Boron	-	-	-	Y
22	7440-29-1	CAS-RN	DTXSID6049800	Thorium	-	-	-	Y

How can we curate our data?

- Crowdsourcing is well proven nowadays
- Comments can be added at a record level



- Submitted comments are reviewed by administrators and responded to

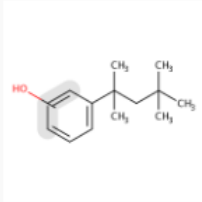
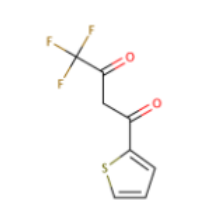
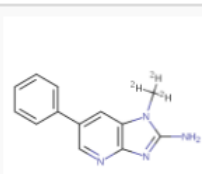
Public Crowdsourced Comments

https://comptox.epa.gov/dashboard/comments/public_index

Crowdsourced Comments

Show 10 entries

Search:

Chemical	Structure	Date	Comment	Status
(1,1,3,3-Tetramethylbutyl)phenol		2017-07-15	Octylphenol redirects here, yet the name and related chemicals are 1,1,3,3-tetramethylbutylphenol - which is only a subset of all octylphenol isomers? Is this CAS only for these alkyl isomers?	★
1,3-Butanedione, 4,4,4-trifluoro-1-(2-thienyl)-		2017-03-30	Synonym: TTFA (Any way to bank these reCAPTCHAs so I don't have to do it everytime?)	★
1-(2H<sup>2</sup>H<sub>3</sub>)-Methyl-6-phenyl-1H-imidazo[4,5-b]pyridin-2-amine		2017-05-06	1-(2H3)Methyl-6-phenyl-1H-imidazo[4,5-b]pyridin-2-amine 210049-13-1 DTXSID70670097 contains an error in the empirical formula due to an error in the deuterium representation and subsequent counting	★


- The majority of comments to date:
 - Structure and names/CASRN do not match
 - Add additional synonyms
 - Request to add specific property data
 - Structure layout/depiction needs improving

Crowdsourcing Comments

Single Cell Commenting added

- Highlight an alphanumeric text string

<u>assessment class</u>	<u>Value</u>	<u>Units</u>	<u>Study type</u>
	50	mg/kg-day	-
	149.999	mg/kg-day	chronic
	50	mg/kg-day	reproductive multigeneration
	500	mg/kg-	reproductive



Crowdsourcing Comments

Details to be submitted with your comment:

Text selected: 149.999


Found On: August 11th 2018, 10:30:02 pm

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

Browser: Chrome 68

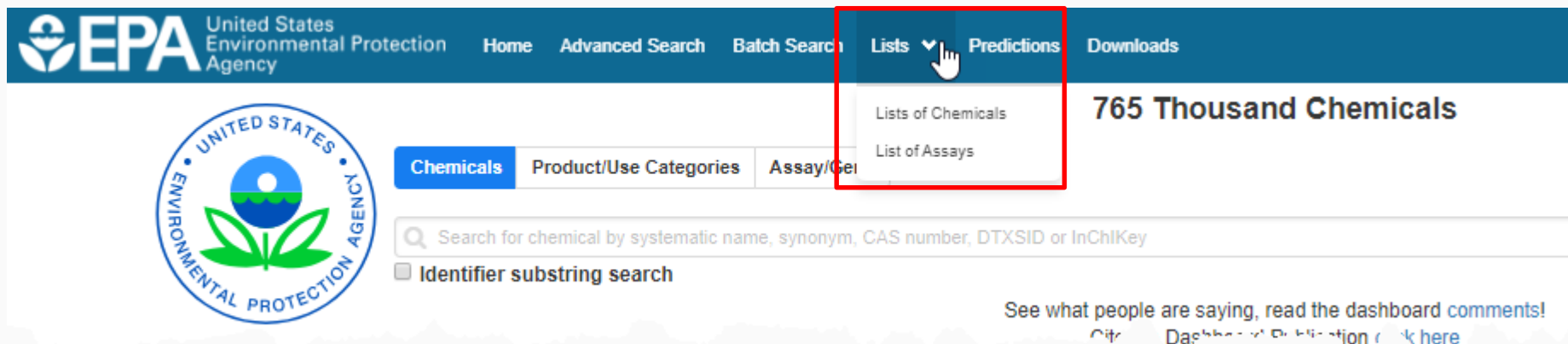
There appears to be a rounding error in this ToxVal data

williams.antony@epa.gov

I'm not a robot  reCAPTCHA
Privacy - Terms

Lists of Lists

- Lists of chemicals – ca. 100 lists
- List of ToxCast/Tox21 assays



The screenshot shows the EPA ToxCast/Tox21 dashboard. The top navigation bar includes links for Home, Advanced Search, Batch Search, Lists, Predictions, and Downloads. The 'Lists' menu is open, showing options for 'Lists of Chemicals' and 'List of Assays'. The main content area features a search bar with the text 'Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey' and a checkbox for 'Identifier substring search'. On the right, it displays '765 Thousand Chemicals'. At the bottom right, there is a link to 'See what people are saying, read the dashboard comments!' and a link to 'Dashboard Publication (click here)'.

11 PFAS Lists

http://comptox-prod.epa.gov/dashboard/chemical_lists

Select List

Show 10 entries

Search: pfas|

Download

List Acronym	List Name	Last Updated	Number of Chemicals	List Description
EPAPFAS75S1	EPA PFAS 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.
EPAPFASCAT	Registered DSSTox "category substances" representing Per- and Polyfluoroalkyl Substances (PFAS) 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 in EPA's 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 in EPA's ToxCast Chemical Inventory	2018-06-29	430	PFAS chemicals included in EPA's expanded ToxCast chemical inventory and available for testing.
EPAPFASRL	EPA PFAS Cross-Agency Research List	2018-07-27	194	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.
PFASEPA	PFAS_EPA List of Perfluorinated alkyl substances	2017-11-03	190	PFAS_EPA (Perfluorinated alkyl substances) is a manually curated listing of mainly straight-chain and branched PFAS substances
PFASEOECOD	PFAS Listed in OECD Global Database	2018-07-26	4725	OECD released a New Comprehensive Global Database of Per- and Polyfluoroalkyl Substances, (PFASs) listing approximately 4700 new PFAS
PFASGRACE	PFASforGrace	2017-02-16	35	A list of polyfluorinated chemicals of interest to Grace Patlewicz
PFASKEMI	PFAS List from the Swedish Chemicals Agency (KEMI) Report	2017-02-09	2397	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.

Showing 1 to 10 of 11 entries (filtered from 96 total entries)



Port

HOME



The OECD releases a new list of PFASs

The OECD releases a new list of Per- and Polyfluoroalkyl Substances (PFASs) based on a comprehensive analysis of information available in the public domain. In total, 4730 PFAS-related CAS numbers have been identified and categorised in this study, including several new groups of PFASs that fulfil the common definition of PFASs (i.e. they contain at least one perfluoroalkyl moiety) but have not yet been commonly regarded as PFASs.

This work has been conducted under the OECD/UN Environment Global PFC Group in support of the Strategic Approach to International Chemicals Management (SAICM) and shifting to safer alternatives for PFASs.

The [New Comprehensive Global Database of Per- and Polyfluoroalkyl Substances \(PFASs\)](#) comes with a [methodology report](#) also detailing the major findings with respect to the total numbers and types of PFASs identified, the limitations, gaps and challenges identified in the development of the new list, and opportunities for improving the future understanding of PFASs production, use on the global market, and presence in the environment, biota, and other matrices.



INARS



The OECD List of PFAS

<http://www.oecd.org/chemicalsafety/portal-perfluorinated-chemicals/>

PFAS Listed in OECD Global Database

Search PFASEUOECD Chemicals



Substring search

List Details

Description: OECD released a New Comprehensive Global Database of Per- and Polyfluoroalkyl Substances (PFASs) listing approximately 4700 new PFAS, including several new groups of PFASs that fulfill the common definition of PFASs (i.e. they contain at least one perfluoroalkyl moiety) but have not yet been commonly regarded as PFASs. The list can be used in conjunction with the methodology report summarising the major findings with respect to the total numbers and types of PFASs identified, the limitations, gaps and challenges identified, and opportunities for improving the future understanding of PFASs production, use on the global market, and presence in the environment, biota, and other matrices.

Source website: <http://www.oecd.org/chemicalsafety/portal-perfluorinated-chemicals>

A major effort was undertaken to register this list within DSSTox, adding chemical structures for as many PFAS entries as possible using both manual and auto-mapping (structures using CAS-matching) curation methods. The result is that approximately 1/3 of the list is curated at the highest two curation levels (DSSTox_High or DSSTox_Low) currently, whereas more than half of this list is registered at the Public_Low curation level (based on PubChem content). The PFASOECD list is undergoing continuous registration and curation.

Number of Chemicals: 4725

4725 chemicals

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Show info:

DTXSID ×

CASRN ×

TOXCAST ×

Select all



Sort by: DTXSID ▼

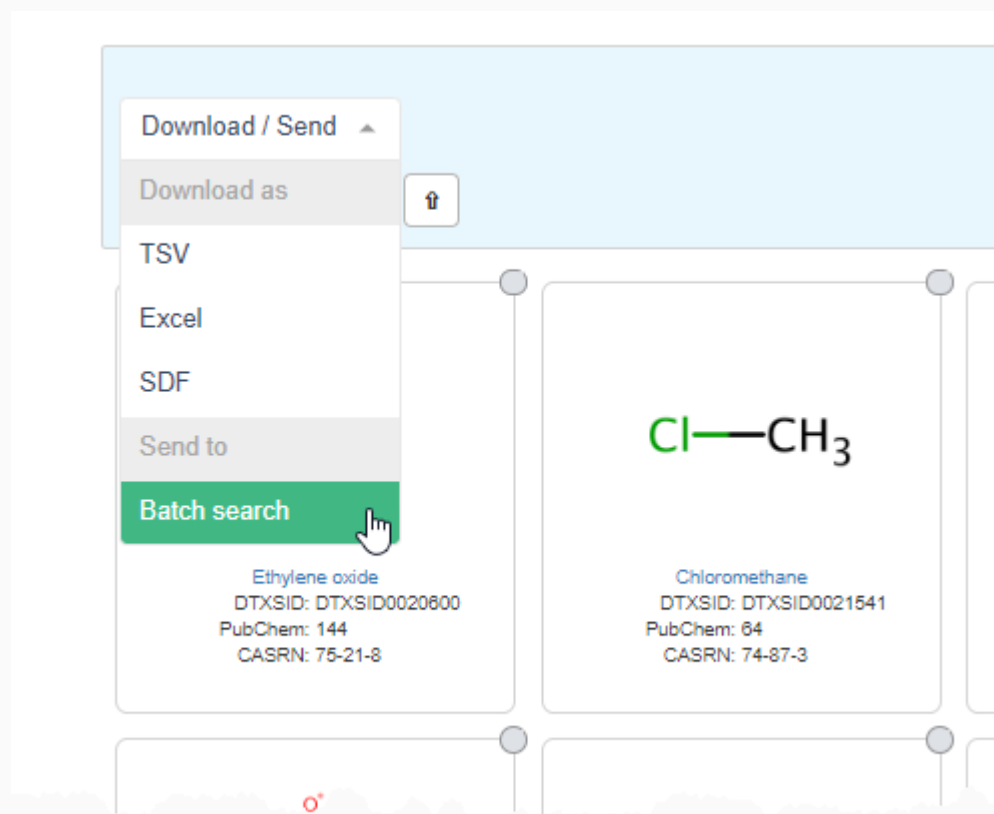


Filter by: Name or CASRN

Hide ▼

Want data for a list???

- Simply send to Batch and choose data...



The screenshot shows a web interface with a 'Download / Send' menu open. The menu options are: Download as (with an upload icon), TSV, Excel, SDF, Send to, and Batch search (highlighted in green with a mouse cursor). Below the menu, two chemical entries are visible:

Chemical Name	DTXSID	PubChem	CASRN
Ethylene oxide	DTXSID0020600	144	75-21-8
Chloromethane	DTXSID0021541	64	74-87-3




The chemical structure for Chloromethane is shown as $\text{Cl}-\text{CH}_3$.

List of Assays

Assay List

Download

Search by Name or Gene

Assay Component Endpoint Name	Details	Active Hits	Description	Gene Symbol
ACEA_T47D_80hr_Negative		469 / 1816	Data from the assay component ACEA_T47D_80hr was analyzed into 2 assay endpoints. This assay endpoint, ACEA_T47D_80hr_Negative, was analyzed in the negative fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of growth reporter, loss-of-signal activity can be used to understand changes in the viability. Furthermore, this assay endpoint can be referred to as a secondary readout, because this assay has produced multiple assay endpoints where this one serves a viability function. To generalize the intended target to other relatable targets, this assay endpoint is annotated to the 'cell cycle' intended target family, where the subfamily is 'cytotoxicity'.	
ACEA_T47D_80hr_Positive		311 / 1816	Data from the assay component ACEA_T47D_80hr was analyzed into 2 assay endpoints. This assay endpoint, ACEA_T47D_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
APR_HepG2_CellCycleArrest_1h_dn		3 / 310	Data from the assay component APR_HepG2_CellCycleArrest_1hr was analyzed into 2 assay endpoints. This assay endpoint, APR_HepG2_CellCycleArrest_1h_dn, was analyzed in the negative fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of morphology reporter, measures of all nuclear dna for loss-of-signal activity can be used to understand the signaling at the pathway-level as they relate to the gene . 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	

Select an Assay to Navigate Tile View

Assay Endpoint Name: ACEA_T47D_80hr_Positive

Assay Details

Assay Endpoint Name: ACEA_T47D_80hr_Positive

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.

311 of 1813 chemicals visible

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Show info:

DTXSID

PubChem

CASRN

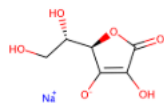
Select all

Sort by:

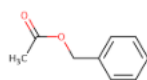
DTXSID

Filter by: Name or CASRN

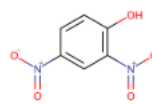
Inactive



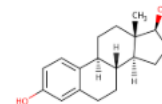
Sodium L-ascorbate
DTXSID: DTXSID0020105
PubChem: 41
CASRN: 134-03-2



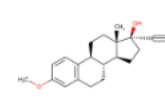
Benzyl acetate
DTXSID: DTXSID0020151
PubChem: 101
CASRN: 140-11-4



2,4-Dinitrophenol
DTXSID: DTXSID0020523
PubChem: 154
CASRN: 51-28-5




17beta-Estradiol
DTXSID: DTXSID0020573
PubChem: 351
CASRN: 50-28-2



Mestranol
DTXSID: DTXSID0020814
PubChem: 97
CASRN: 72-33-3

Select an Assay to Navigate Table View

 United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Share Search all data

Assay Endpoint Name: ACEA_T47D_80hr_Positive

Assay Details

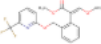
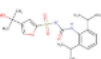

Assay Endpoint Name: ACEA_T47D_80hr_Positive

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.

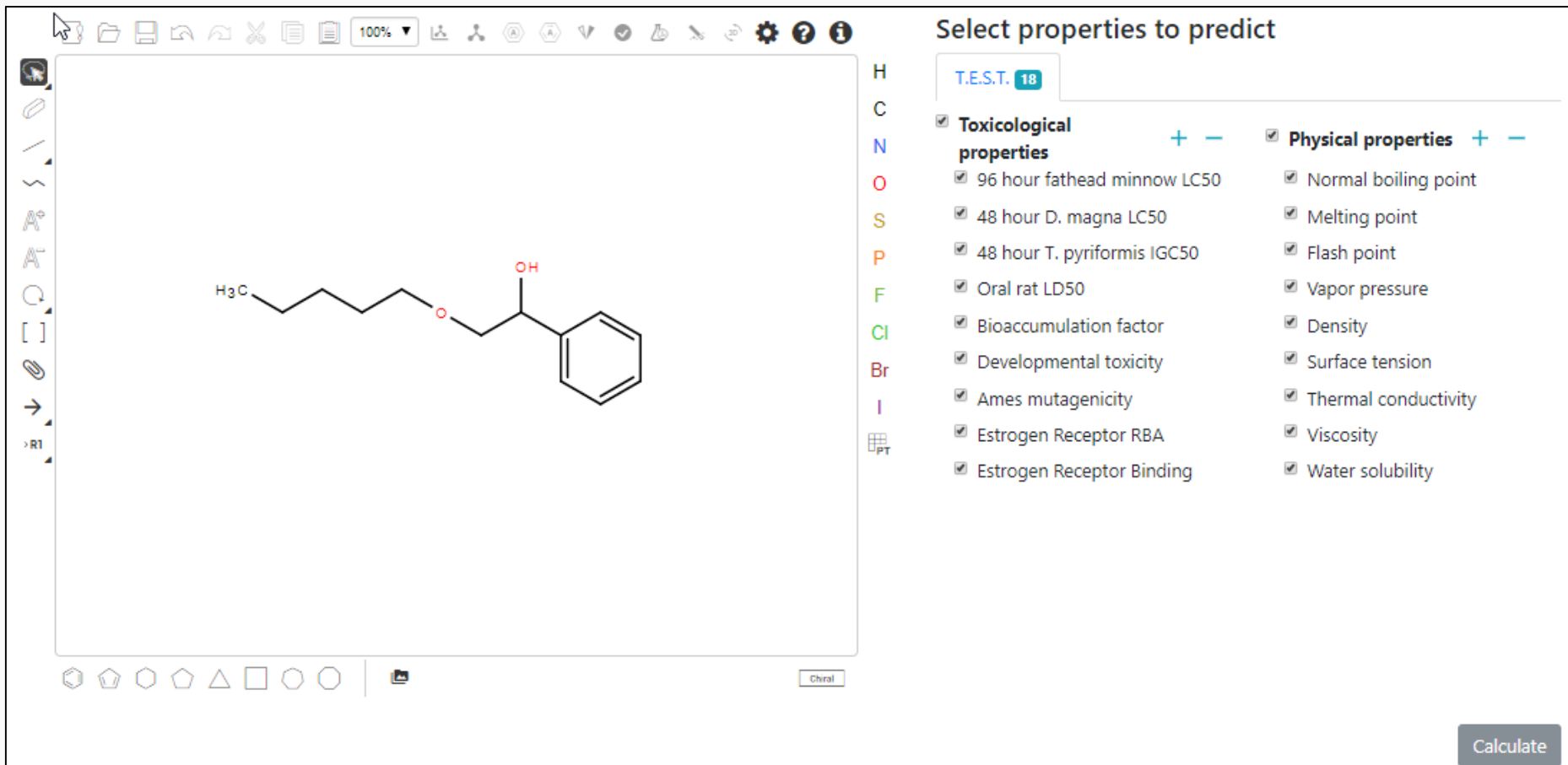
311 of 1813 chemicals visible

Download / Send Select all

Sort by: DTXSID Filter by: Name or CASRN Inactive

Structure	DTXSID	Preferred Name	# ToxCast Active	% ToxCast Active	Hit Call	Top	Scaled Top	AC50 (uM)	logAC50 (uM)
	DTXSID9047542 ToxCast™	Picoxystrobin	127/558	23%	Active	56.0	2.30	10.9	1.04
	DTXSID9047255 ToxCast™	CP-465304	16/538	3%	Active	30.1	1.24	82.2	1.91
	DTXSID9047178 ToxCast™	2-Ethylhexyl octadecanoate	10/469	2%	Active	24.8	1.02	20.7	1.32

Real-Time Predictions



Select properties to predict

T.E.S.T. 18

<input checked="" type="checkbox"/> Toxicological properties + -	<input checked="" type="checkbox"/> Physical properties + -
<input checked="" type="checkbox"/> 96 hour fathead minnow LC50	<input checked="" type="checkbox"/> Normal boiling point
<input checked="" type="checkbox"/> 48 hour D. magna LC50	<input checked="" type="checkbox"/> Melting point
<input checked="" type="checkbox"/> 48 hour T. pyriformis IGC50	<input checked="" type="checkbox"/> Flash point
<input checked="" type="checkbox"/> Oral rat LD50	<input checked="" type="checkbox"/> Vapor pressure
<input checked="" type="checkbox"/> Bioaccumulation factor	<input checked="" type="checkbox"/> Density
<input checked="" type="checkbox"/> Developmental toxicity	<input checked="" type="checkbox"/> Surface tension
<input checked="" type="checkbox"/> Ames mutagenicity	<input checked="" type="checkbox"/> Thermal conductivity
<input checked="" type="checkbox"/> Estrogen Receptor RBA	<input checked="" type="checkbox"/> Viscosity
<input checked="" type="checkbox"/> Estrogen Receptor Binding	<input checked="" type="checkbox"/> Water solubility

Calculate

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

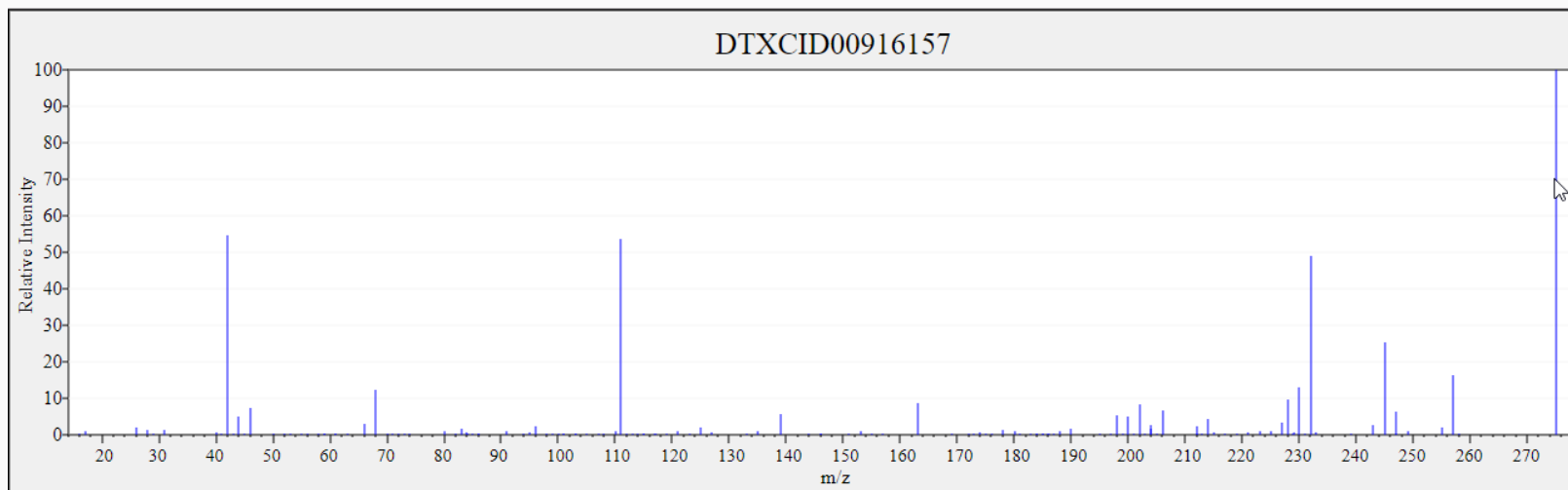
- **CFM-ID**
 - Viewing and Downloading pre-predicted spectra
 - Search spectra against the database
- **Structure/substructure/similarity search**
- **pKa prediction**

Predicted Mass Spectra

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

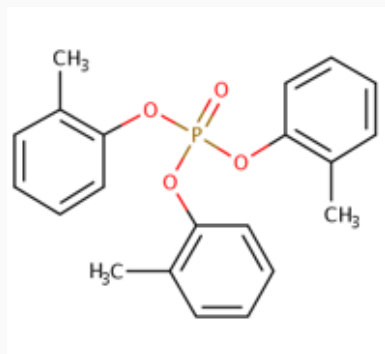


- MS/MS spectra prediction for ESI+, ESI-, and EI
- Predictions generated and stored for >700,000 structures, to be accessible via Dashboard

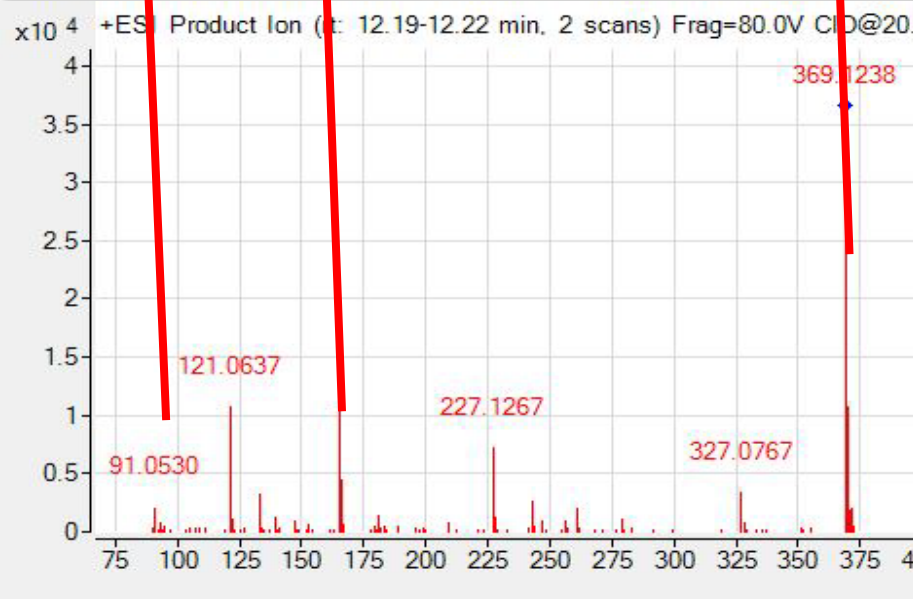
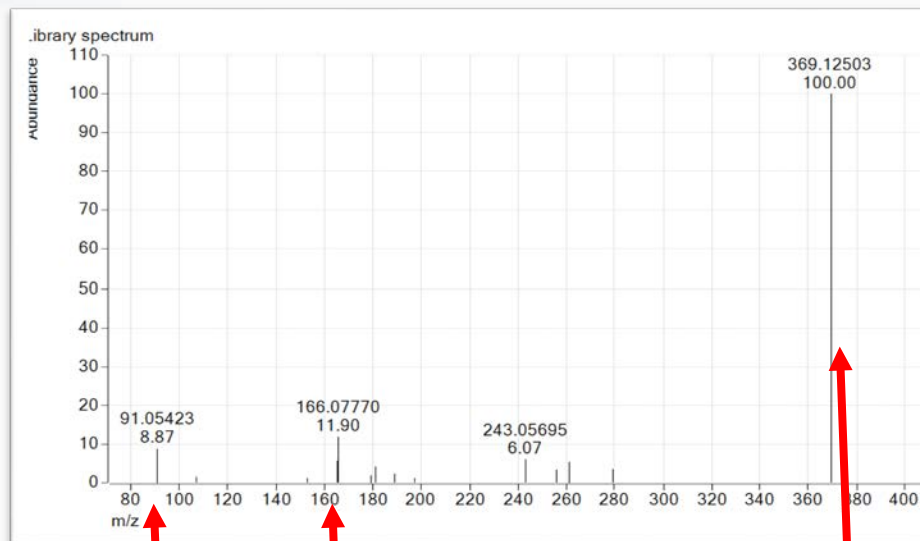


Predicted Mass Spectra

Library Fragmentation
Spectra (20eV)



Observed Fragmentation
Spectra (20eV)



Match
Score

Search Expt. vs. Predicted Spectra

Mass Search

Min/Max

Mass Da Error Da ppm

Molecular Formula Search

Molecular Formula

Mass or Formula must be entered before searching spectrum

Ionization Type

ESI+

Spectra Input

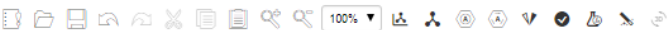

Single Energy

Peak Match Window: Da ppm

Prototype Development

AADashboard

atrazine Search

100%  


Select properties to predict

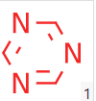
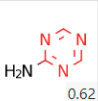
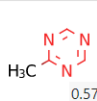
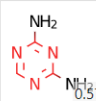
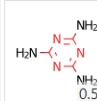
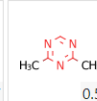
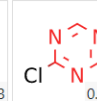
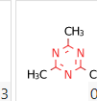
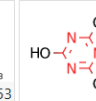
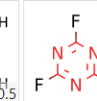
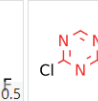
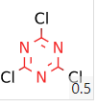
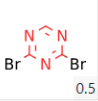

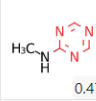
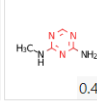
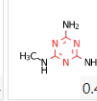
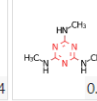
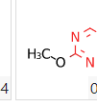
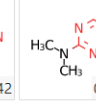
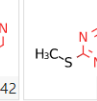
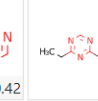
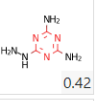
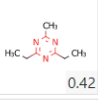
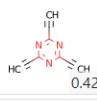
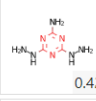
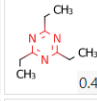
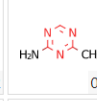
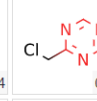
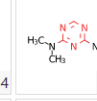
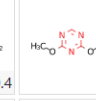
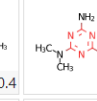
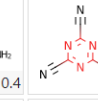
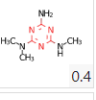
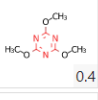
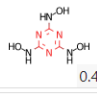
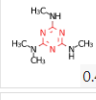
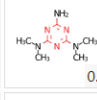
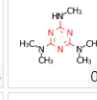
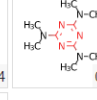
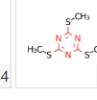
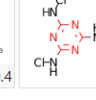
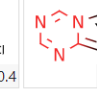
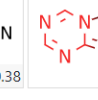
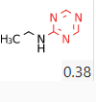
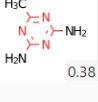
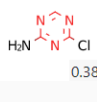
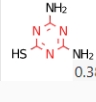
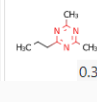
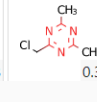

H T.E.S.T. 18 OPERA Search

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				

Search result 2540 Show Isotopically Labeled

Prototype Development

atrazine Search

100%

Select properties to predict

H T.E.S.T. 18 OPERA Search

C

N

O

S

P

F

Cl

Br

Exact

Substructure

Similarity

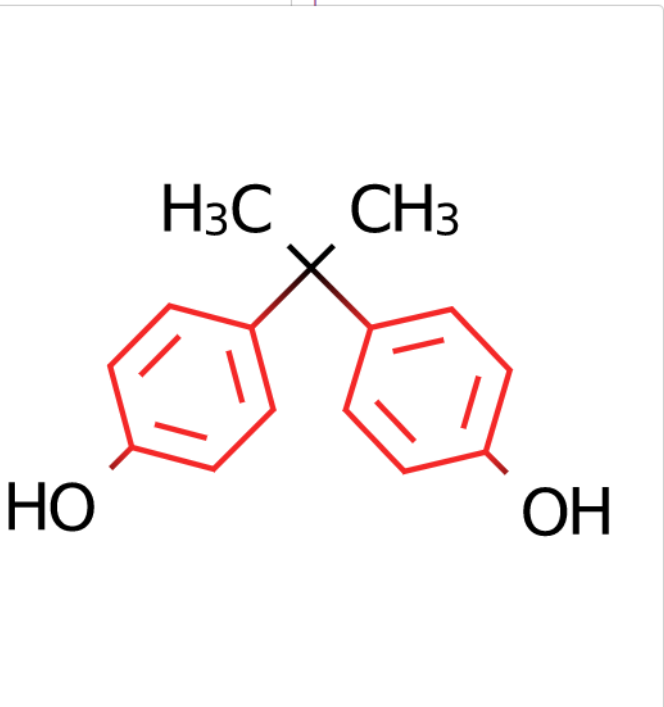
Molecular Formula

Molecular Weight

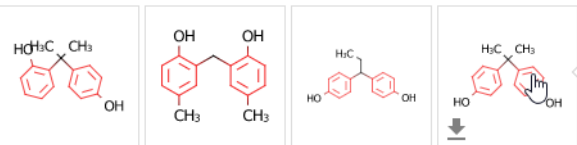
Input formula (e.g. C6 H6):

C15H16O2

Search



Search result 5 Show Isotopically Labeled Cl

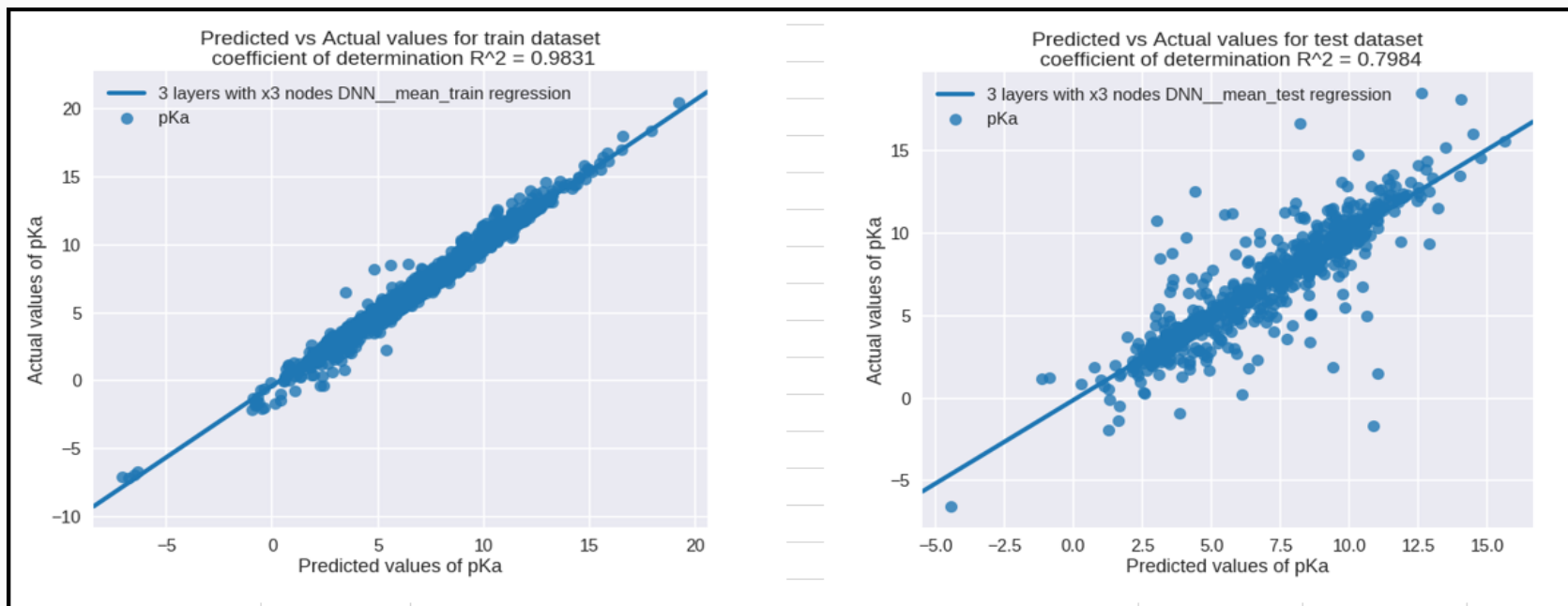


Elements per page 50

1

<https://comptox.epa.gov/dashboard/DTXSID7020182>

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



- The last public release of ToxCast data (invitroDB_v2) was in 3rd Quarter of 2015
- The next release invitroDB_v3 is Fall 2018
- Data includes new assays, new chemicals, new pipelining, results of data curation
- Data will also release via CompTox Dashboard
- Data will be available at <https://www.epa.gov/chemical-research/exploring-toxcast-data-downloadable-data>

Downloadable Data Being Updated

Chemistry Dashboard

Downloads

[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	casn	dssstox_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

- The CompTox Chemistry Dashboard provides access to data for ~765,000 chemicals
- An expanding list of data types and sources has been integrated
- New searches based on Product Use and Categories and Assay and Gene
- The chemical lists of interest grows with each release
- Next release scheduled for Fall 2018 with InvitroDB_v3 data – more chemicals, more assays

Williams et al. *J Cheminform* (2017) 9:61
DOI 10.1186/s13321-017-0247-6


 Journal of Cheminformatics

DATABASE

Open Access



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

Antony J. Williams^{1*} , Christopher M. Grulke¹, Jeff Edwards¹, Andrew D. McEachran², Kamel Mansouri^{1,2,4}, Nancy C. Baker³, Grace Patlewicz¹, Imran Shah¹, John F. Wambaugh¹, Richard S. Judson¹ and Ann M. Richard¹

- Our NCCT CompTox Chemical Dashboard Development and IT Team
- The NCCT Team of Scientists
- NERL scientists - Mass Spectrometry
- Kamel Mansouri – OPERA models
- Todd Martin – TEST predictions

Antony Williams

US EPA Office of Research and Development

National Center for Computational Toxicology (NCCT)

Williams.Antony@epa.gov

ORCID: <https://orcid.org/0000-0002-2668-4821>