

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

The CompTox Portal

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



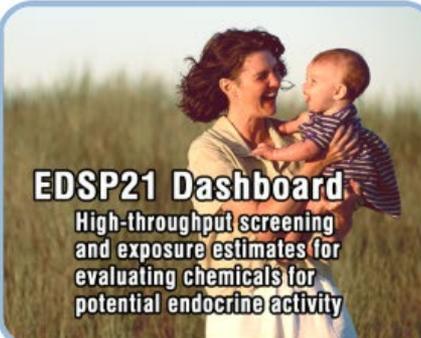
**CompTox
Chemicals
Dashboard**



**Aggregated
Publicly Available
Chemical Data
ACToR**



**ToxCast
Dashboard
High-throughput
screening data**



EDSP21 Dashboard
High-throughput screening
and exposure estimates for
evaluating chemicals for
potential endocrine activity



RapidTox
Decision support workflows
to integrate chemistry,
toxicity, and exposure
information



Downloadable Data

- A **publicly accessible website** delivering access:
 - ~**765,000 chemicals** with related property data
 - Experimental and predicted physicochemical property data
 - Experimental Human and Ecological hazard data
 - Integration to “biological assay data” for 1000s of chemicals
 - Information regarding consumer products containing chemicals
 - Links to other agency websites and public data resources
 - “Literature” searches for chemicals using public resources
 - “Batch searching” for thousands of chemicals
 - Real time prediction of physchem and toxicity endpoints

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

CompTox Chemicals Dashboard

https://comptox.epa.gov/dashboard



762 Thousand Chemicals

Chemicals Product/Use Categories Assay/Gene

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

Identifier substring search

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

Latest News

[Read more news](#)

YouTube video regarding using the Dashboard for Non-Targeted Analysis

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

Ar
Mar

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.](#)



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CompTox Dashboard Chemicals

 United States Environmental Protection Agency

Home Advanced Search Batch Search Lists ▼ Predictions Downloads Share ▼

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

762 Thousand Chemicals

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-prod.epa.gov/dashboard

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

Q estrogen

GENE: ESR1
estrogen receptor 1

GENE: ESR2
estrogen receptor 2 (ER beta)

GENE: ESRR A
estrogen-related receptor alpha

GENE: ESRR B
estrogen-related receptor beta

GENE: ESRR G
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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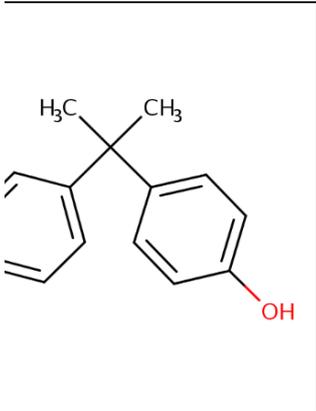
Detailed Chemical Pages New User Interface Design

- 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	<u>BMDL-10</u>	-	chronic	0.609	mg/kg-day	human	-	mouse	EFSA CEF	EFSA
	5	<u>NOEL</u>	Systemic	repeat dose	3.75	mg/kg-day	repeat dose toxicity : oral	oral	rat	-	ECHA
	6	<u>NOAEL</u>	-	reproductive	3.75	mg/kg-day	reproductive	oral	rat	-	HPVIS
	5	<u>NOEL</u>	Systemic	repeat dose	3.75	mg/kg-day	repeat dose toxicity : oral	oral	rat	-	ECHA
	5	<u>NOEL</u>	Systemic	repeat dose	4.5	mg/kg-day	repeat dose toxicity : oral	oral	mouse	-	ECHA
	5	<u>NOEL</u>	Systemic	repeat dose	4.5	mg/kg-day	repeat dose toxicity : oral	oral	mouse	-	ECHA
	7	<u>LEL</u>	-	subchronic	5	mg/kg-day	subchronic	oral	rat	unpublished_submission	ToxRefDB
	7	<u>nel</u>	-	chronic	5	mg/kg-day	reproductive multigeneration	oral	rat	open_lit	ToxRefDB
	5	<u>NOAEL</u>	-	chronic	5	mg/kg-day	human	-	mouse	EFSA AFC	EFSA
	7	<u>nel</u>	-	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

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

EXPOSURE

PRODUCT & USE CATEGORIES

CHEMICAL WEIGHT FRACTION

CHEMICAL FUNCTIONAL USE

TOXICS RELEASE INVENTORY

MONITORING DATA

EXPOSURE PREDICTIONS

PRODUCTION VOLUME

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

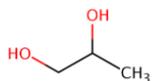
182 chemicals

Download / Send

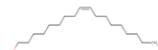
Show info: **DTXSID** **CASRN** **TOXCAST** Select all

Sort by: **DTXSID**

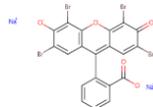
Filter by: Name or CASRN Hide



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



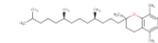
cis-Oleyl alcohol
DTXSID: DTXSID0022010
CASRN: 143-28-2
TOXCAST: 0



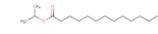
Eosin
DTXSID: DTXSID0025234
CASRN: 17372-87-1
TOXCAST: 45/302

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

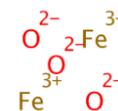
Paraffin waxes and Hydrocarbon waxes...
DTXSID: DTXSID0028115
CASRN: 63231-60-7
TOXCAST: 0

1 related chemical
structure with this
substance

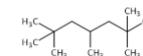
Alcohols, C16-18
DTXSID: DTXSID0028323
CASRN: 67762-27-0
TOXCAST: 1/163

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



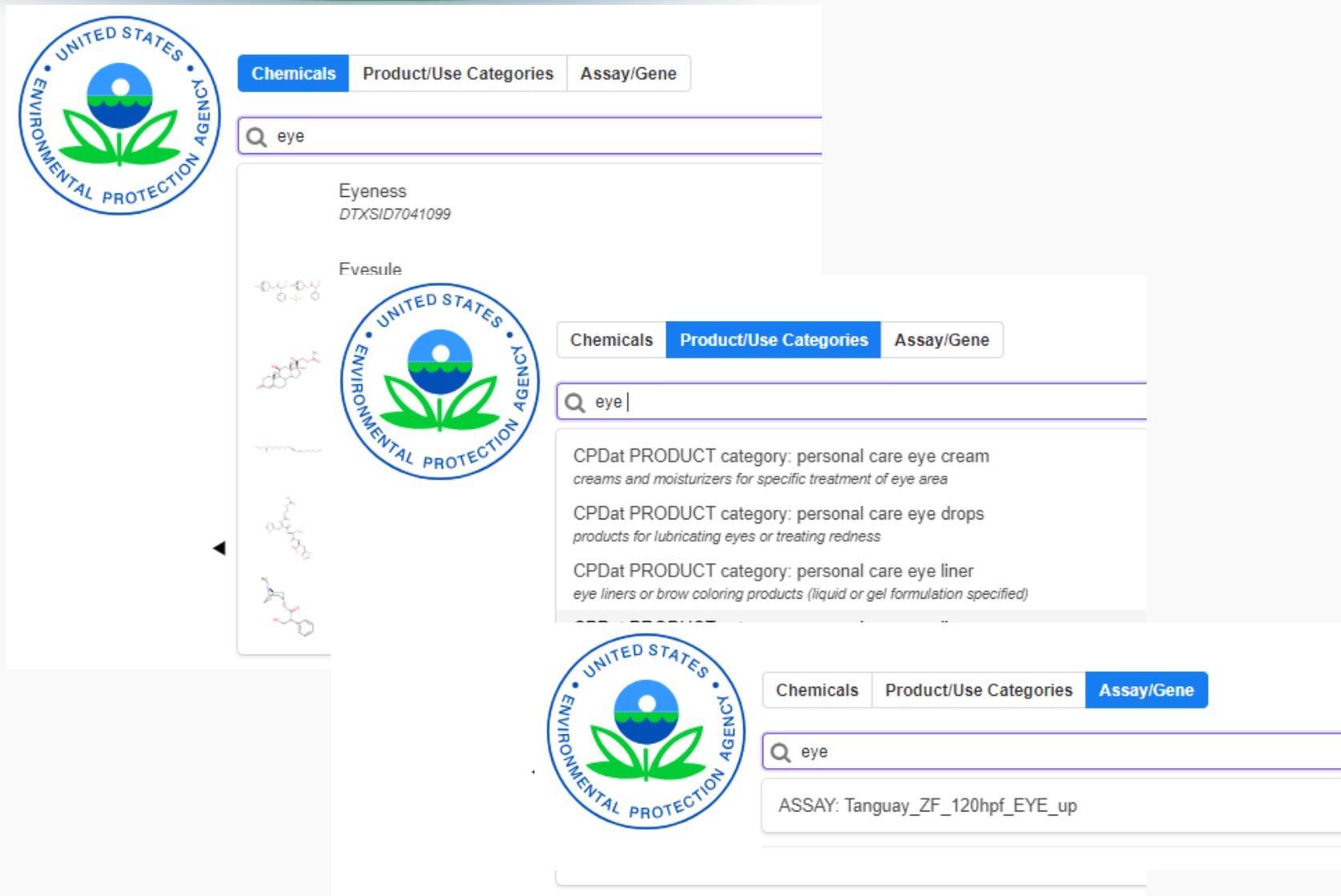
2,2,4,6,6-Pentamethylheptane
DTXSID: DTXSID0042034
CASRN: 13475-82-6
TOXCAST: 0



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

Remember home page searches

Searching for “eye” ...



The image shows three overlapping screenshots of the EPA's search interface. The top-left screenshot shows the search results for 'eye', listing 'Eyeness' (DTXSID7041099) and 'Evesule' with chemical structures. The top-right screenshot shows the search bar with 'eye' and the 'Product/Use Categories' tab selected, displaying CPDat product categories for eye cream, eye drops, and eye liner. The bottom screenshot shows the search bar with 'eye' and the 'Assay/Gene' tab selected, displaying the result 'ASSAY: Tanguay_ZF_120hpf_EYE_up'.

Chemicals Product/Use Categories Assay/Gene

Q eye

Eyeness
DTXSID7041099

Evesule

Chemicals Product/Use Categories Assay/Gene

Q eye |

CPDat PRODUCT category: personal care eye cream
creams and moisturizers for specific treatment of eye area

CPDat PRODUCT category: personal care eye drops
products for lubricating eyes or treating redness

CPDat PRODUCT category: personal care eye liner
eye liners or brow coloring products (liquid or gel formulation specified)

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

Q eye

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

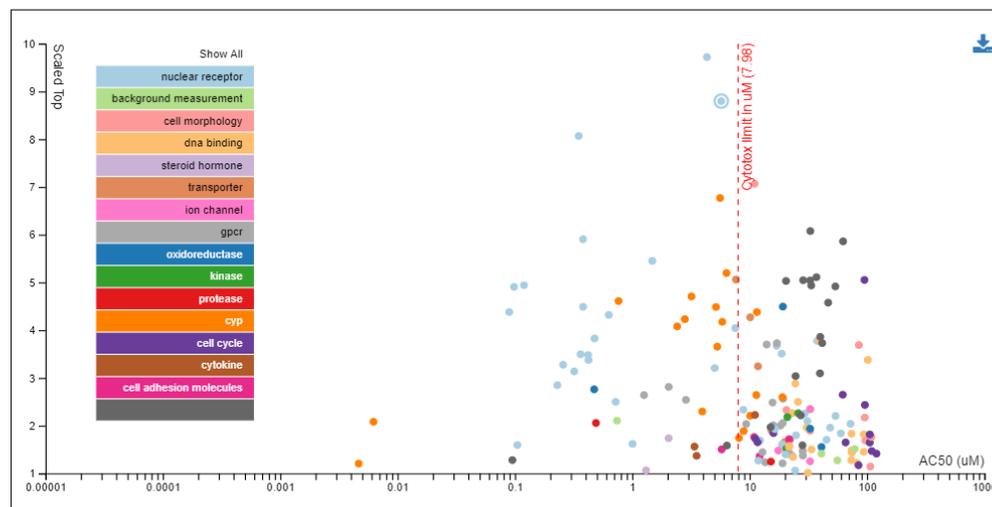
SIMILAR COMPOUNDS

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
-	-	-	-	-	ACTIVE	4.49	5.05	95.2	1.98	cell cycle
-	-	-	-	-	ACTIVE	2.71	3.69	85.3	1.93	cell morphology
-	-	-	-	-	ACTIVE	1.66	1.17	84.7	1.93	cell cycle
-	-	-	-	-	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

In Vitro Bioassay Screening

ToxCast and Tox21

Download

Columns 10

Search query 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

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Bisphenol A

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

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

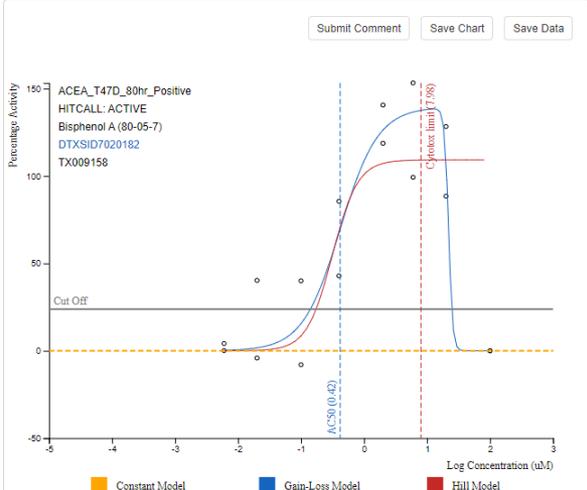
Assay Selection 1 Selected A Single Assay Can Have Multiple Charts Number of Charts: 6

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

ACEA_T47D_80hr_Positive
HITCALL: ACTIVE
Bisphenol A (80-05-7)
DTXSID7020182
TX009158



Submit Comment Save Chart Save Data

Percentage Activity

Log Concentration (µM)

Constant Model Gain-Loss Model Hill Model



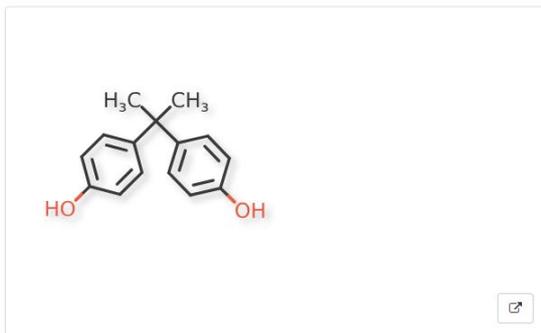
Structure Search

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

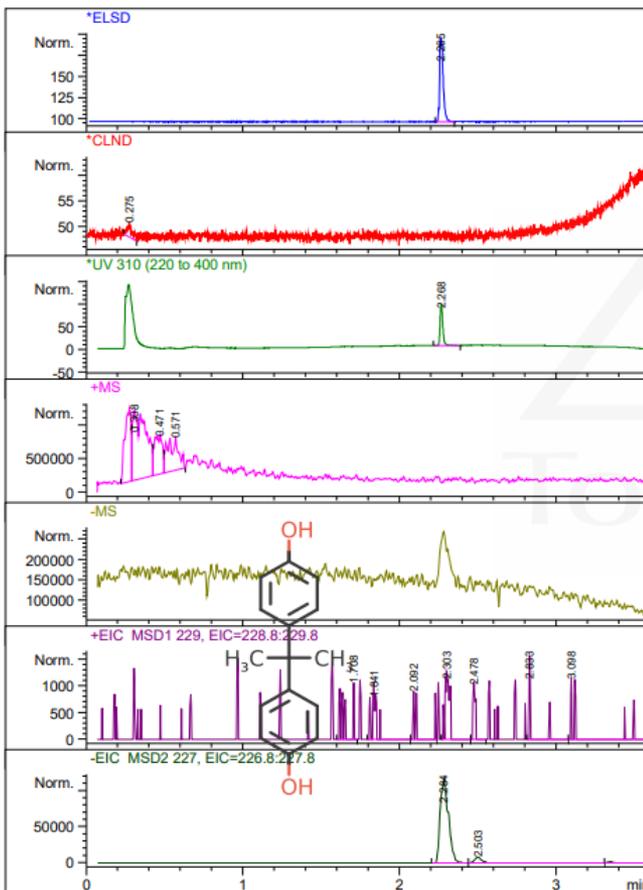
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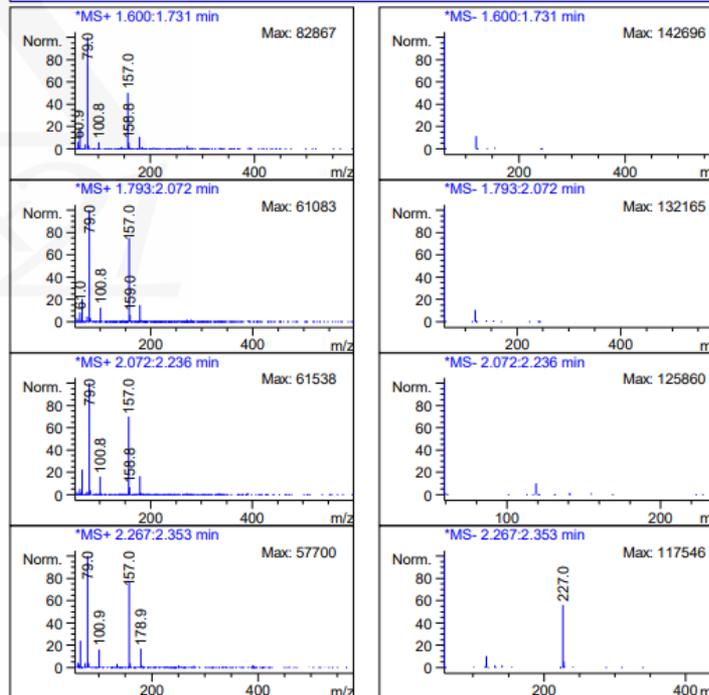
Access to Analytical QC Data

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



A MW Confirmed, Purity >90%

OpAns_Process.MAC Version A.01.10 - Dec 9, 2010



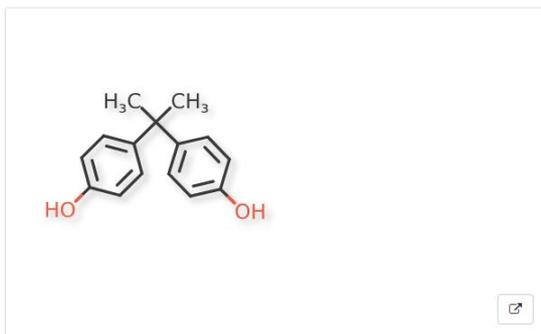
Structure Search

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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In Vitro Bioassay Screening

ToxCast and Tox21

 United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Copy Share Submit Comment Search all data

Bisphenol A

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

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

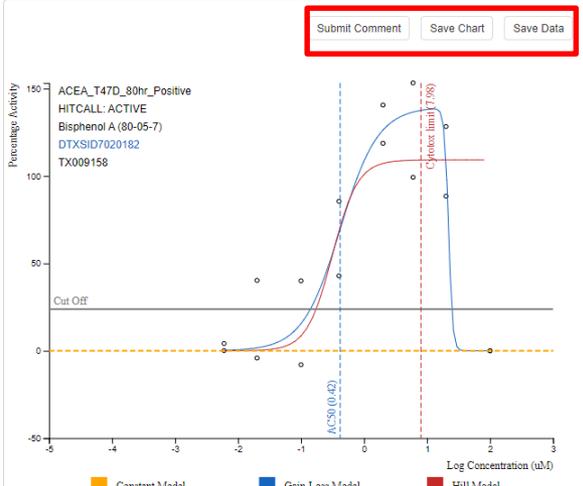
Active Inactive All
Filter

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

Submit Comment Save Chart Save Data



ACEA_T47D_80hr_Positive
HITCALL: ACTIVE
Bisphenol A (80-05-7)
DTXSID7020182
TX009158

Cut Off

AC50 (0.42) Cmax (7.96)

Percentage Activity

Log Concentration (µM)

Constant Model Gain-Loss Model Hill Model

In Vitro Bioassay Screening

ToxCast and Tox21

 United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Copy Share Submit Comment Search all data

Bisphenol A

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

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

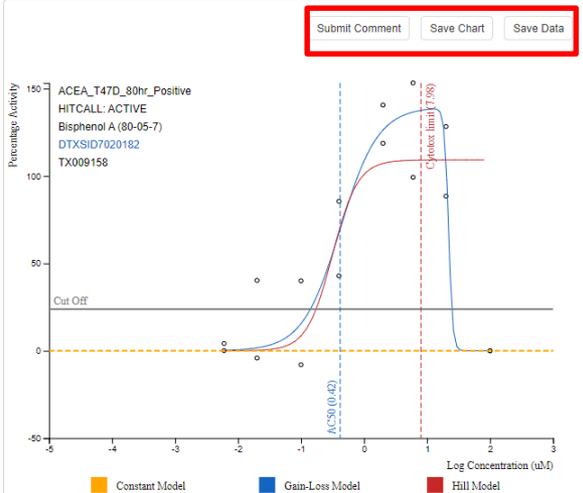
Assay Selection 1 Selected ← A Single Assay Can Have Multiple Charts Number of Charts: 6

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



Submit Comment Save Chart Save Data

ACEA_T47D_80hr_Positive
HITCALL: ACTIVE
Bisphenol A (80-05-7)
DTXSID7020182
TX009158

Percentage Activity

Log Concentration (uM)

Legend: Constant Model, Gain-Loss Model, Hill Model

Assay Modal Details

All Chemicals in Assay Endpoint: ACEA_T47D_80hr_Negative

Annotations Citations tcpl Processing Reagents AOPs

Excel

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.	

All Chemicals in Assay Endpoint: ACEA_T47D_80hr_Negative

Annotations Citations tcpl Processing Reagents AOPs

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.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)

All Chemicals in Assay Endpoint: ACEA_T47D_80hr_Negative

Annotations Citations tcpl Processing Reagents AOPs

- 4 MULTI
- 5 MULTI
- 6 MULTI
- 7 MULTI
- 8 MULTI

	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.

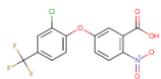
1813 chemicals

Download / Send 

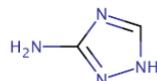
Show info: DTXSID x CASRN x TOXCAST x  Select all 

Sort by: DTXSID  

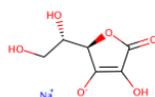
Filter by: Name or CASRN Hide 



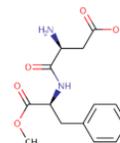
Acifluorfen
DTXSID: DTXSID0020022
CASRN: 50594-66-6
TOXCAST: 23/694



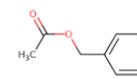
Amitrole
DTXSID: DTXSID0020076
CASRN: 61-82-5
TOXCAST: 1/303



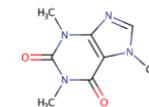
Sodium L-ascorbate
DTXSID: DTXSID0020105
CASRN: 134-03-2
TOXCAST: 19/561



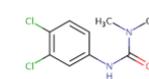
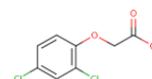
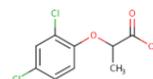
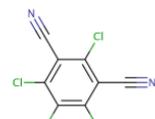
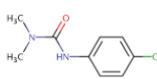
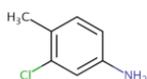
Aspartame
DTXSID: DTXSID0020107
CASRN: 22839-47-0
TOXCAST: 1/296



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



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



Choose Display Details

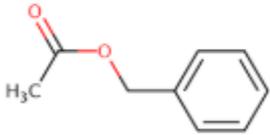
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Filter by:

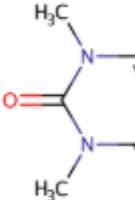
Hide ▲

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

107



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



Caffeine
DTXSID:
CASRN:
TOXCAST: 21/546

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

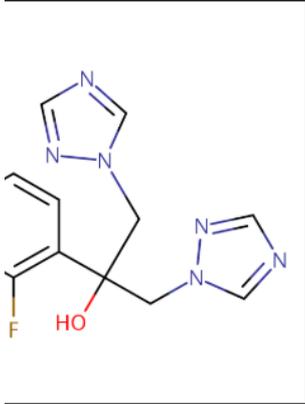
GenRA (Generalised Read-Across)

- 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

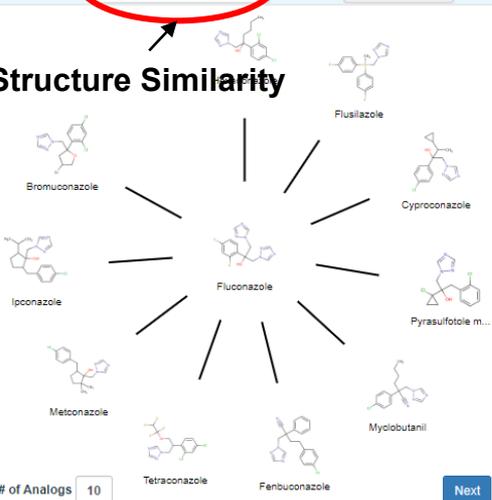
Searched by DSSTox Substance Id.

- 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

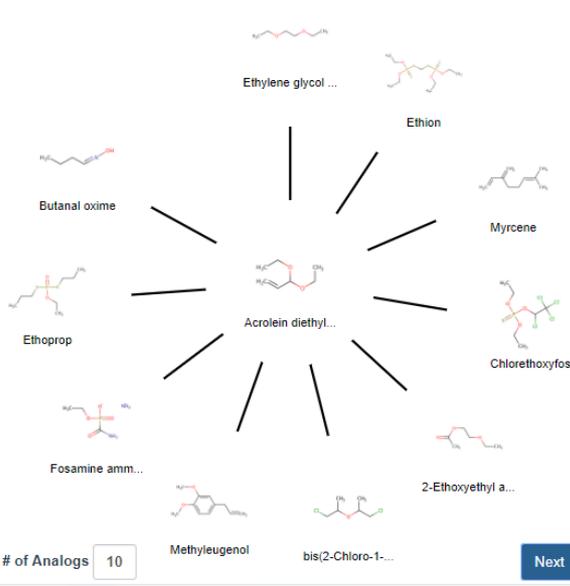
Select and Review Analogs

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	chl_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											
CHR:Adrenal Gland											
CHR:Artery (General)											
CHR:Auditory Startle Re...											
CHR:Bile duct											
CHR:Blood											
CHR:Blood vessel											
CHR:Body Weight											
CHR:Bone											
CHR:Bone Marrow											
CHR:Brain											
CHR:Tracheus											

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

Summary Data Gap Analysis:

bio_tox21	14	0	4	0
bio_tox	7	0	4	95
chem_ct				
tox_l_tox				

Source analogues: Acrolein diethylacetal, Ethylene glycol diethyl e..., Ethion, Myrcene, Chloretoxyfats, 2-Ethoxyethyl acetate, bis(2-Chloro-1-meth..., Methylcyclopent..., Fosamine ammonium, Ethionprop, Butanal oxime

Run Read-Across (circled in red)

Target: Fluconazole

Similarity Weight: 0.39 ✓, 0.31 ✓, 0.29 ✓, 0.29 ✓, 0.26 ✓, 0.24 ✓, 0.22 ✓, 0.21 ✓, 0.21 ✓, 0.20 ✓ (circled in red with arrow)

	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	Blue	Blue	Blue	Blue	Red
CHR:Bone	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue	Blue

Run GenRA

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

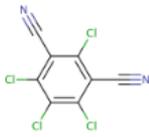
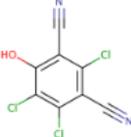
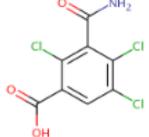
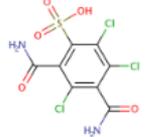
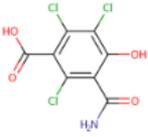
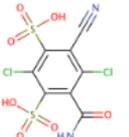
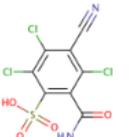
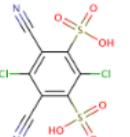
8 chemicals

Download / Send

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

Sort by: Relationship

Filter by:

Searched Chemical	Transformation Product	Transformation Product	Transformation Product	Transformation Product
 <p>Chlorothalonil DTXSID: DTXSID0020319 CASRN: 1897-45-6</p>	 <p>4-Hydroxy-2,5,6-trichloroisophthalonitrile DTXSID: DTXSID00182588 CASRN: 28343-81-6</p>	 <p>3-Carbamoyl-2,4,5-trichlorobenzoic acid DTXSID: DTXSID10597537 CASRN: 142733-37-7</p>	 <p>2,4-dicarbamoyl-3,5,6-trichlorobenzene DTXSID: DTXSID30891327 CASRN: NOCAS_891327</p>	 <p>3-carbamoyl-2,5,6-trichloro-4-hydroxybenzoic acid DTXSID: DTXSID00891328 CASRN: NOCAS_891328</p>
 <p>4-carbamoyl-2,5-dichloro-6-cyanobenzamide DTXSID: DTXSID00891329 CASRN: NOCAS_891329</p>	 <p>2-carbamoyl-3,5,6-trichloro-4-cyanobenzamide DTXSID: DTXSID00891330 CASRN: NOCAS_891330</p>	 <p>2,5-dichloro-4,6-dicyanobenzene-1,3-diamine DTXSID: DTXSID20891331 CASRN: NOCAS_891331</p>		

(C10-C16) Alkylbenzenesulfonic acid

68584-22-5 | DTXSID2028723

Searched by CAS-RN.

DETAILS

[RELATED SUBSTANCES](#)

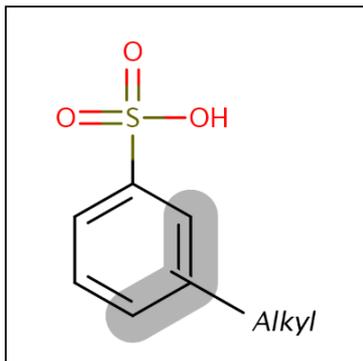
[PROPERTIES](#)

[ENV. FATE/TRANSPORT](#)

[BIOACTIVITY](#)

[SYNONYMS](#)

[COMMENTS](#)



Intrinsic Properties

Molecular Formula: Not Found

Average Mass: 0 g/mol

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

EPA United States Environmental Protection Agency

Home Advanced Search Batch Search Lists Predictions Downloads

Copy Share Submit Comment Search all data

27 chemicals

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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

GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

▶ LITERATURE

LINKS

COMMENTS

25

Search query

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 Belstein Registry Number

Belstein

(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

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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

List of Chemicals

Lists of Chemicals

List of Assays

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

Algal Toxins

54 chemicals

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Show info:

DTXSID

CASRN

Select all



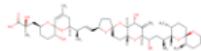
Sort by:

DTXSID

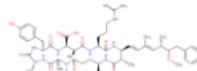


Filter by: Name or CASRN

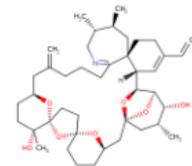
Hide



Dinophysistoxin 1
DTXSID: DTXSID00880001
CASRN: 81720-10-7



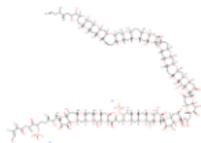
Microcystin YR
DTXSID: DTXSID00880086
CASRN: 101064-48-6



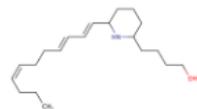
Pinnatoxin G
DTXSID: DTXSID00880102
CASRN: NOCAS_880102



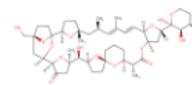
CTX 4B
DTXSID: DTXSID00880107
CASRN: 123676-76-6



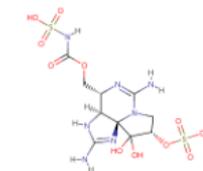
Maitotoxin
DTXSID: DTXSID10880012
CASRN: 59392-53-9



Euglenophycin
DTXSID: DTXSID10880017
CASRN: 1219817-69-2



Peclenotoxin-1
DTXSID: DTXSID10880092
CASRN: 97564-90-4



Gonyautoxin
DTXSID: DTXSID10880097
CASRN: 80226-62-6

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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](#) 

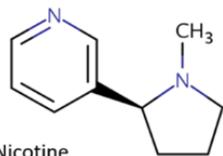
Journal of Cheminformatics 2018 **10**:45

<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

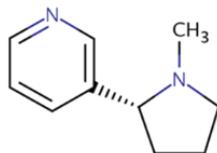
MS-Ready Structures

Exact Formula Match and MS-Ready Match



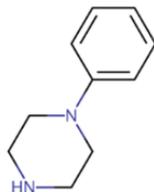
Nicotine

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



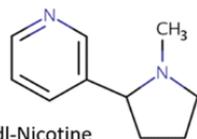
D-Nicotine

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



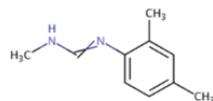
Phenylpiperazine

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



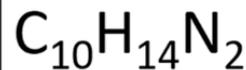
dl-Nicotine

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

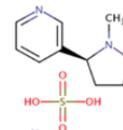


N'-(2,4-Dimethylphenyl)-N-methylformamide

DTXSID1037696 | DTXCID9017696
Tox: no | Expo: Yes | Bioassay: yes
 $C_{10}H_{14}N_2$ | 33089-74-6 | 27

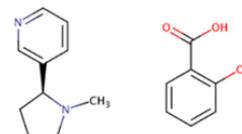


MS-Ready Match Only



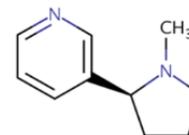
Nicotine sulfate

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

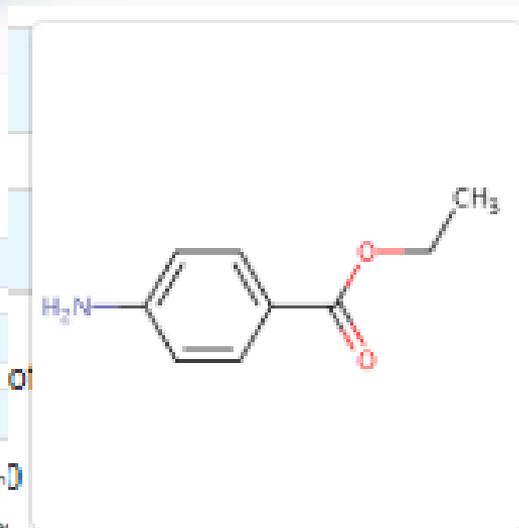
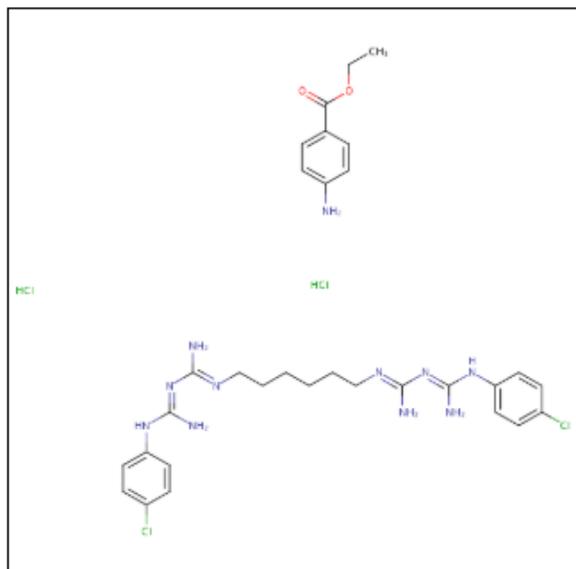
LEGEND: Preferred Name
DTXSID | MS-ready DTXCID
Avail. Data: Toxicity | Exposure | Bioassay
Formula | CAS | Data Sources

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)

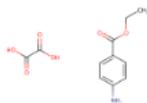
9 of 11 chemicals visible

Download / Send

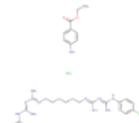
Sort by: DTXSID

Show info: DTXSID CASRN Select all

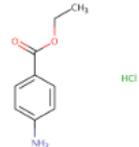
Filter by: Name or CASRN Isotopes



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



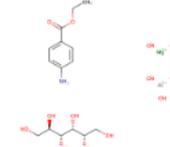
Progaron
DTXSID: DTXSID20148679
CASRN: 108532-15-8



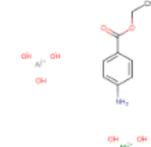
Benzocaine hydrochloride
DTXSID: DTXSID50177812
CASRN: 23239-88-5



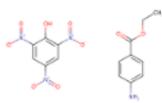
Anesthesine succinate
DTXSID: DTXSID60148336
CASRN: 107948-46-9



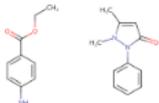
Almagel A-neo
DTXSID: DTXSID80227559
CASRN: 76741-92-9



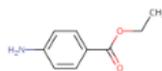
Almagel
DTXSID: DTXSID70227680
CASRN: 76741-95-2



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



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



Benzocaine
DTXSID: DTXSID8021804
CASRN: 94-09-7

Mass and Formula Searches Supporting Mass Spectrometry

Advanced Search

Mass Search

Select Adduct: ▼

Da

Molecular Formula Search

MS Ready Formula 

Exact Formula 

Generate Molecular Formula(e)

Da

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

Search Results

Searched by Mass: 191.131 +/- 5.0 ppm.

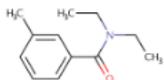
298 of 298 chemicals visible

Download / Send

Show info:

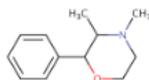
Sort by:

Filter by:



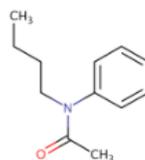
DEET

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TOXCAST: 14/663
Mass Diff: 0.000014



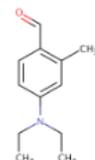
Phendimetrazine

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



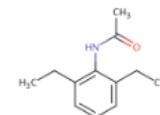
N-Butylacetanilide

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



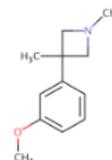
Benzaldehyde, 4-(diethylamino)-2-methyl-

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



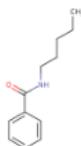
Acetanilide, 2',6'-diethyl-

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



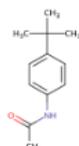
Azetidine, 1,3-dimethyl-3-(m-methoxyphenyl)-

DTXSID: DTXSID40173560
CASRN: 19832-26-9
TOXCAST: 0
Mass Diff: 0.000014



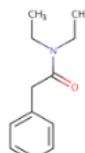
Benzamide, N-pentyl-

DTXSID: DTXSID20174198
CASRN: 20308-43-4



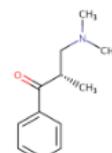
p-t-Butylacetanilide

DTXSID: DTXSID80174238
CASRN: 20330-45-4



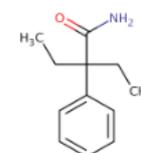
N,N-Diethylphenylacetamide

DTXSID: DTXSID00179048
CASRN: 2431-98-1



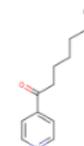
3-(Dimethylamino)-2-methylpropiofenone

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

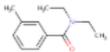
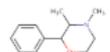
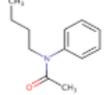
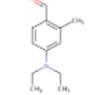
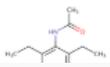


Sort by: Mass Difference



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

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

- ~3000 chemicals added since last release
- Human and Ecological hazard data added and curated
- PFAS lists added (and many others)
- Production volume data added

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

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

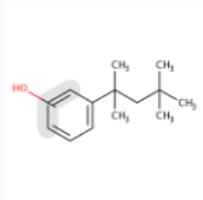
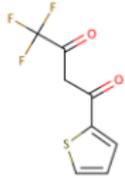
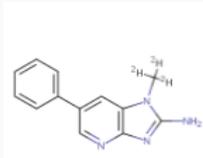
Public Crowdsourced Comments

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>3</sup>)-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

Submit

A List of Lists of Chemicals

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



Home

Advanced Search

Batch Search

Lists

Predictions

Downloads

Search All Data



Chemistry Dashboard

Aa ▾

Aa

Aa ▲

Select List



List Name ▲	Number of Chemicals ▲	List Description
40CFR355	354	Extremely Hazardous Substance List and Threshold Planning Quantities; Emergency Planning and Release Notification Requirements; Final Rule. (52 FR 13378)
Algal Toxins	54	A set of algal toxins of interest
Androgen Receptor Chemicals	110	The list of chemicals used to identify references with in vitro AR binding . From Kleinstrauer et al http://pubs.acs.org/doi/abs/10.1021/acs.chemrestox.6b00347
ATSDR Toxic Substances Portal Chemical List	200	The Agency for Toxic Substances and Disease Registry (ATSDR) is a federal public health agency of the U.S. Department of Health and Human Services.
Bisphenol Compounds	52	This list represents a collection of Bisphenol Compounds
California Office of Environmental Health Hazard Assessment	972	The OEHHA Chemical Database is a compilation of health hazard information including reference exposure levels, California public health goals, child-specific reference doses, Propos. 65 safe harbor numbers, soil-screening levels, and fish advisories
Chemicals with interesting names	17	This is a list of chemicals with interesting and fun names
EPA Integrated Risk Information System (IRIS)	510	EPA's IRIS Program identifies and characterizes the health hazards of chemicals found in the environment. Each IRIS assessment can cover a chemical, a group of related chemicals, or a complex mixture.
EPAHFR - EPA Chemicals associated with hydraulic fracturing	1640	EPAHFR lists chemicals associated with hydraulic fracturing from 2005-20013, as reported in EPA's Hydraulic Fracturing Drinking Water Assessment Final Report (Dec 2016)
EU Cosmetic Ingredients Inventory (Combined 2000/2006)	2878	EUCOSMETICS contains the Combined Inventory of Ingredients Employed in Cosmetic Products (2000, SCCNFP/0389/00 Final) and Revised Inventory (2006, Decision 2006/257/EC), prepared for NORMAN by P. von der Ohe (UBA) and R. Aalizadeh (Uni. Athens).
EU Toxrisk Dataset	230	Compounds of interest to the EU-ToxRisk Case Studies.
French Monitoring List	1171	FRENCHLIST contains substances for prospective monitoring activities in France, developed in cooperation with the NORMAN Network Working Group 1 on Prioritization. Provided by Valeria Dulio, INERIS, France. Further details on the website.

The EPA List of Hydraulic Fracturing Chemicals

EPAHFR - EPA Chemicals associated with hydraulic fracturing

Search EPAHFR Chemicals 

List Details

Description: Chemicals used in hydraulic fracturing fluids and/or identified in produced water from 2005-2013, corresponding to chemicals listed in Appendix H of EPA's Hydraulic Fracturing Drinking Water Assessment Final Report (Dec 2016). Citation: U.S. EPA, Hydraulic Fracturing for Oil and Gas: Impacts from the Hydraulic Fracturing Water Cycle on Drinking Water Resources in the United States (Final Report). U.S. Environmental Protection Agency, Washington, D.C. EPA/600/R-16/236F, 2016. <https://www.epa.gov/hfstudy>

*Note that Appendix H chemical listings in Tables H-2 and H-4 were mapped to current DSSTox content, which has undergone additional curation since the publication of the original EPA HF Report (Dec 2016). In the few cases where a Chemical Name and CASRN from the original report map to distinct substances (as of Jan 2018), both were included in the current EPAHFR chemical listing for completeness; additionally, 34 previously unmapped chemicals in Table H-5 are now registered in DSSTox (all but 2 assigned CASRN) and, thus, have been added to the current EPAHFR listing.

Number of Chemicals: 1640

Download / Send 

Sort by:

DTXSID 



1640 chemicals

Hide:

Select all 

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

Download / Send ▼

Show info:

DTXSID ×

CASRN ×

TOXCAST ×

Select all



Sort by: DTXSID ▼

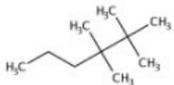
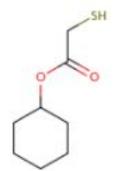
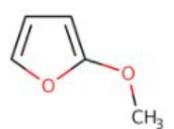
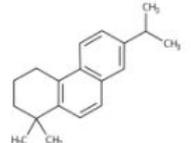
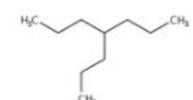
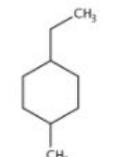
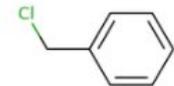
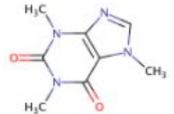


Filter by: Name or CASRN

Hide ▼

The List as "Structures"

Download / Send Sort by: DTXSID 1640 chemicals Hide: Select all

 <p>2,2,3,3-Tetramethylhexane 13475-81-5</p>	 <p>Cyclohexyl mercaptoacetate 16849-98-2</p>	 <p>2-Methoxyfuran 25414-22-6</p>	 <p>Simonellite 27530-79-6</p>	 <p>4-Propylheptane 3178-29-8</p>
 <p>7-Tetradecyne 35216-11-8</p>	 <p>1-Ethyl-4-methylcyclohexane 3728-56-1</p>	 <p>Ammonium chloride 12125-02-9</p>	 <p>Benzyl chloride 100-44-7</p>	 <p>Caffeine 58-08-2</p>

Real Time Predictions

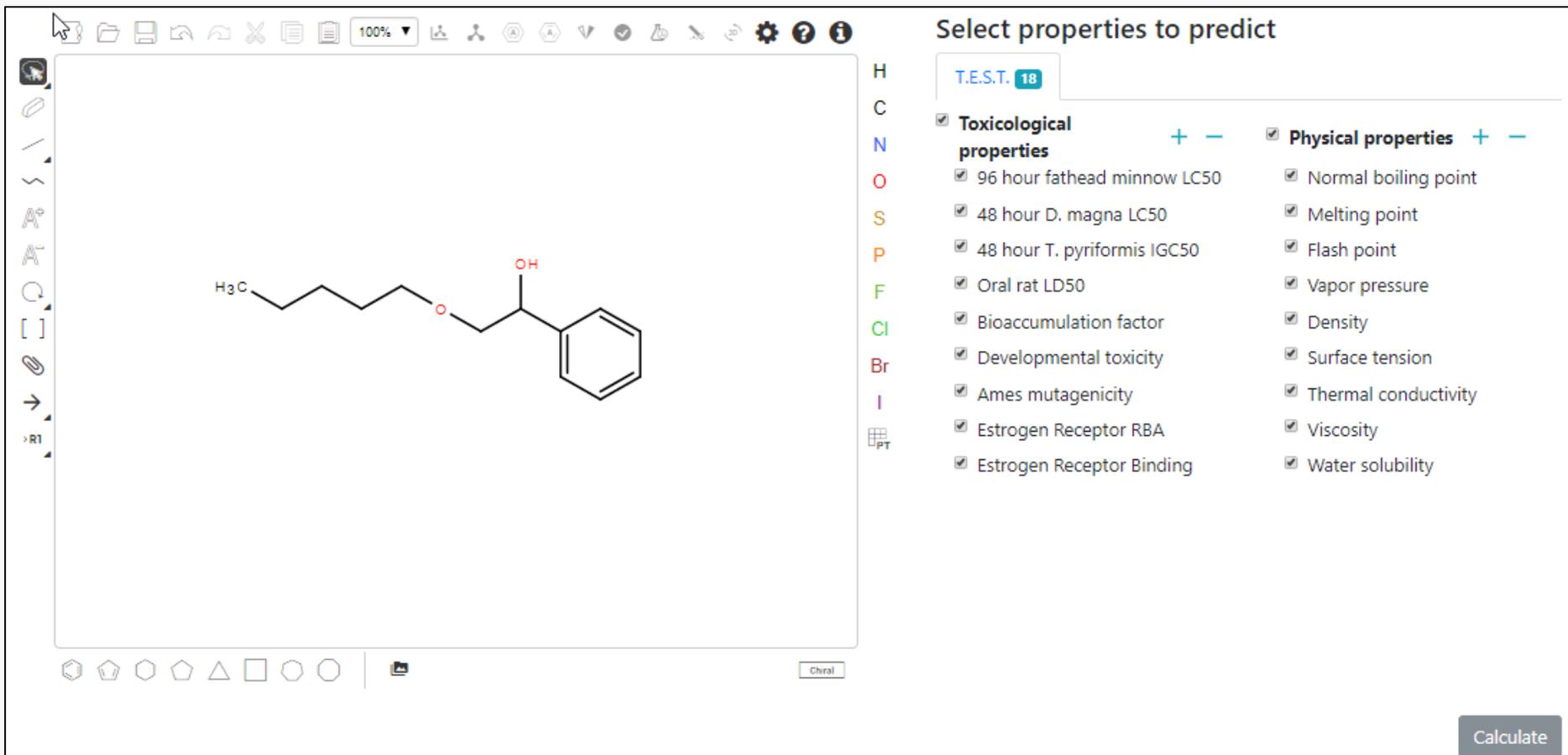
10 Years of EPA T.E.S.T Models



The screenshot shows the EPA website header with the EPA logo and navigation links for Environmental Topics, Laws & Regulations, and About EPA. A search bar is visible on the right. Below the header, there is a section for Related Topics, including Safer Chemicals Research, and social media sharing options for Facebook, Twitter, Pinterest, and Email. The main heading is "Toxicity Estimation Software Tool (TEST)". Underneath, it says "On this page:" followed by two links: "QSAR Methodologies" and "What's New in Version 4.2.1?".

- Over 10 years of QSAR modeling at the desktop – installable Java module (from National Risk Management Research Laboratory)
- Now 750,000 chemicals predicted and real time predictions are available

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

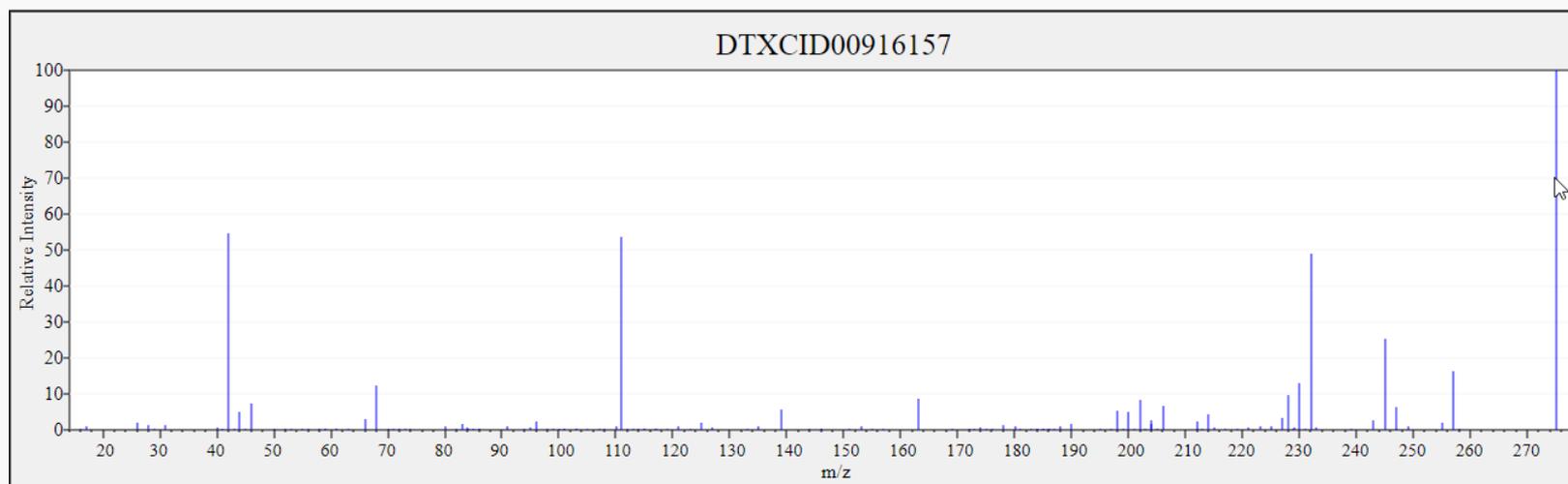
- CFM-ID
 - Viewing and Downloading pre-predicted spectra
 - Search spectra against the database
- Structure/substructure/similarity search
- pKa prediction

Predicted Mass Spectra

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

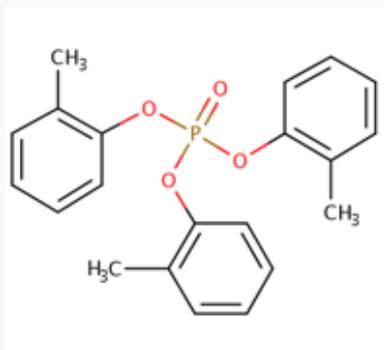


- MS/MS spectra prediction for ESI+, ESI-, and EI
- Predictions generated and stored for >700,000 structures, to be accessible via Dashboard

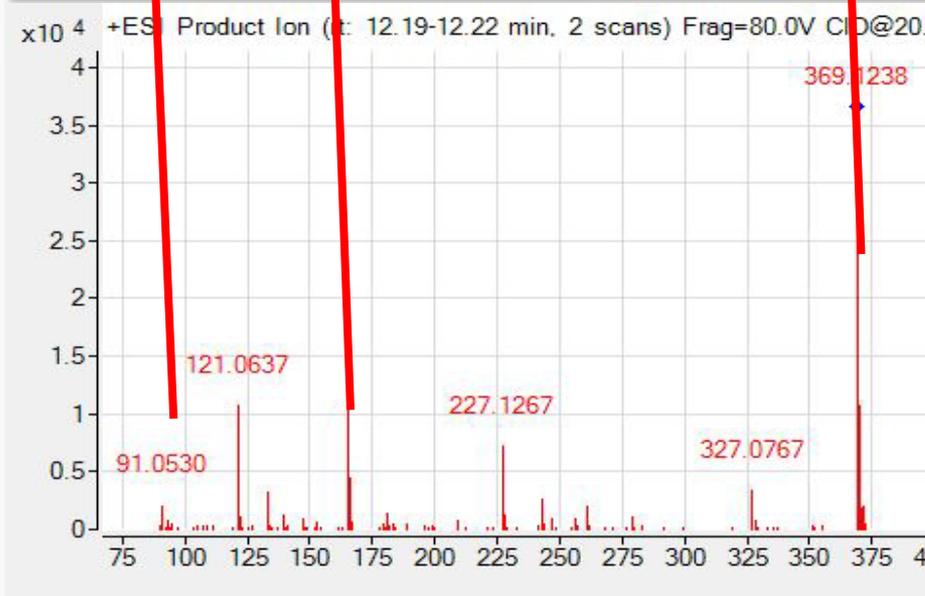
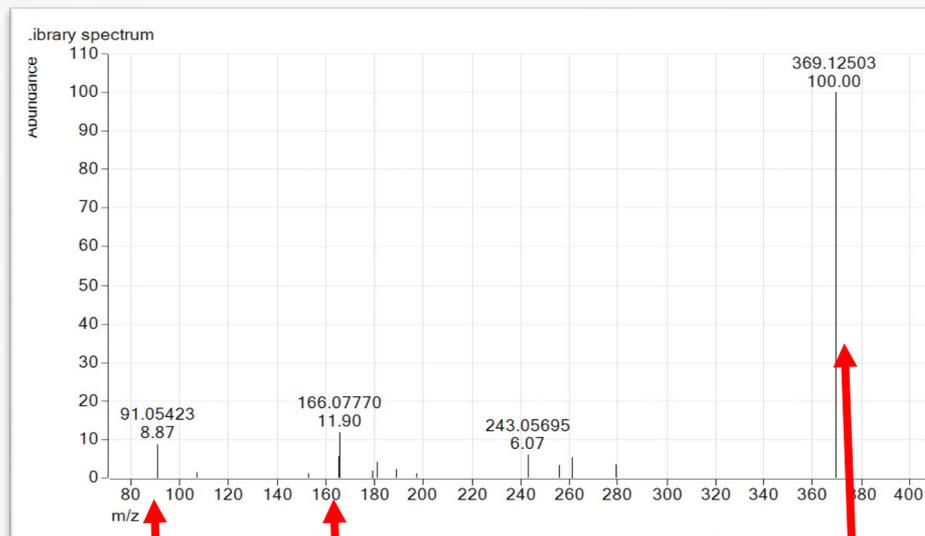


Predicted Mass Spectra

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 Multiple

Peak Match Window:

0.02

Da ppm

Prototype Development

AADashboard

atrazine Search

100%  

Select properties to predict

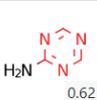
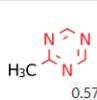
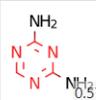
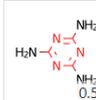
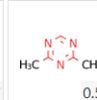
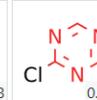
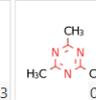
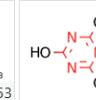
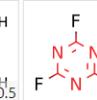
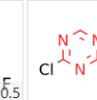
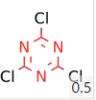
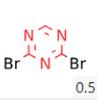
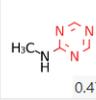
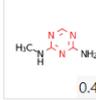
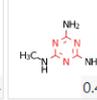
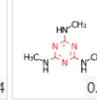
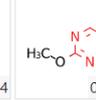
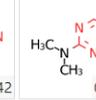
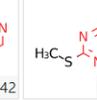
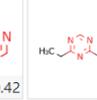
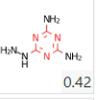
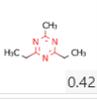
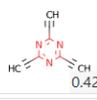
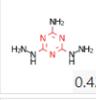
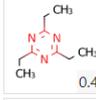
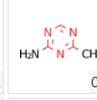
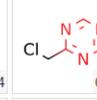
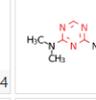
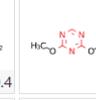
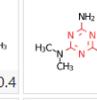
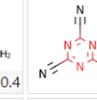
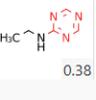
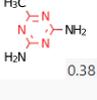
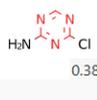
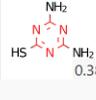
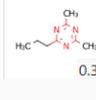
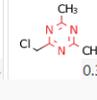
H T.E.S.T. 18 OPERA Search

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	 0.4	 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

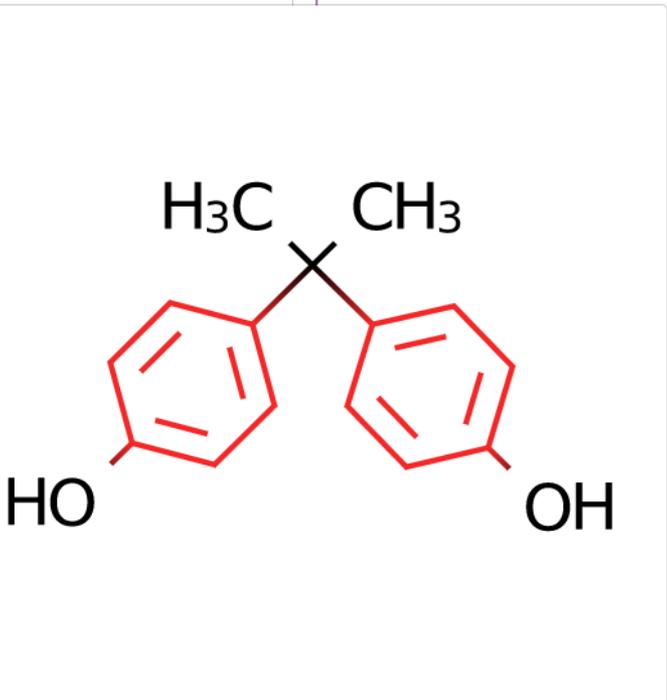
Molecular Formula

Molecular Weight

Input formula (e.g. C6 H6):

C15H16O2

Search



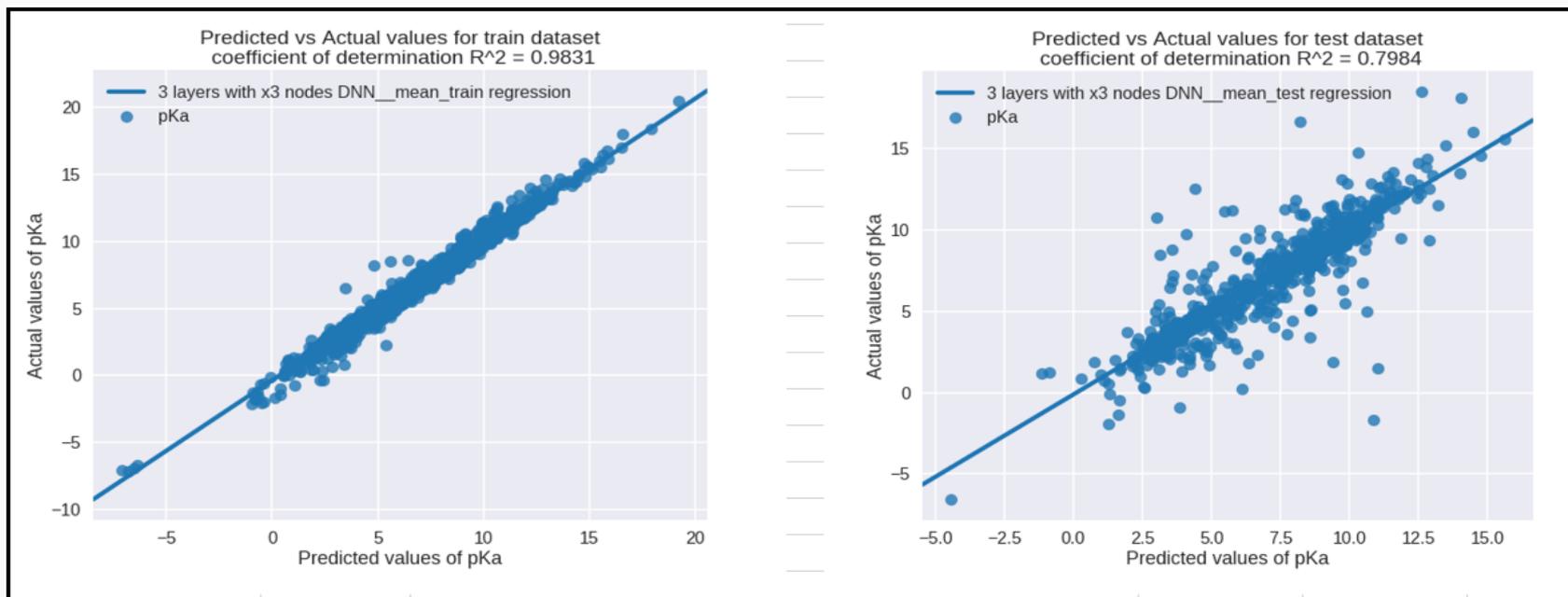
Search result 5 Show Isotopically Labeled Cl

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>

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 ~760,000 chemicals
- An expanding list of data types and sources has been integrated
- The chemical lists of interest grows with each release
- Real time prediction models rollout has started

- Exciting array of additional searches in development

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>