The EPA CompTox Chemicals Dashboard: An Integration Hub for Data Supporting Computational Toxicology

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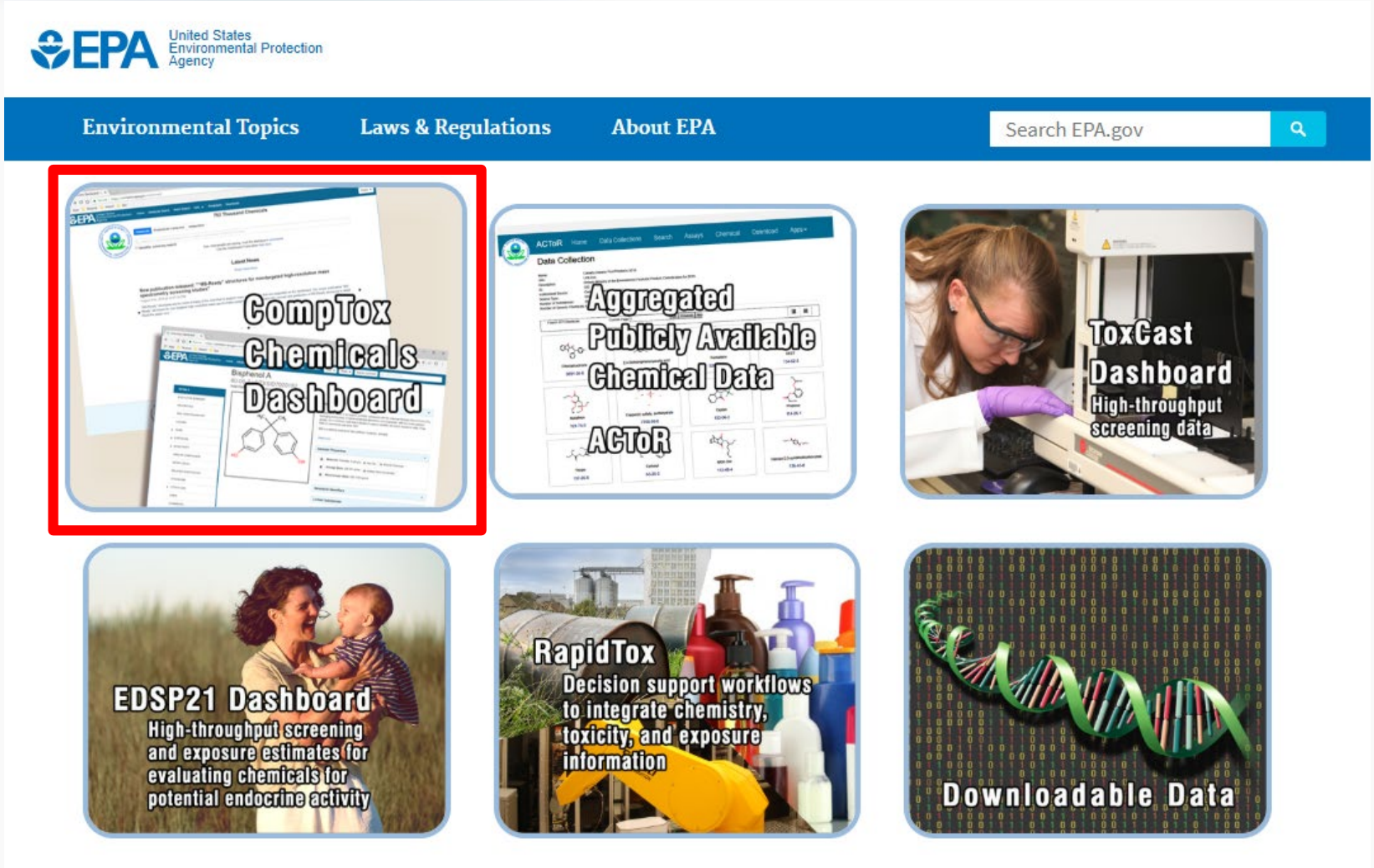
This work was reviewed by the U.S. EPA and approved for presentation but does not necessarily reflect official Agency policy.

May 21st 2019

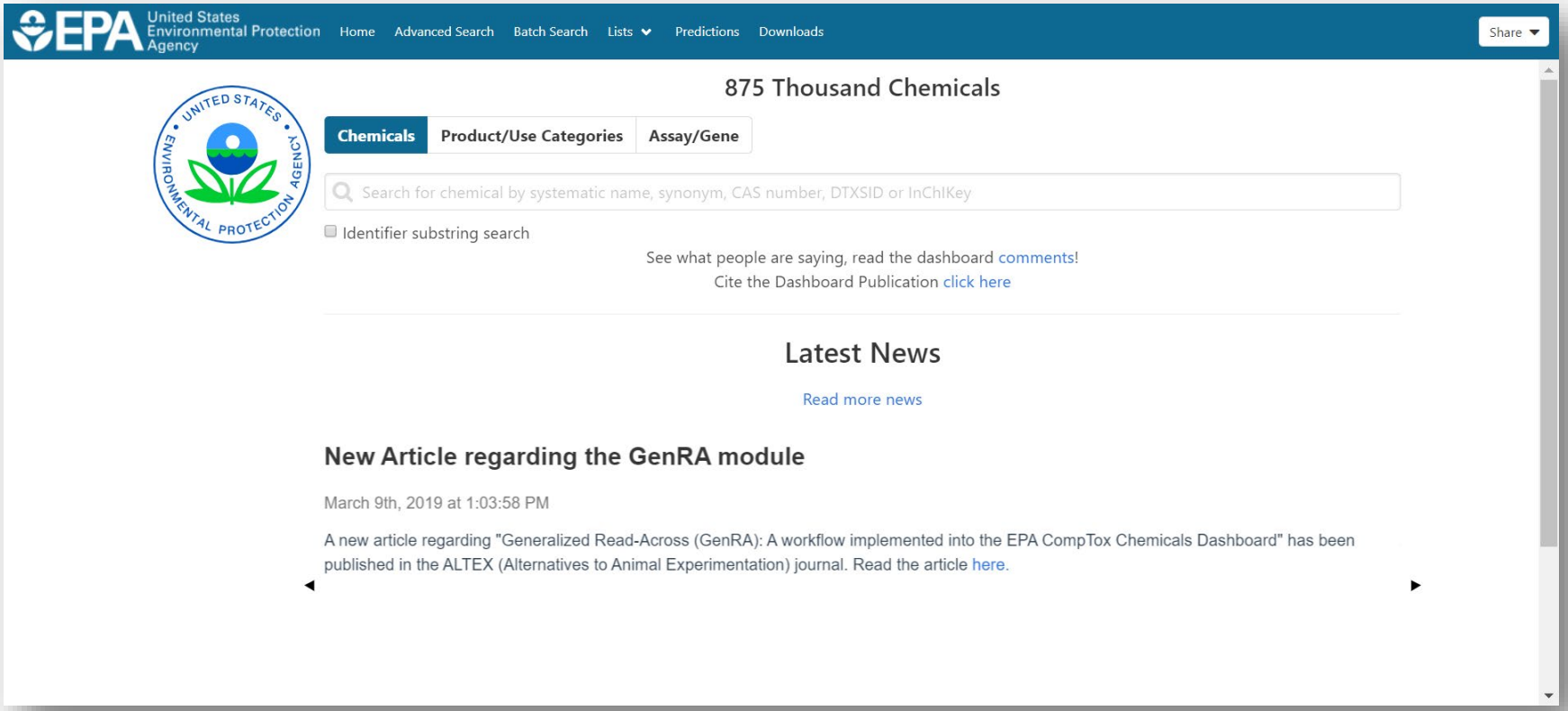
The CompTox Portal
https://comptox.epa.gov/



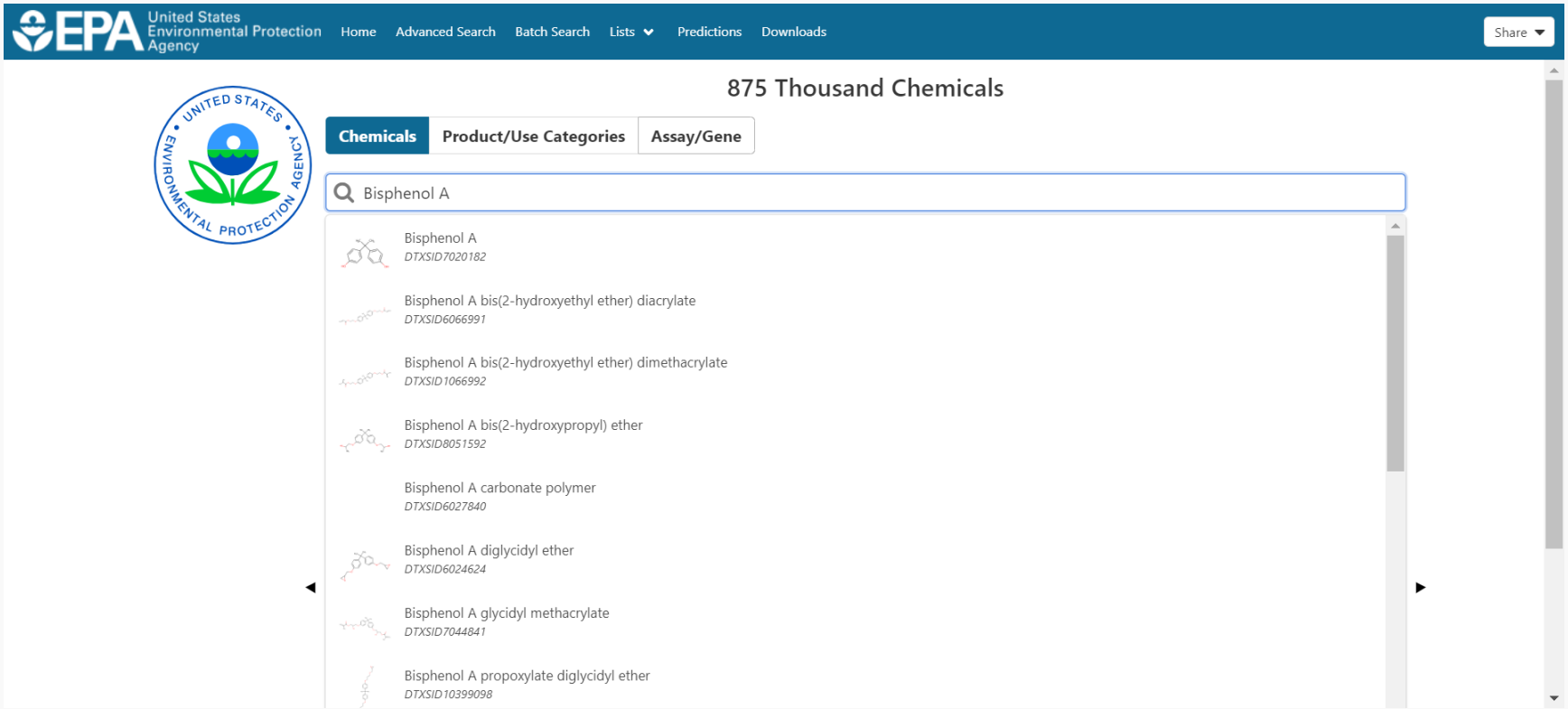
CompTox Chemicals Dashboard

- A **publicly accessible website** delivering access:
  - ~875,000 chemicals with related property data
  - Experimental and predicted physicochemical property 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
  - DOWNLOADABLE Open Data for reuse and repurposing

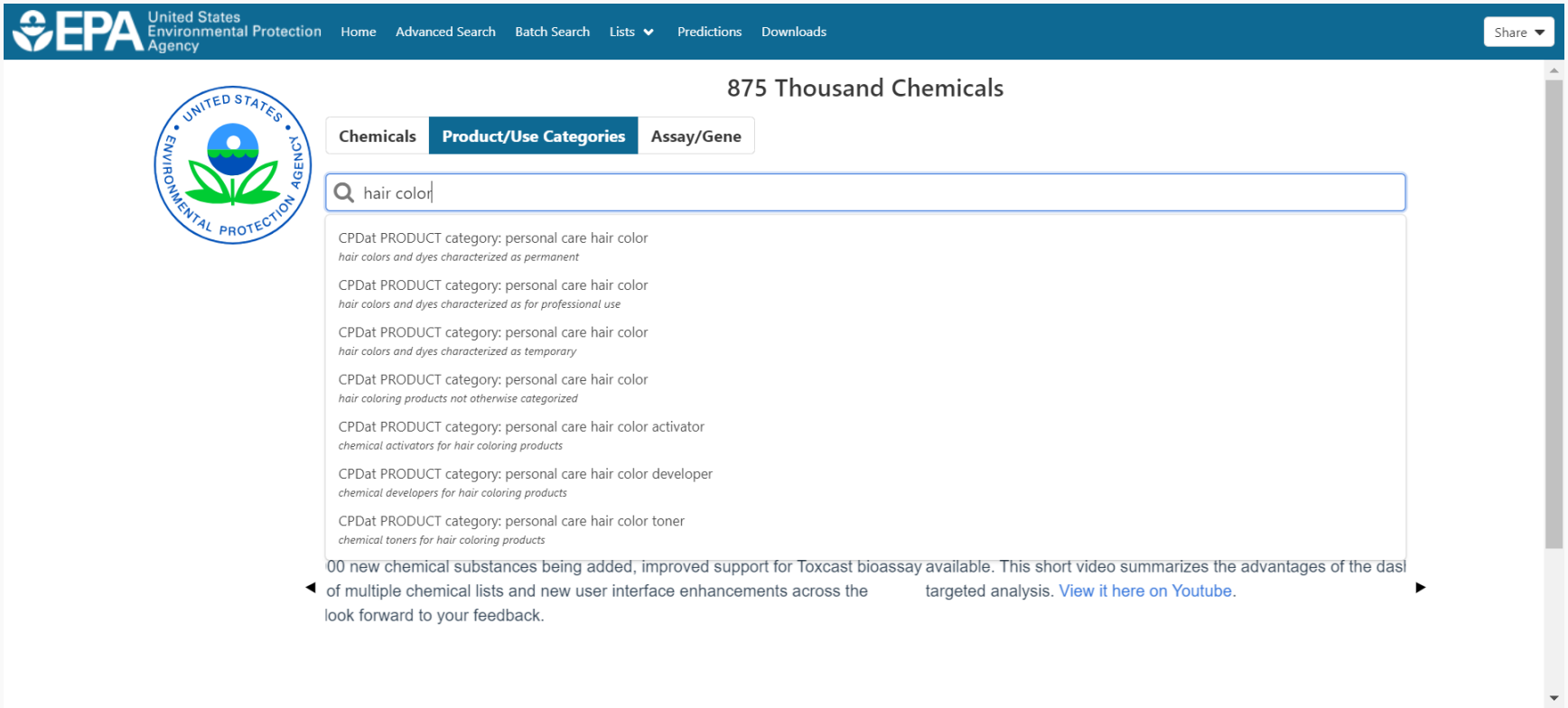
CompTox Chemicals Dashboard



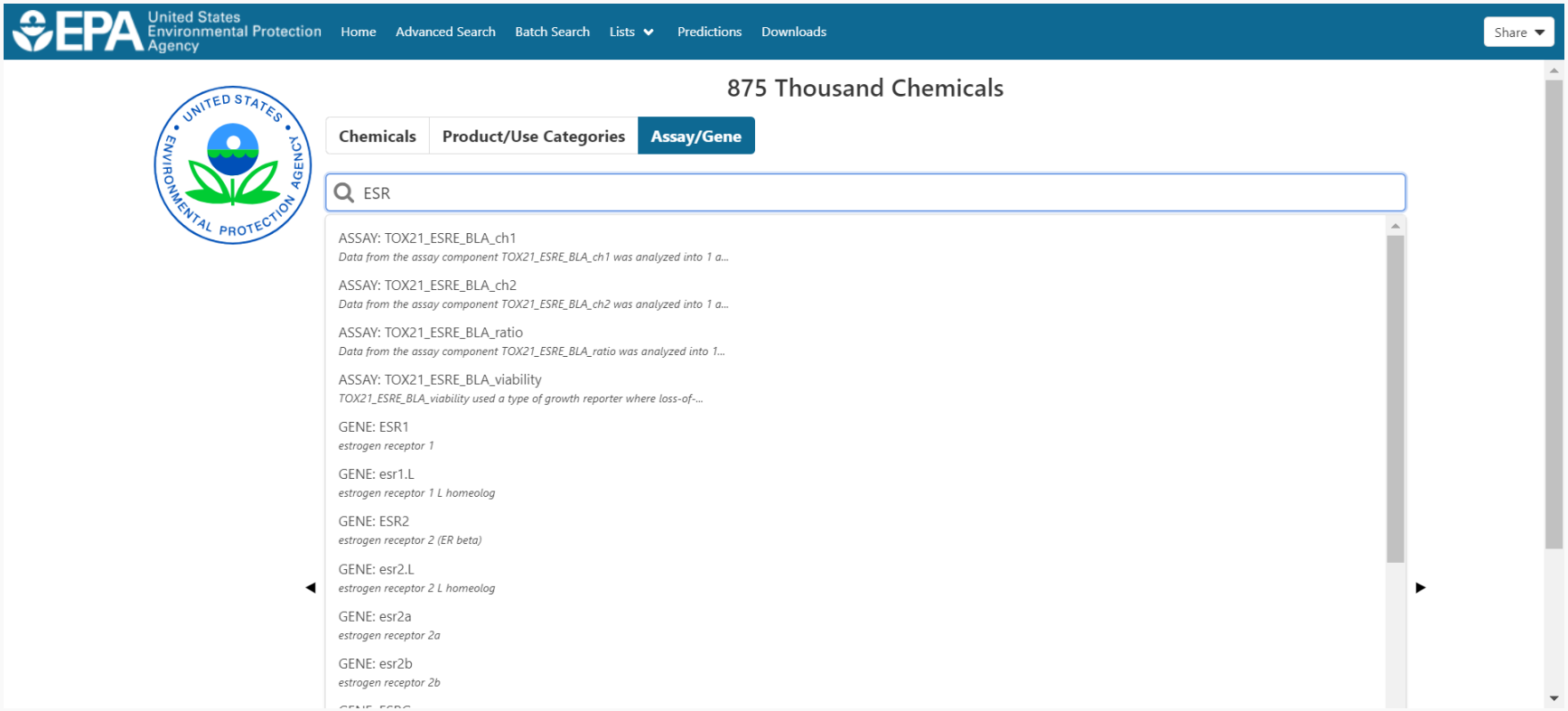
CompTox Chemicals Dashboard
Chemicals



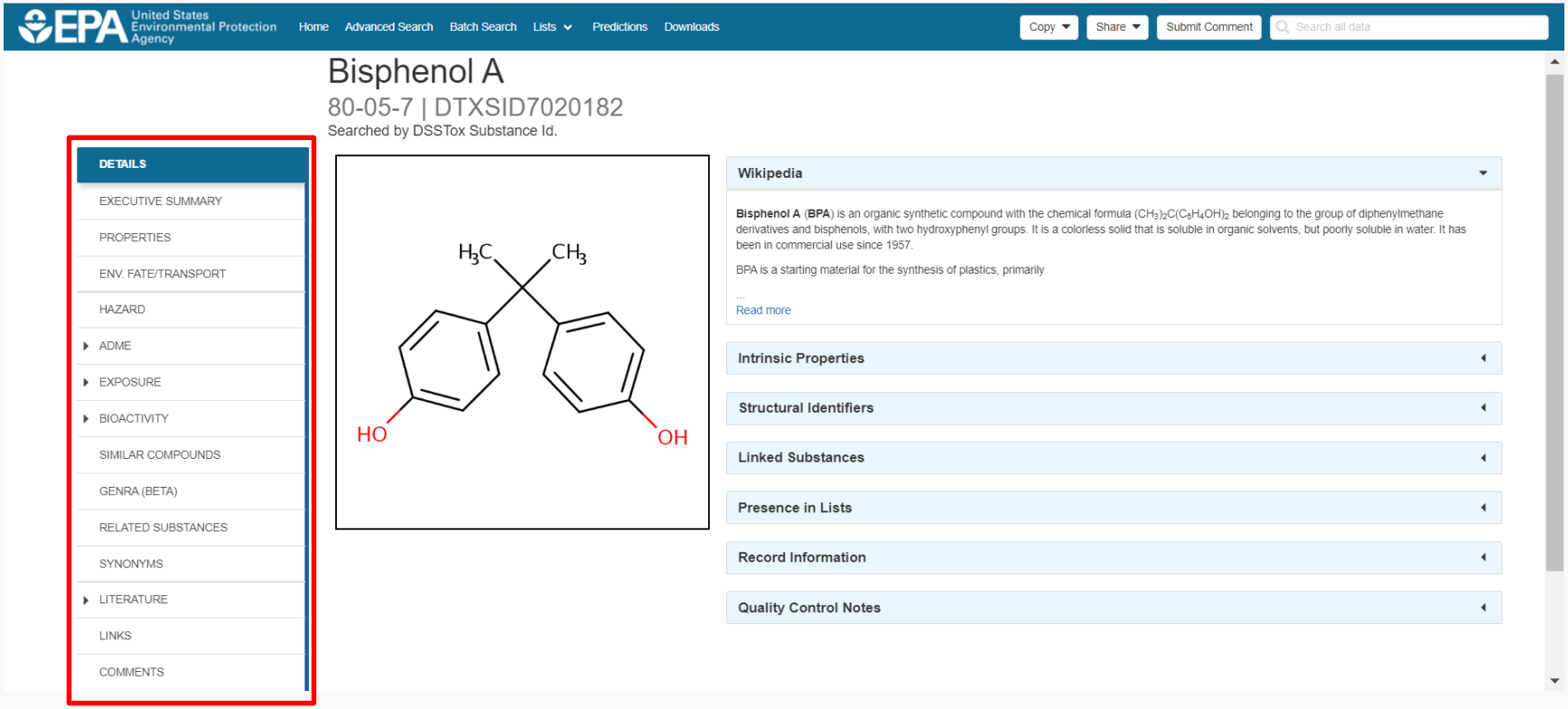
CompTox Chemicals Dashboard
Products and Use Categories



CompTox Chemicals Dashboard
Assays and Genes



Detailed Chemical Pages



An “Executive Summary”

EPA United States Environmental Protection Agency

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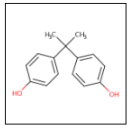

Bisphenol A

80-05-7 | DTXSID7020182

Searched by Expert Validated Synonym.

- DETAILS
- **EXECUTIVE SUMMARY**
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- ADME
- EXPOSURE
- BIOACTIVITY
  - TOXCAST: SUMMARY
  - EDSP21
  - TOXCAST/TOX21
  - PUBCHEM

Executive Summary

Quantitative Risk Assessment Values

- IRIS values available
- No PPRTV values
- EPA RSL values available
- Minimum RfD: **0.050 mg/kg-day** (chronic, IRIS, oral, 8)
- No RfC calculated
- IVIVE POD not calculated

Quantitative Hazard Values

- Minimum oral POD: **3.8 mg/kg-day** (reproductive, HPVIS, oral, 6)
- No inhalation POD values
- Lowest Observed Bioactivity Equivalent Level: CYP1A1, CYP1A2, Tpo, ESR2, ESR1, ESR1, NR1I3, PPARA, NR1I2, Cyp2c11, MMP3, Esr1

Cancer Information

- No cancer slope factor
- No inhalation unit risk value
- Carcinogenicity data available: University of Maryland carcinogenicity warning;
- No genotoxicity findings reported

Reproductive Toxicology

- 200 Reproductive toxicity PODs available

REGIONAL SCREENING

Class	THQ	Value
risk-based SSL (mg/kg)	THQ = 0.1	5.8
GIABS (unspecified)	THQ = 1	1
GIABS (unspecified)	THQ = 0.1	1
ABS (unspecified)	THQ = 0.1	0.1
RFDo (mg/kg-day)	THQ = 0.1	0.05
screening level (residential Soil) (mg/kg)	THQ = 0.1	320
screening level (industrial soil) (mg/kg)	THQ = 0.1	4100

An "Executive Summary" Quick Look Tox Info

EPA United States Environmental Protection Agency

Executive Summary

Quantitative Risk Assessment Values
- IRIS values available
- No PPRTV values
- EPA RSL values available
- Minimum RfD: **0.050 mg/kg-day** (chronic, IRIS, oral, 8)
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Cancer Information
- No cancer slope factor
- No inhalation unit risk value
- Carcinogenicity data available: University of Maryland carcinogenicity warning;
- No genotoxicity findings reported

Reproductive Toxicology
- 200 Reproductive toxicity PODs available

Chronic Toxicology
- 340 Chronic toxicity PODs available

Subchronic Toxicology
- 12 Subchronic toxicity PODs available

Developmental Toxicology
- 6 Developmental toxicity PODs available

Acute Toxicology
- 391 Acute toxicity PODs available

Subacute Toxicology
- 1 subacute toxicity PODs available

Neurotoxicology
- No neurotoxicology data available.

Endocrine System
- Endocrine Disruption Potential. Significant Estrogen and Androgen Receptor activity seen. Chemical was positive in **21 ER assays (out of 35)** and was positive in **9 AR assays (tested in 19)**.

ADME
- HTTK Css data are available

Fate and Transport
- No bioaccumulation concern.
- No volatility concern.
- Biodegradation predictions are available
- BCF predictions are available
- Vapor Pressure predictions are available

Exposure
- Exposure estimates are available based on NHANES and SEEM

AOP Information
- AOP Links: 13, 33, 36, 58, 60, 61, 66, 107, 124, 150, 163, 175, 187, 200

Other Notes
- No water quality values available.
- No air quality values available.
- 14 Occupational exposure values available.

POINT-OF-DEPARTURE PLOTS

REGIONAL SCREENING

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risk-based SSL (mg/kg)	THQ = 0.1	5.8
GIABS (unspecified)	THQ = 1	1
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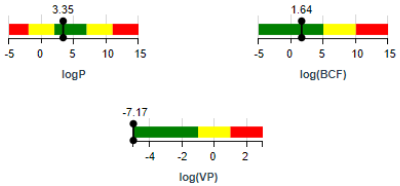
RFDo (mg/kg-day)	THQ = 0.1	0.05
screening level (residential Soil) (mg/kg)	THQ = 0.1	320
screening level (industrial soil) (mg/kg)	THQ = 0.1	4100
screening level (tap water) (ug/L)	THQ = 0.1	77
RFDo (mg/kg-day)	THQ = 1	0.05
screening level (residential Soil) (mg/kg)	THQ = 1	3200
screening level (industrial soil) (mg/kg)	THQ = 1	41000
ABS (unspecified)	THQ = 1	0.1
risk-based SSL (mg/kg)	THQ = 1	58
screening level (tap water) (ug/L)	THQ = 1	770

PHYSCHEM PARAMETERS



ASSAY PLOTS

Quantitative Risk Assessment Values
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Physicochemical properties

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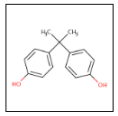

Bisphenol A

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  - TOXCAST/TOX21
  - PUBCHEM
  - TOXCAST: MODELS
- SIMILAR COMPOUNDS

Property

Summary

Summary

Download | Columns | Search query

Property	Experimental average	Predicted average	Experimental median	Predicted median	Experimental range	Predicted range	Unit
LogP: Octanol-Water	3.32 (1)	3.29		3.43	3.32	2.40 to 3.64	
Melting Point	155 (7)	139	156	138	153 to 156	125 to 157	°C
Boiling Point	200 (1)	363		360	200	343 to 401	°C
Water Solubility	5.26e-4 (1)	9.62e-4		1.00e-3	5.26e-4	5.35e-4 to 1.31e-3	mol/L
Vapor Pressure	-	8.37e-7		3.43e-7	-	6.83e-8 to 2.59e-6	mmHg
Flash Point	-	190		190	-	188 to 192	°C
Surface Tension	-	46.0			-	46.0	dyn/cm
Index of Refraction	-	1.60			-	1.60	
Molar Refractivity	-	68.2			-	68.2	cm^3
Polarizability	-	27.0			-	27.0	Å^3
Density	-	1.17		1.17	-	1.14 to 1.20	g/cm^3
Molar Volume	-	200			-	200	cm^3

Detailed OPERA Prediction Reports

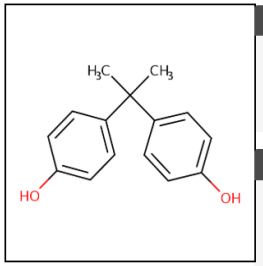
(we heard about from Kamel…)

OPERA Models: LogP: Octanol-Water

Bisphenol A

80-05-7 | DTXSID7020182

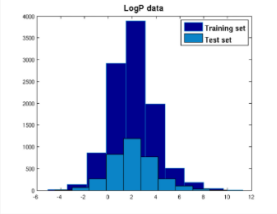
Print PDF

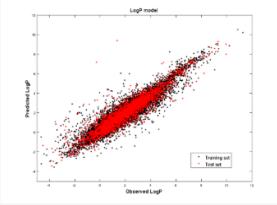


Model Results

Predicted value: 3.35
Global applicability domain: Inside
Local applicability domain index: 0.877
Confidence level: 0.813

Model Performance



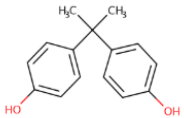


QMRF

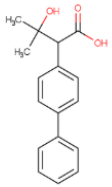
Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.850	0.690	0.860	0.670	0.860	0.780

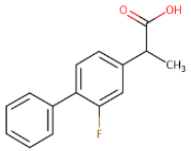
Nearest Neighbors from the Training Set



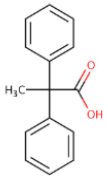
Bisphenol A
Measured:3.32
Predicted: 3.35076



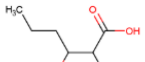
BUTANOIC ACID,2-(4-BIPHENYLYL)-3-HYDROXY-3-METHY
Measured:3.25
Predicted: 3.39062



Flurbiprofen
Measured:4.16
Predicted: 3.94445



2,2-Diphenylpropionic acid
Measured:2.69
Predicted: 2.84603



Other Data: Human and Ecological Chemical Hazard Data

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

Data Type: Point of Departure

Download

Human | Eco

Columns | 10 | Search query

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

Hazard Data from “ToxVal_DB”

- ToxVal Database contains following data:
  - ~30,000 chemicals
  - ~750,000 toxicity values
  - ~30 sources of data
  - ~4500 journals cited
  - ~70,000 literature citations

Sources of Exposure to Chemicals

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Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
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- HAZARD
- ADME
- EXPOSURE
  - PRODUCT & USE CATEGORIES
  - CHEMICAL WEIGHT FRACTION
  - CHEMICAL FUNCTIONAL USE
  - TOXICS RELEASE INVENTORY
  - MONITORING DATA
  - EXPOSURE PREDICTIONS
  - PRODUCTION VOLUME

Product and Use Categories (PUCs)

Download | Columns | 10 | Search query

Product or Use Categorization	Categorization type	Number of Unique Products
manufacturing, metals	CPCat Cassette	17
adhesive	CPCat Cassette	17
	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

Weight Fraction Details

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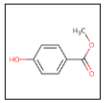

Methylparaben

99-76-3 | DTXSID4022529

Searched by Synonym from Valid Source.

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
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  - CHEMICAL FUNCTIONAL USE
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  - EXPOSURE PREDICTIONS
  - PRODUCTION VOLUME
- BIOACTIVITY
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS

Chemical Weight Fractions

Download | Columns | 50 | Search query

Product Name	Product Use Category	Minimum Weight Fraction	Maximum Weight Fraction	Data Type	Source
hairsil accelerator shampoo 1	personal care: shampoo	1.00e-2	9.00e-2	MSDS	Retail Product Categories/Walmart
simple cleansing facial wipes	-	1.00e-3	5.06e-2	Ingredients List	Unilever
simple facial spot liquid spotless skin spot zapper	-	1.00e-3	5.06e-2	Ingredients List	Unilever
simple facial cream pore minimising facial cleanser	-	1.00e-3	5.06e-2	Ingredients List	Unilever
body butter (bldetox) 1	personal care: hand/body lotion	1.00e-2	5.00e-2	MSDS	Retail Product Categories/Walmart
neulmsfe-neutrogena mineral sheers for eyes 1	personal care: eye shadow	1.00e-2	5.00e-2	MSDS	Retail Product Categories/Walmart
nyc hair streakers 973a-04, 05, 06, 07 1	personal care: hair styling	1.00e-2	5.00e-2	MSDS	Retail Product Categories/Walmart
room spray 1	inside the home: air freshener	1.00e-2	5.00e-2	MSDS	Retail Product Categories/Walmart
soap (bldetox) 1	personal care: bar soap	1.00e-2	5.00e-2	MSDS	Retail Product Categories/Walmart
signal family protection original toothpaste	-	1.00e-3	4.69e-2	Ingredients List	Unilever
simple facial cream purifying cleansing lotion	-	1.00e-3	4.69e-2	Ingredients List	Unilever
simple kind to eyes eye make up remover pads	-	1.00e-3	4.69e-2	Ingredients List	Unilever
simple facial scrub smoothing	-	1.00e-3	4.55e-2	Ingredients List	Unilever
vaseline cream intensive rescue	-	1.00e-3	4.55e-2	Ingredients List	Unilever
vaseline intensive rescue relief and repair balm	-	1.00e-3	4.55e-2	Ingredients List	Unilever
simple exfoliating facial wipes	-	1.01e-3	4.41e-2	Ingredients List	Unilever
simple soothing facial toner	-	1.00e-3	4.39e-2	Ingredients List	Unilever
simple facial wash clear skin oil balancing exfoliating	-	1.00e-3	4.39e-2	Ingredients List	Unilever
simple facial wash spotless skin triple active	-	1.00e-3	4.39e-2	Ingredients List	Unilever

Functional Use Predictions (FUSE)

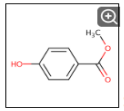
EPA United States Environmental Protection Agency

CrossMark click for updates

Cite this: *Green Chem.*, 2017, **19**, 1063

High-throughput screening of chemicals as functional substitutes using structure-based classification models†

Katherine A. Phillips,*[a,c] John F. Wambaugh,[b] Christopher M. Grulke,[b] Kathie L. Dionisio[c] and Kristin K. Isaacs[c]



Methylparaben

99-76-3 | DTXSID4022529

Searched by Synonym from Valid Source.

Collected Data on Functional Use

Download

Search query

Harmonized functional use	Reported functional use
fragrance	COLORANT
fragrance	fragrance
fragrance	Fragrance Component
-	preservative

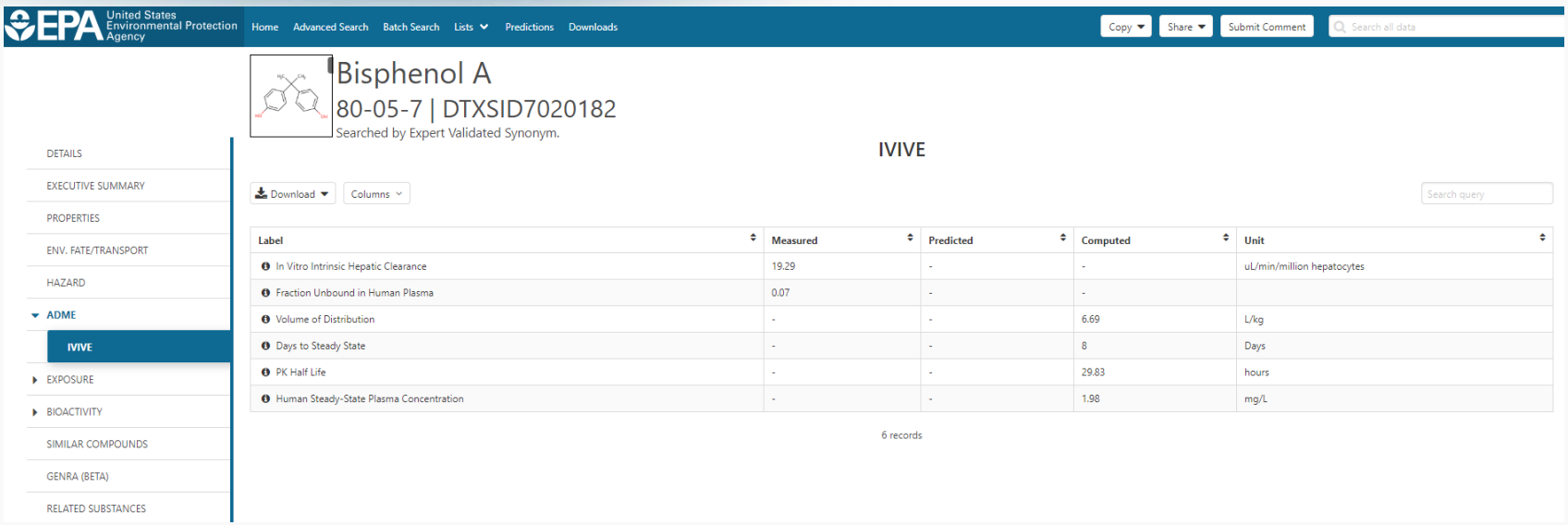
Predicted Probability of Associated Functional Use
QSAR Version/Date: 2015-11-06

Download 10

Search query

Harmonized functional use	Probability
preservative	0.988
UV absorber	0.885
fragrance	0.653
antioxidant	0.608
skin conditioner	0.475
skin protectant	0.411
chelator	0.364
colorant	0.285
antimicrobial	0.279
crosslinker	0.187

ADME-IVIVE



Label	Measured	Predicted	Computed	Unit
In Vitro Intrinsic Hepatic Clearance	19.29	-	-	uL/min/million hepatocytes
Fraction Unbound in Human Plasma	0.07	-	-	
Volume of Distribution	-	-	6.69	L/kg
Days to Steady State	-	-	8	Days
PK Half Life	-	-	29.83	hours
Human Steady-State Plasma Concentration	-	-	1.98	mg/L

- Barbara Wetmore will cover this in detail

In Vitro Bioassay Screening

ToxCast and Tox21

EPA United States Environmental Protection Agency

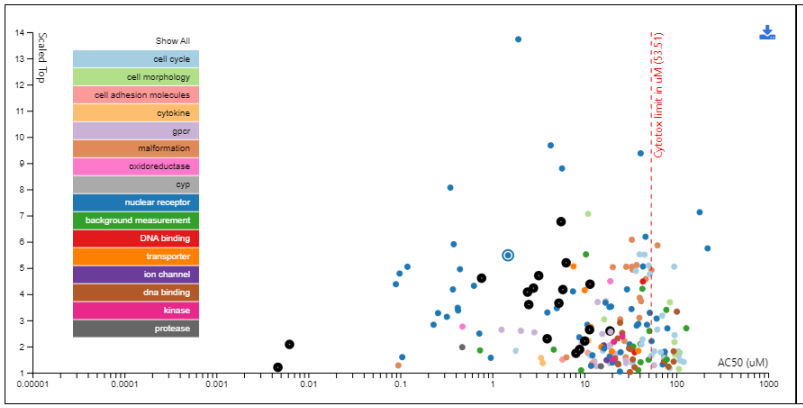
EPA United States Environmental Protection Agency | Home | Advanced Search | Batch Search | Lists | Predictions | Downloads | Copy | Share | Submit Comment | Search all data

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- ADME
- EXPOSURE
- BIOACTIVITY
  - TOXCAST: SUMMARY
  - EDSP21
  - TOXCAST/TOX21
  - PUBCHEM
  - TOXCAST: MODELS
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE
- LINKS
- COMMENTS

Searched by Expert Validated Synonym.

Chemical Activity Summary

TOXCAST DATA



ASSAY DETAILS

AC50 (uM): 1.48
Scaled top: 5.48
Assay Endpoint Name: ATG_PXRE_CIS_up
Gene Symbol: NR1I2
Organism: human
Tissue: liver
Assay Format Type: cell-based
Biological Process Target: regulation of transcription factor activity
Detection Technology: RT-PCR and Capillary electrophoresis
Analysis Direction: positive
Intended Target Family: nuclear receptor
Description: Data from the assay component ATG_PXRE_CIS was analyzed into 1 assay endpoint. This assay endpoint, ATG_PXRE_CIS_up, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of inducible reporter, measures of mRNA for gain-of-signal activity can be used to understand the reporter gene at the transcription factor-level as they relate to the gene NR1I2. Furthermore, this assay endpoint can be referred to as a primary readout, because this assay has produced multiple assay endpoints where this one serves a reporter gene function. To generalize the intended target to other relatable targets, this assay endpoint is annotated to the "nuclear receptor" intended target family, where the subfamily is "non-steroidal".

185 active of 839 assays

Download | Columns | 10 | Search query | Show Inactive | Show Background

Name	Modal	SeqaPASS	AOP	Event	Hit Call	Top	AC50	logAC50	MaxMed	Cutoff	ModlAcc	Intended Target Family
ACEA_ER_80hr		NP_000116.2	200	1181	ACTIVE	112	0.373	-0.428	113	26.9	-0.686	nuclear receptor
APR_HepG2_CellLoss_24h_dn		-	-	-	ACTIVE	1.20	106	2.02	1.20	0.663	2.04	cell cycle
APR_HepG2_MitoMass_24h_dn		-	-	-	ACTIVE	0.874	109	2.04	0.867	0.496	2.05	cell morphology

In Vitro Bioassay Screening

ToxCast and Tox21

EPA United States Environmental Protection Agency

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Bisphenol A

80-05-7 | DTXSID7020182

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- DETAILS
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  - TOXCAST/TOX21
  - PUBCHEM
  - TOXCAST: MODELS
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES
- SYNONYMS
- LITERATURE

ToxCast/Tox21

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

Assay Selection **136 Selected**

Active Inactive All

Filter assays

- Ceetox/OpAns **(2 of 24 selected)**
- Odyssey Thera **(6 of 17 selected)**
- Attagene **(4 of 165 selected)**
- Tox21/NCGC **(44 of 211 selected)**
- CellzDirect **(3 of 48 selected)**
- Bioseek **(4 of 174 selected)**
- Apredica **(8 of 107 selected)**
- NHEERL Padilla Lab **(1 of 1 selected)**
- Novascreen **(46 of 167 selected)**
- NHEERL's Hunter Lab **(0 of 4 selected)**
- NCCT's Lab **(4 of 4 selected)**
- ACEA Biosciences **(4 of 6 selected)**
- Tanguay Lab **(9 of 19 selected)**

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

Bioactivity: Downloadable Data

https://www.epa.gov/chemical-research/exploring-toxcast-data-downloadable-data

EPA United States Environmental Protection Agency

Exploring ToxCast Data: Downloadable Data

The results after processing through the Pipeline are available on the ToxCast Dashboard, and for most users EPA recommends accessing the data there.

- ToxCast Chemicals
- ToxCast Assays

Resources

- Toxicity Forecaster (ToxCast) Fact Sheet
- ToxCast Publications
- ToxCast Citation
- About ToxCast

ToxCast Data and Information

- **ToxCast & Tox21 Summary Files.** Data for a single chemical endpoint pair for thousands of chemicals and assay endpoints for 20 variables such as the activity or hit call, activity concentrations, whether the chemical was tested in a specific assay, etc.
  - Download ToxCast Summary Information
  - Download ReadMe
- **ToxCast & Tox21 Data Spreadsheet.** A spreadsheet of EPA's analysis of the chemicals screened through ToxCast and the Tox21 collaboration which includes EPA's activity calls from the screening of over 1,800 chemicals.
  - Download Data
  - Download ReadMe
- **ToxCast Data Pipeline R Package.** The R computer programming package used to process and model all EPA ToxCast and Tox21 chemical screening data. The files include the R programming package as well as documents that provide overviews of the data analysis pipeline used and the R package. Users will need experience with R to use these files.
  - Download Package
  - TCPL Overview

BUILT-IN "MODULES"

Generalized Read-Across (GenRA)

EPA United States Environmental Protection Agency

Bisphenol A

80-05-7 | DTXSID7020182

Searched by Expert Validated Synonym.

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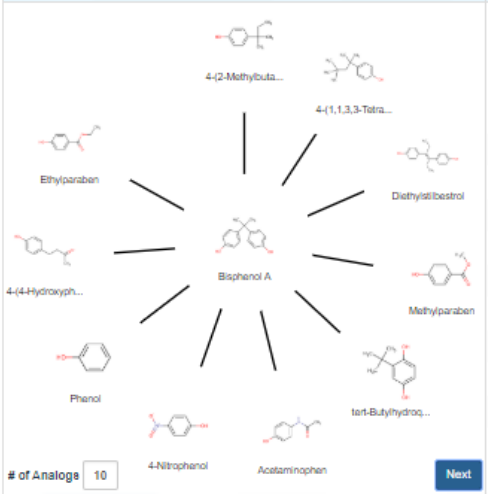
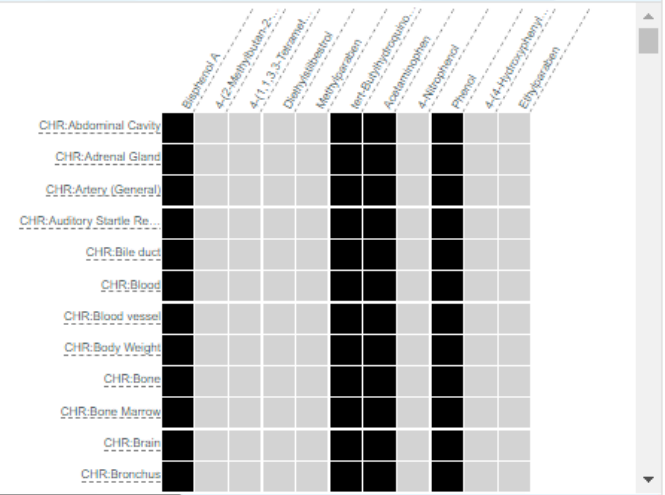
- COMMENTS

Step Two: Data Gap Analysis & Generate Data Matrix

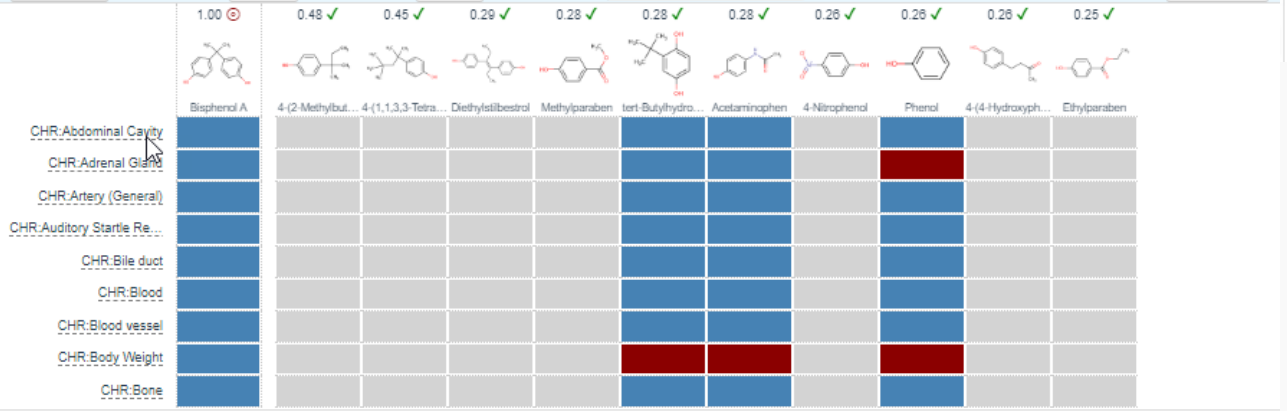
Neighbors by: Chem: Morgan Fgrprts | Filter by: Invivo data | Summary Data Gap Analysis | Group: ToxRef | By: Tox Fingerprint | Generate Data Matrix



	bio_bd21	bio_bnd	chm_ct	tox_bnd
Bisphenol A	23	821	10	402
4-(2-Methylbutan-2-yl)ph...	5	714	10	180
4-(1,1,3,3-Tetramethylbu...	15	726	9	177
Diethylstilbestrol	38	726	11	234
Methylparaben	7	714	7	48
tert-Butylhydroquinone	12	714	9	168
Acetaminophen	4	714	8	313
4-Nitrophenol	15	706	6	95
Phenol	3	714	5	280
4-(4-Hydroxyphenyl)but...	14	0	16	85
Ethylparaben	3	714	8	48



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



Related Publications

Chemical Research in Toxicology

Article

Cite This: Chem. Res. Toxicol. 2017, 30, 2046-2059 pubs.acs.org/crt

Predicting Organ Toxicity Using *in Vitro* Bioactivity Data and Chemical Structure

Jie Liu,[‡,§] Grace Patlewicz,[†] Antony J. Williams,[†] Russell S. Thomas,[†] and Imran Shah*,[†]

[†]National Center for Computational Toxicology, Office of Research and Development, U.S. Environmental Protection Agency, Research Triangle Park, Durham, North Carolina 27711, United States

[‡]Department of Information Science, University of Arkansas at Little Rock, Arkansas 72204, United States

[§]Oak Ridge Institute for Science Education, National Center for Computational Toxicology, Office of Research and Development, U.S. Environmental Protection Agency, Research Triangle Park, Durham, North Carolina 27711, United States

ELSEVIER

Regulatory Toxicology and Pharmacology

Volume 79, August 2016, Pages 12-24

Systematically evaluating read-across prediction and performance using a local validity approach characterized by chemical structure and bioactivity information

Imran Shah [a], Jie Liu [b, c], Richard S. Judson [a], Russell S. Thomas [a], Grace Patlewicz [a]

ELSEVIER

Computational Toxicology

Available online 23 July 2018

In Press, Corrected Proof

Extending the Generalised Read-Across approach (GenRA): A systematic analysis of the impact of physicochemical property information on read-across performance

George Helman [a, b], Imran Shah [b], Grace Patlewicz [b]

ELSEVIER

Contents lists available at ScienceDirect

Computational Toxicology

journal homepage: www.elsevier.com

Journal Cover Image

Navigating through the minefield of read-across frameworks: A commentary perspective

Grace Patlewicz[a, *], Mark T.D. Cronin[b], George Helman[a, c], Jason C. Lambert[d], Lucina E. Lizarraga[d], Imran Shah[a]

[a] National Center for Computational Toxicology (NCCT), Office of Research and Development, US Environmental Protection Agency (US EPA), 109 TW Alexander Dr, Research Triangle Park (RTP), NC 27711, USA

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

[c] Oak Ridge Institute for Science and Education (ORISE), 1299 Bethel Valley Road, Oak Ridge, TN 37830, USA

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

Names and CASRNs to Support Searches

EPA United States Environmental Protection Agency

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Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

- DETAILS
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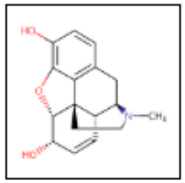
- GENRA (BETA)
- RELATED SUBSTANCES
- **SYNONYMS**
- LITERATURE
- LINKS
- COMMENTS

25 | Search query

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

Literature Searching



Morphine

57-27-2 | DTXSID9023336

Searched by Approved Name.

Abstract Sifter

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
- Disaster / Emergency

Optionally, edit the query before retrieving.

"57-27-2" OR "Morphine"

Literature Searching

Child (infant through adolescent)
Dust and Exposure
Food and Exposure
Water and Exposure
Algae
Disaster / Emergency

Optionally, edit the query before retrieving.

("57-27-2" OR "Morphine") AND ((water OR groundwater OR drinking water) AND Environmental Exposure)

Literature Searching

37 of 37 articles loaded...

To find articles quickly, enter terms to sift abstracts.

wastewater | Spectrometry | EPA | Clear Terms

Download / Send to... | Download Sifter for Excel

	wastewater	Spectrometry	EPA	Total	PMID	Year	Title	Authors	Journal	Rev
	4	2	0	6	29274731	2017	Simultaneous analysis of opioid analgesics and thei...	Krizman-Matasic; Kostanjevecki; Ahel; Terzic	Journal of chromatography. A	
	0	1	0	1	25768972	2015	Evaluating external contamination of polybrominate...	Poon; Aleksa; Carnevale; Kapur; Goodyer; Koren	Therapeutic drug monitoring	
	0	1	0	1	22544551	2012	Spatial distribution of illicit drugs in surface waters o...	Vazquez-Roig; Andreu; Blasco; Morillas; Picó	Environmental science and pollution research inter...	
	1	1	0	2	20801487	2010	Analysis of llicit and illicit drugs in waste, surface an...	Berset; Brenneisen; Mathieu	Chemosphere	
	1	1	0	2	17935751	2007	Illicit drugs, a novel group of environmental contami...	Zuccato; Castiglioni; Bagnati; Chiabrando; Grassi; ...	Water research	
	2	1	1	4	17607391	2007	Using environmental analytical data to estimate lev...	Bones; Thomas; Paull	Journal of environmental monitoring : JEM	
	3	1	2	6	17180984	2006	Simultaneous determination of psychoactive drugs ...	Hummel; Löffler; Fink; Ternes	Environmental science & technology	
	6	0	0	6	30583189	2018	Assessment of drugs of abuse in a wastewater trea...	Kumar; Tscharke; O'Brien; Mueller; Wilkins; Padhye	The Science of the total environment	
	0	0	3	3	30488421	2018	Effect of enriched environment during adolescence ...	Mohammadian; Najafi; Miladi-Gorji	Developmental psychobiology	
	3	0	0	3	29574368	2018	Estimation of the consumption of illicit drugs during ...	Foppe; Hammond-Weinberger; Subedi	The Science of the total environment	
	1	0	0	1	28787791	2017	Evaluation of in-sewer transformation of selected illi...	Gao; Banks; Li; Jiang; Lai; Mueller; Thai	The Science of the total environment	
	9	0	0	9	28472697	2017	Occurrence and fate of illicit drugs and pharmaceuti...	Causanilles; Ruepert; Ibáñez; Emke; Hernández; d...	The Science of the total environment	
	0	0	0	0	28010888	2016	Dose-dependent effects of morphine on lipopolysac...	Mottaz; Schönenberger; Fischer; Eggen; Schirmer; ...	Environmental pollution (Barking, Essex : 1987)	
	0	0	0	0	27746311	2016	Effects of voluntary exercise on the viability, prolifer...	Haydari; Safari; Zarbakhsh; Bandegi; Miladi-Gorji	Neuroscience letters	
	0	0	0	0	27261879	2016	Genotoxic effects induced by the exposure to an en...	Parolini; Magni; Castiglioni; Binelli	Ecotoxicology and environmental safety	
	3	0	0	3	27179320	2016	Temporal trends in drug use in Adelaide, South Aus...	Tscharke; Chen; Gerber; White	The Science of the total environment	

External Links to ~80 websites

EPA United States Environmental Protection Agency

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Bisphenol A

80-05-7 | DTXSID7020182

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General

- EPA Substance Registry Service
- Household Products Database
- Chemical Entities of Biological Interest (ChEBI)
- PubChem
- Chemspider
- 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

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

CHEMICAL LISTS AND CATEGORIES

Category example – PAHs

EPA United States Environmental Protection Agency

Polycyclic aromatic hydrocarbons

130498-29-2 | DTXSID3044043

Searched by DSSTox Substance Id.

Wikipedia

Polycyclic aromatic hydrocarbons (**PAHs**, also ***polyaromatic hydrocarbons*** or ***polynuclear aromatic hydrocarbons***) are hydrocarbons—organic compounds containing only carbon and hydrogen—that are composed of multiple aromatic rings (organic rings in which the electrons are delocalized). The simplest such chemicals are naphthalene, having two aromatic rings, and the three-ring compounds anthracene and phenanthrene.
PAHs are uncharged, non-polar molecules found

...

Read more

Presence in Lists

Federal

ATSDR: Toxic Substar

EPA: Toxicity Values

US State

None.

Polycyclic aromatic hydrocarbons

130498-29-2 | DTXSID3044043

Searched by DSSTox Substance Id.

- DETAILS
- RELATED SUBSTANCES
- SYNONYMS
- LINKS
- BIOACTIVITY
- EXPOSURE
- HAZARD
- COMMENTS
- PROPERTIES
- LITERATURE

73 chemicals

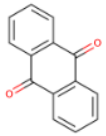
Select all | Download | Send to Batch Search | Relationship | DTXSID | PubChem | CPDAT | Hide chemicals that are: | Filter by Name or CASRI

Searched Chemical

73 related chemical structures with this substance

Polycyclic aromatic hydrocarbons
DTXSID: DTXSID3044043
PubChem: 0
CPDAT: 87

Component

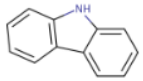


Anthraquinone
DTXSID: DTXSID3020095
PubChem: 138
CPDAT: 34

Component

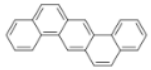
Benzo(a)pyrene
DTXSID: DTXSID2020139
PubChem: 161
CPDAT: 81

Component



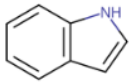
Carbazole
DTXSID: DTXSID4020248
PubChem: 147
CPDAT: 2

Component



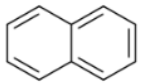
Dibenz(a,h)anthracene
DTXSID: DTXSID9020409
PubChem: 73
CPDAT: 28

Component



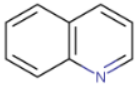
Indole
DTXSID: DTXSID0020737

Component



Naphthalene
DTXSID: DTXSID8020913

Component

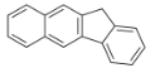


Quinoline
DTXSID: DTXSID1021798

Component

Chrysene
DTXSID: DTXSID0022432

Component



2,3-Benzofluorene
DTXSID: DTXSID1022477

List of Chemicals

EPA United States Environmental Protection Agency

Select List

Download | Columns | PFAS | Copy Filtered Lists URL

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

An Example List

EPA United States Environmental Protection Agency

EPA United States Environmental Protection Agency | Home | Advanced Search | Batch Search | Lists | Predictions | Downloads | Share | Search all data

Hepatic metabolic clearance and plasma protein binding data PHASE 1

Search WETMORE2012 Chemicals

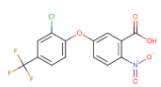
Identifier substring search

List Details

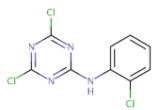
Description: Data from the Wetmore *et al.* paper Integration of dosimetry, exposure, and high-throughput screening data in chemical toxicity assessment. Hepatic metabolic clearance and plasma protein binding data were experimentally measured for ca. 240 ToxCast Phase I chemicals. The experimental data were used in a population-based *in vitro*-to-*in vivo* (IVIVE) extrapolation model to estimate the daily human oral dose, called the oral equivalent dose, necessary to produce steady-state *in vivo* blood concentrations equivalent to *in vitro* AC(50) (concentration at 50% of maximum activity) or lowest effective concentration values across more than 500 *in vitro* assays. The work was split into two phases. This is phase 1 (2012) and the second phase is available here (2015).
Number of Chemicals: 238

238 chemicals

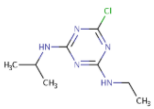
Select all | Download | Send to Batch Search | Default | CASRN | DTXSID | Mass | Hide chemicals that are: | Filter by Name or CASRN



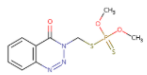
Acifluorfen
CASRN: 50594-66-6
DTXSID: DTXSID0020022
Mass: 360.996485



Anilazine
CASRN: 101-05-3
DTXSID: DTXSID9020089
Mass: 273.957979



Atrazine
CASRN: 1912-24-9
DTXSID: DTXSID9020112
Mass: 215.093773



Azinphos-methyl
CASRN: 86-50-0
DTXSID: DTXSID3020122
Mass: 317.005771

List of Assays

EPA United States Environmental Protection Agency

Assay List

Download | 10 | ATG × | OT × | NHEERL_PADILLA × | Search query | Copy page URL

ACEA Biosciences
Apredica
Attagene
Bioseek
Novascreen
Odyssey Thera
Tox21/NCGC
Ceetox/OpAns
CellzDirect
NHEERL Padilla Lab
NCCT's Lab
Tanguay Lab
NHEERL's Hunter Lab
NHEERL Stoker & Laws Lab
NHEERL Med Lab

Assay Component Endpoint Name	Details	Active Hits	Description	Gene Symbols
ATG_Ahr_CIS_up		573 / 3807	Data from the assay component ATG_A assay endpoint. This assay endpoint, ATG_Ahr_CIS_up, was analyz ction relative to DMSO as the negative control and baseline of activi reporter, measures of mRNA for gain-of-signal activity can be used to u e at the transcription factor-level as they relate to the gene AHR. Furtherm be referred to as a primary readout, because this assay has produ s where this one serves a reporter gene function. To generalize the intend targets, this assay endpoint is annotated to the "dna binding" intend subfamily is "basic helix-loop-helix protein".	AHR
ATG_AP_1_CIS_up		658 / 3807	Data from the assay component ATG_A assay endpoint. This assay endpoint, ATG_AP_1_CIS_up, was analy ection relative to DMSO as the negative control and baseline of activi reporter, measures of mRNA for gain-of-signal activity can be used to u e at the transcription factor-level as they relate to the gene FOS and JUN. F oint can be referred to as a primary readout, because this assay has produ s where this one serves a reporter gene function. To generalize the intend targets, this assay endpoint is annotated to the "dna binding" intended target family, where the subfamily is "basic leucine zipper".	FOS JUN
ATG_AP_2_CIS_up		47 / 3807	Data from the assay component ATG_AP_2_CIS was analyzed into 1 assay endpoint. This assay endpoint, ATG_AP_2_CIS_up, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of inducible reporter, measures of mRNA for	TFAP2A TFAP2B TFAP2D

From Assay to Chemicals…

EPA United States Environmental Protection Agency

Assay Endpoint Name: ACEA_ER_80hr

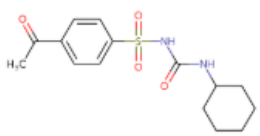
Assay Details

Assay Endpoint Name: ACEA_ER_80hr

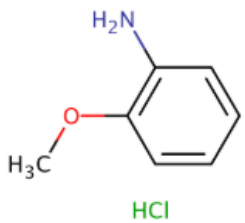
Assay Source Description: ACEA Biosciences, Inc. (ACEA) is a privately owned biotechnology company that developed a real-time, label-free, cell-based assay system based on a microelectronic readout called xCELLigence.

425 of 3031 chemicals visible

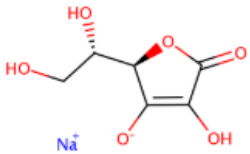
Select all | Download | Send to Batch Search | Default | CASRN ✕ | TOXCAST ✕ | PubMed ✕ | Inactive ✕ | Filter by Name or CASRN



Acetohexamide
CASRN: 968-81-0
TOXCAST: 4/376
PubMed: 235



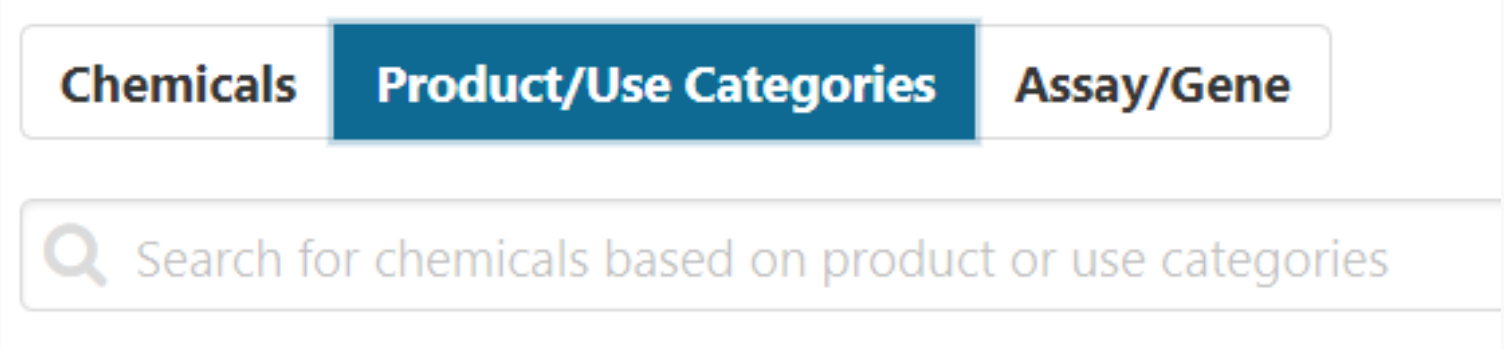
2-Methoxyaniline hydrochloride
CASRN: 134-29-2
TOXCAST: 17/385
PubMed: 46



Sodium L-ascorbate
CASRN: 134-03-2
TOXCAST: 20/662
PubMed: 38756

Sodium azide
CASRN: 26628-22-8
TOXCAST: 26/644
PubMed: 1866

Other Searches



Product/Use Categories

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

lubricant

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

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

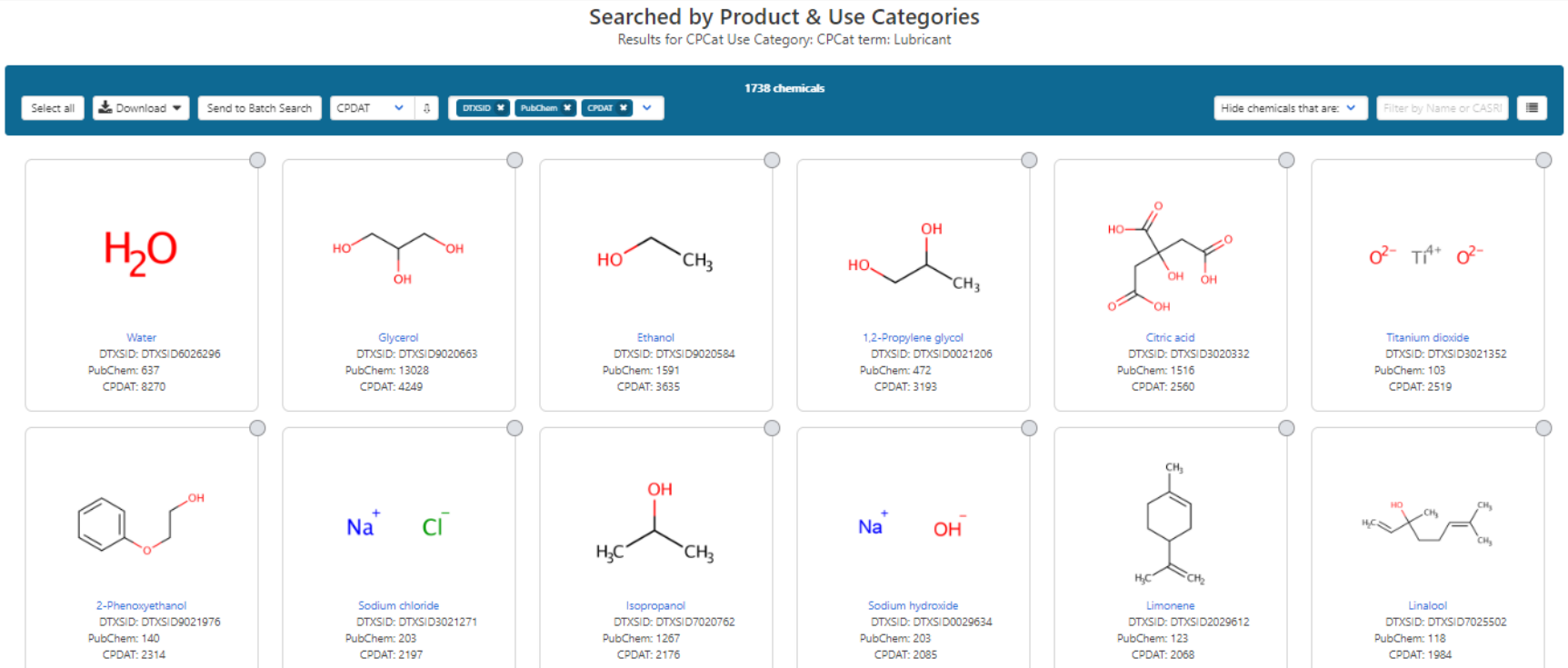
CPDat PRODUCT category: home maintenance lubricant
household maintenance lubricants (spray or aerosol formulation specified)

CPDat PRODUCT category: home maintenance lubricant
household maintenance lubricants

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

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

Lubricant


Searched by Product & Use Categories
Results for CPCat Use Category: CPCat term: Lubricant
1738 chemicals
Select all
Download
Send to Batch Search
CPDAT
DTXSID
PubChem
CPDAT
Hide chemicals that are:
Filter by Name or CASRN
Water
DTXSID: DTXSID6026296
PubChem: 637
CPDAT: 8270
Glycerol
DTXSID: DTXSID9020663
PubChem: 13028
CPDAT: 4249
Ethanol
DTXSID: DTXSID9020584
PubChem: 1591
CPDAT: 3635
1,2-Propylene glycol
DTXSID: DTXSID0021206
PubChem: 472
CPDAT: 3193
Citric acid
DTXSID: DTXSID3020332
PubChem: 1516
CPDAT: 2560
Titanium dioxide
DTXSID: DTXSID3021352
PubChem: 103
CPDAT: 2519
2-Phenoxyethanol
DTXSID: DTXSID9021976
PubChem: 140
CPDAT: 2314
Sodium chloride
DTXSID: DTXSID3021271
PubChem: 203
CPDAT: 2197
Isopropanol
DTXSID: DTXSID7020762
PubChem: 1267
CPDAT: 2176
Sodium hydroxide
DTXSID: DTXSID0029634
PubChem: 203
CPDAT: 2085
Limonene
DTXSID: DTXSID2029612
PubChem: 123
CPDAT: 2068
Linalool
DTXSID: DTXSID7025502
PubChem: 118
CPDAT: 1984

Lots of UVCBS in Commerce….

1 related chemical structure with this substance

Butoxypolypropylene glycol
DTXSID: DTXSID3034404
PubChem: 0
CPDAT: 437

0 related chemical structures with this substance

Fatty acids, tall-oil
DTXSID: DTXSID0028088
PubChem: 0
CPDAT: 436

Poly(oxy-1,2-ethanediyl), alpha-tridecyl-...
DTXSID: DTXSID8043993
PubChem: 0
CPDAT: 435

1 related chemical structure with this substance

Polyoxyethylene (20) oleylether
DTXSID: DTXSID1027714
PubChem: 0
CPDAT: 435

0 related chemical structures with this substance

Soy oil
DTXSID: DTXSID8027660
PubChem: 0
CPDAT: 435

0 related chemical structures with this substance

Bentonite
DTXSID: DTXSID6030782
PubChem: 0
CPDAT: 433

0 related chemical structures with this substance

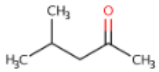
Distillates, petroleum, hydrotreated heav...
DTXSID: DTXSID3028217
PubChem: 0
CPDAT: 433

1 related chemical structure with this substance

Edifas B
DTXSID: DTXSID2020555
PubChem: 0
CPDAT: 433

0 related chemical structures with this substance

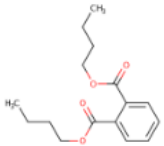
Coconut oil
DTXSID: DTXSID8027664
PubChem: 0
CPDAT: 432



4-Methyl-2-pentanone
DTXSID: DTXSID5021889
PubChem: 173
CPDAT: 428

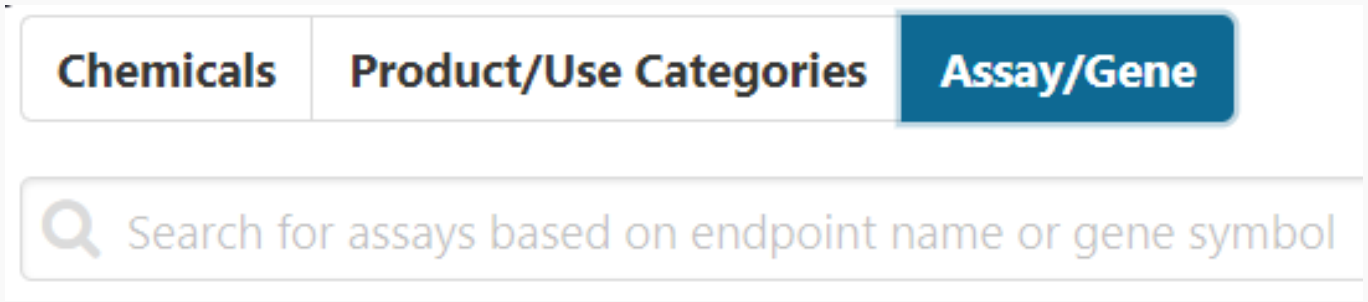
0 related chemical structures with this substance

Distillates, petroleum, solvent-refined he...
DTXSID: DTXSID9028172
PubChem: 0
CPDAT: 426



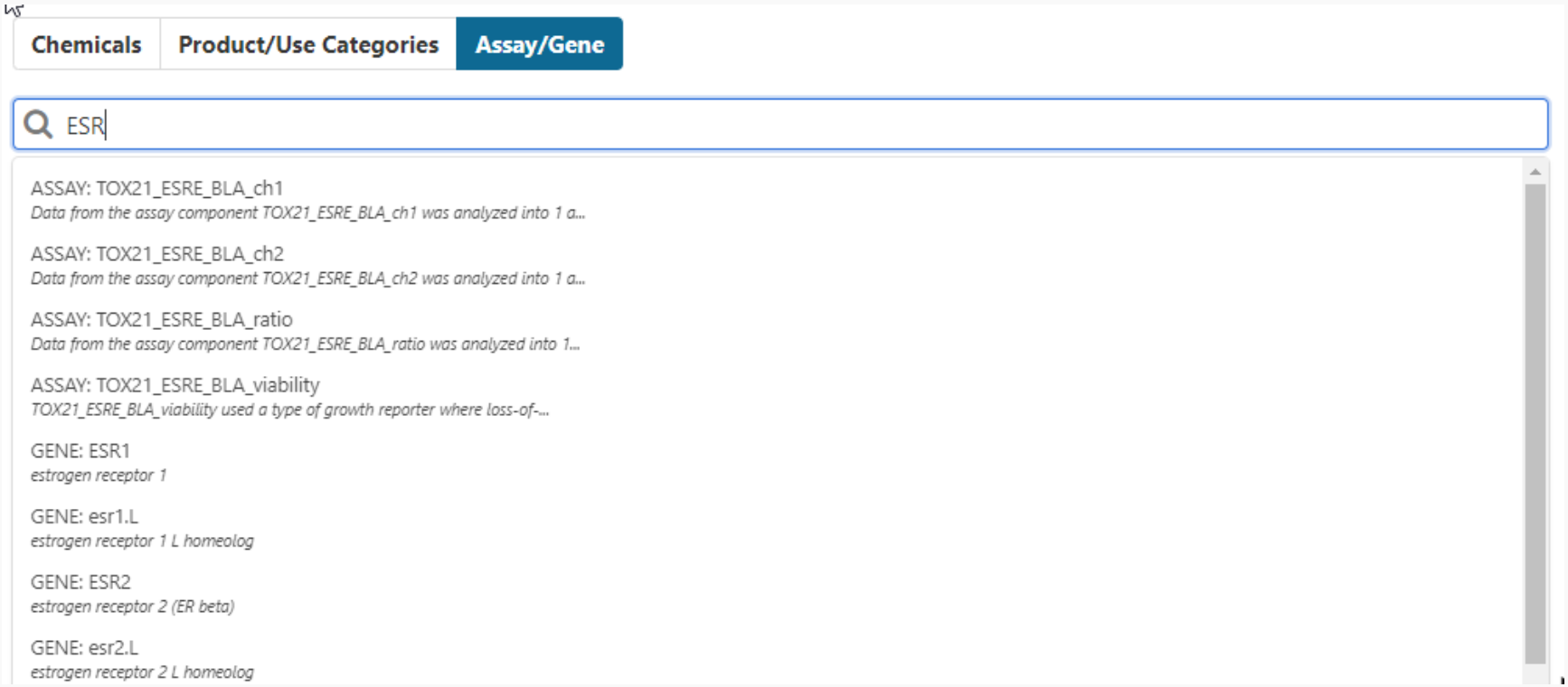
Dibutyl phthalate
DTXSID: DTXSID2021781
PubChem: 138
CPDAT: 421

Other Searches



Chemical-Biology

Assay/Gene Search



Assay/Gene Search

Assay List

Download | 10 | Filter by vendor | ESR1 | Copy Filtered Lists URL

Assay Component Endpoint Name	Details	Active Hits	Description	Gene Symbols
ACEA_ER_80hr		425 / 3031	Data from the assay component ACEA_ER_80hr was analyzed into 2 assay endpoints. This assay endpoint, ACEA_ER_80hr_Positive, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of growth reporter, measures of the cells for gain-of-signal activity can be used to understand the signaling at the pathway-level as they relate to the gene ESR1. Furthermore, this assay endpoint can be referred to as a primary readout, because this assay has produced multiple assay endpoints where this one serves a signaling function. To generalize the intended target to other relatable targets, this assay endpoint is annotated to the "nuclear receptor" intended target family, where the subfamily is "steroidal".	ESR1
ATG_ERE_CIS_up		992 / 3807	Data from the assay component ATG_ERE_CIS was analyzed into 1 assay endpoint. This assay endpoint, ATG_ERE_CIS_up, was analyzed in the positive fitting direction relative to DMSO as the negative control and baseline of activity. Using a type of inducible reporter, measures of mRNA for gain-of-signal activity can be used to understand the reporter gene at the transcription factor-level as they relate to the gene ESR1. Furthermore, this assay endpoint can be referred to as a primary readout, because this assay has produced multiple assay endpoints where this one serves a reporter gene function. To generalize the intended target to other relatable targets, this assay endpoint is annotated to the "nuclear receptor" intended target family, where the subfamily is "steroidal".	ESR1

<< < 1 2 3 4 > >>

Showing 1 to 10 of 32 records

Batch Searching

Batch Searching

- Singleton searches are useful but people generally want data on LOTS 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?
  - Can I include properties in the download file?

- I'll demo this in the breakout session

Real-Time Predictions

Real-Time Predictions

EPA United States Environmental Protection Agency

EPA United States Environmental Protection Agency
Home Advanced Search Batch Search Lists Predictions Downloads
Share
Search all data

Atrazine

100%

Select properties to predict

T.E.S.T.

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

H C N O S P F Cl Br I PT

Calculate

Chiral

Real-Time Predictions with detailed calculation reports

EPA United States Environmental Protection Agency

EPA United States Environmental Protection Agency | Home | Advanced Search | Batch Search | Lists | Predictions | Downloads | Share | Search all data

Provider: T.E.S.T.

Download Summary

Property	Experimental Value	Consensus	Hierarchical clustering	Single model	Group contribution	Nearest neighbor
96 hour fathead minnow LC50		4.951 -Log10(mol/L) 3.425 mg/L	5.198 -Log10(mol/L) 1.943 mg/L	5.257 -Log10(mol/L) 1.693 mg/L	5.287 -Log10(mol/L) 1.581 mg/L	4.064 -Log10(mol/L) 26.452 mg/L
48 hour D. magna LC50		4.430 -Log10(mol/L) 11.374 mg/L	4.764 -Log10(mol/L) 5.269 mg/L	5.006 -Log10(mol/L) 3.020 mg/L	4.430 -Log10(mol/L) 11.386 mg/L	3.521 -Log10(mol/L) 92.353 mg/L
48 hour T. pyriformis IGC50			5.272 -Log10(mol/L) 1.639 mg/L			
Oral rat LD50		1.989 -Log10(mol/kg) 3141.571 mg/kg	1.867 -Log10(mol/kg) 4157.591 mg/kg			2.111 -Log10(mol/kg) 2373.843 mg/kg
Bioaccumulation factor		1.321 Log10 20.956	1.209 Log10 16.192	1.585 Log10 38.452	1.517 Log10 32.923	0.974 Log10 9.409
Developmental toxicity		true	true	true		
Ames mutagenicity		false	false			false
Estrogen Receptor RBA						
Estrogen Receptor Binding		false	false	false	false	
Normal boiling point		357.4 °C	334.0 °C		432.8 °C	305.5 °C
Melting point		111.3 °C	98.3 °C		99.1 °C	136.7 °C
Flash point		219.9 °C	272.7 °C		211.4 °C	175.7 °C
Vapor pressure		-6.849 Log10(mmHg) 1.417*10^-7 mmHg	-6.471 Log10(mmHg) 3.382*10^-7 mmHg		-7.617 Log10(mmHg) 2.415*10^-8 mmHg	-6.458 Log10(mmHg) 3.486*10^-7 mmHg
Density		1.211 g/cm³	1.157 g/cm³		1.278 g/cm³	1.197 g/cm³

I'll demo this in the breakout session

Conclusion

- Transparent access to data supporting computational toxicology
- CompTox Chemicals Dashboard provides access to data for ~875,000 chemicals
- Ongoing expansion of functionality to serve all data streams for NCCT
- A clear development path ahead to add more data, models and expanded support for agency efforts around computational toxicology

Acknowledgements

EPA-RTP

- *An enormous team of contributors from NCCT, especially the IT software development team*
- *Our curation team for their care and focus on data quality*
- *Multiple centers and laboratories across the EPA*
- *Many public domain databases and open data contributors*

Contact

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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. Grulke[1], Jeff Edwards[1], Andrew D. McEachran[2], Kamel Mansouri[1,2,4], Nancy C. Baker[3], Grace Patlewicz[1], Imran Shah[1], John F. Wambaugh[1], Richard S. Judson[1] and Ann M. Richard[1]

https://doi.org/10.1186/s13321-017-0247-6