

Forward thinking data-driven and evidence-based approach to the questions

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The Charge for the Dashboard



- Develop a “first-stop-shop” for environmental chemical data to support EPA and partner decision making:
 - **Centralized location** for relevant chemical data
 - Chemistry, exposure, hazard and dosimetry
 - Combination of existing data and predictive models
 - Publicly accessible, periodically updated, curated
- Easy access to data improves efficiency and ultimately accelerates chemical risk assessment

CompTox Chemicals Dashboard

>1.2 million chemicals

CompTox Chemicals Dashboard

Home Search ▾ Lists ▾ About ▾ Tools ▾

Submit Comments

CompTox Chemicals Dashboard

Search 1,200,059 Chemicals

Chemicals




Products/Use Categories

Assay/Gene

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

Start typing to search.


☐ Identifier substring search




BASIC Search

Chemicals Product/Use Categories Assay/Gene


Q Benzo(a)pyrene




Benzo(a)pyrene
DTXSID2020139




Benzo(a)pyrene diolepoxide 1
DTXSID9036779




Benzo(a)pyrene- 7,8,9-triol,7,8,9,10-tetrahydro-, (7-alpha,8-beta,9-beta)-
DTXSID00210066




Benzo(a)pyrene-1-methanol
DTXSID40235374




Benzo(a)pyrene-1,6-dione, 7-methyl-
DTXSID70229645




Benzo(a)pyrene-10-methanol
DTXSID20235817



Benzo(a)pyrene-10-sulfonic acid, 7,8,9,10-tetrahydro-7,8,9-trihydroxy-, (7alpha,8beta,9beta)
DTXSID80154378



Benzo(a)pyrene-11,12-diol
DTXSID70215609



Benzo(a)pyrene-11,12-diol, 11,12-dihydro-, cis-
DTXSID20214501

- Type ahead search using Names, synonyms and CASRNs
- Millions of identifiers
- Substring search

Search Results

Searched with 'Synonym Substring': Benzo(A)Pyrene

183 chemicals

Detailed Chemical Pages

One more identifier – the **DTXSID**

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

▶ SAFETY

▶ ADME

▶ EXPOSURE

▶ BIOACTIVITY

SIMILAR COMPOUNDS


GENRA (BETA)

RELATED SUBSTANCES

SYNONYMS

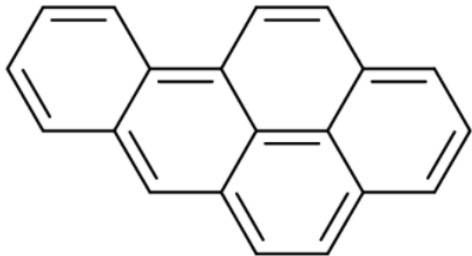
▶ LITERATURE

LINKS



Benzo(a)pyrene
50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.





Wikipedia


Benzo[a]pyrene is a polycyclic aromatic hydrocarbon and the result of incomplete combustion of organic matter at temperatures between 300 °C (572 °F) and 600 °C (1,112 °F). The ubiquitous compound can be found in coal tar, tobacco smoke and many foods, especially grilled meats. The substance with the formula C₂₀H₁₂ is one of the benzopyrenes, formed by a benzene ring fused to pyrene. Its diol epoxide metabolites (more commonly known as BPDE) react and bind to ...
[Read more](#)


Quality Control Notes


Intrinsic Properties


 Molecular Formula: C₂₀H₁₂

 Mol File

 Find All Chemicals

 Average Mass: 252.316 g/mol

 Isotope Mass Distribution

 Monoisotopic Mass: 252.0939 g/mol

Structural Identifiers

Linked Substances

Presence in Lists

- Chemical page: Wikipedia snippet when available, intrinsic properties, structural identifiers, linked substances

“Executive Summary”

Executive Summary

Quantitative Risk Assessment Values

- ✓ IRIS values available [↗](#)
- ✗ No PPRTV values
- ✓ EPA RSL values available [↗](#)
- ✓ Minimum RfD: **0.00030 mg/kg-day** (chronic, IRIS, oral, 8) [↗](#)
- ✓ Minimum RfC: **0.0000020 mg/m3** (chronic, IRIS, inhalation, 8) [↗](#)
- ✗ IVIVE POD not calculated

Quantitative Hazard Values

- ✓ Minimum oral POD: **0.070 mg/kg-day** (chronic, EFSA, oral, 5) [↗](#)
- ✓ Minimum inhalation POD: **0.0046 mg/m3** (chronic, IRIS, inhalation, 8) [↗](#)
- ✓ Lowest Observed Bioactivity Equivalent Level: [AR](#)

Cancer Information

- ✓ Cancer slope factor: **23.5 (mg/kg-day)⁻¹** (ACToR, dermal, 4) [↗](#)
- ✓ Inhalation unit risk: **2.4 (mg/m3)⁻¹** (IRIS, inhalation, 8) [↗](#)
- ✓ Carcinogenicity data available: IARC: undefinedEPA OPP cancer class: undefinedNTP Report on Carcinogens (ROC 12): undefinedNLM ToxNet HSDB carcinogenicity warningUniversity of Maryland carcinogenicity warning, [↗](#)
- ✗ No genotoxicity findings reported

Reproductive Toxicology

- ✓ Reproductive toxicity PODs available [↗](#)

Chronic Toxicology

- ✓ Chronic toxicity PODs available [↗](#)

Subchronic Toxicology

- ✓ Subchronic toxicity PODs available [↗](#)

Developmental Toxicology

- ✗ No developmental toxicity data available.

Acute Toxicology

- ✓ Acute toxicity PODs available [↗](#)

Subacute Toxicology

- ✗ No subacute toxicity data available.

Neurotoxicology

- ✗ No neurotoxicology data available.

Endocrine System

- ✓ Endocrine Disruption Potential: Significant Estrogen Receptor activity seen. Chemical was positive in **7 ER assays** (out of 12) and was positive in **3 AR assays** (tested in 6).

ADME

- ✗ No HTTK data

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 have been predicted using the SEEM modeling methodology [↗](#)

AOP Information

- ✓ AOP Links: [36](#), [61](#), [66](#), [107](#), [150](#), [163](#), [187](#), [200](#)

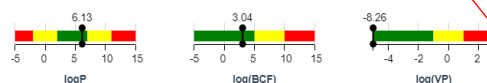
Other Notes

- ✗ No water quality values available.
- ✓ 18 Air quality values available [↗](#)
- ✓ Occupational exposure values available [↗](#)

REGIONAL SCREENING

Class	THQ	Value
GIABS (-)	THQ = 0.1	1
ABS (-)	THQ = 0.1	0.13
MCL (ug/L)	THQ = 0.1	0.2
MCLbased SSL (mg/kg)	THQ = 0.1	0.24
cancer slope factor ((mg/kg-day) ⁻¹)	THQ = 0.1	1
cancer unit risk ((ug/m3) ⁻¹)	THQ = 0.1	0.0006
RfDo (mg/kg-day)	THQ = 0.1	0.0003
RfCi (mg/m3)	THQ = 0.1	0.000002
Resident soil (mg/kg)	THQ = 0.1	0.11
Industrial soil (mg/kg)	THQ = 0.1	2.1
Resident air (ug/m3)	THQ = 0.1	0.00021
Industrial air (ug/m3)	THQ = 0.1	0.00088
Tapwater (ug/L)	THQ = 0.1	0.025
Riskbased SSL (mg/kg)	THQ = 0.1	0.029
GIABS (-)	THQ = 1	1
ABS (-)	THQ = 1	0.13
MCL (ug/L)	THQ = 1	0.2
MCLbased SSL (mg/kg)	THQ = 1	0.24
cancer slope factor ((mg/kg-day) ⁻¹)	THQ = 1	1
cancer unit risk ((ug/m3) ⁻¹)	THQ = 1	0.0006
RfDo (mg/kg-day)	THQ = 1	0.0003
RfCi (mg/m3)	THQ = 1	0.000002
Resident soil (mg/kg)	THQ = 1	0.11
Industrial soil (mg/kg)	THQ = 1	2.1
Resident air (ug/m3)	THQ = 1	0.0017
Industrial air (ug/m3)	THQ = 1	0.0088
Tapwater (ug/L)	THQ = 1	0.025
Riskbased SSL (mg/kg)	THQ = 1	0.029

PHYSICHEM PARAMETERS



- Overview of toxicity-related info
 - Quantitative values
 - Info re. toxicology subsets
 - Physchem. and Fate & Transport
 - Adverse Outcome Pathway links
 - *In vitro* bioactivity summary plot


Quantitative Risk Assessment Values

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Experimental and Predicted Data



Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

Property

Summary

Download Columns

Property	Experimental average	Predicted average
Water Solubility	8.40e-9 (4)	1.75
LogKow: Octanol-Water	6.13 (2)	6.24
Vapor Pressure	5.49e-9 (1)	3.61e-9
Boiling Point	495 (3)	480
Henry's Law	4.57e-7 (1)	4.59e-7
Melting Point	177 (8)	189
Surface Tension	-	53.9
Flash Point	-	234
Density	-	1.28

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

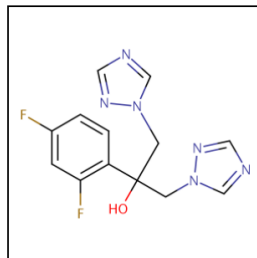
OPERA Reports

OPERA Models: LogKow: Octanol-Water

Fluconazole

86386-73-4 | DTXSID3020627

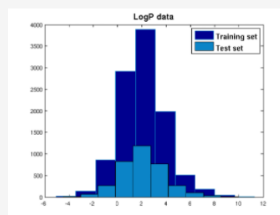
Print PDF



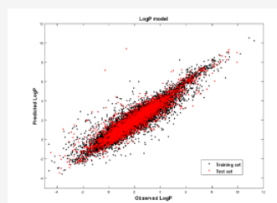
Model Results

Predicted value: 0.501
Global applicability domain: Inside
Local applicability domain index: 0.998
Confidence level: 0.732

Model Performance



QMRP

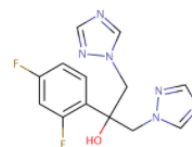


Weighted KNN model

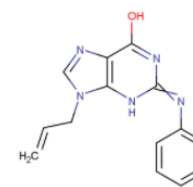
Weighted KNN model

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

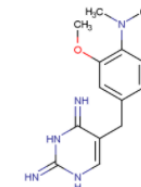
Nearest Neighbors from the Training Set



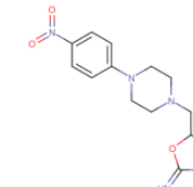
Fluconazole
Measured: 0.5
Predicted: 0.50



GUANINEN2PHENYL9ALLYL
Measured: 1.75
Predicted: 1.75




2,4-PYRIMIDINEDIAMINE, 5-[(4-(DIMETHYLAMINO)-3-M
Measured: 1.87
Predicted: 1.87



5-(1-P-NITROPHENYL-4-PIPERAZINYL)METHYL-2-AMINO-
Measured: 1.23
Predicted: 1.23

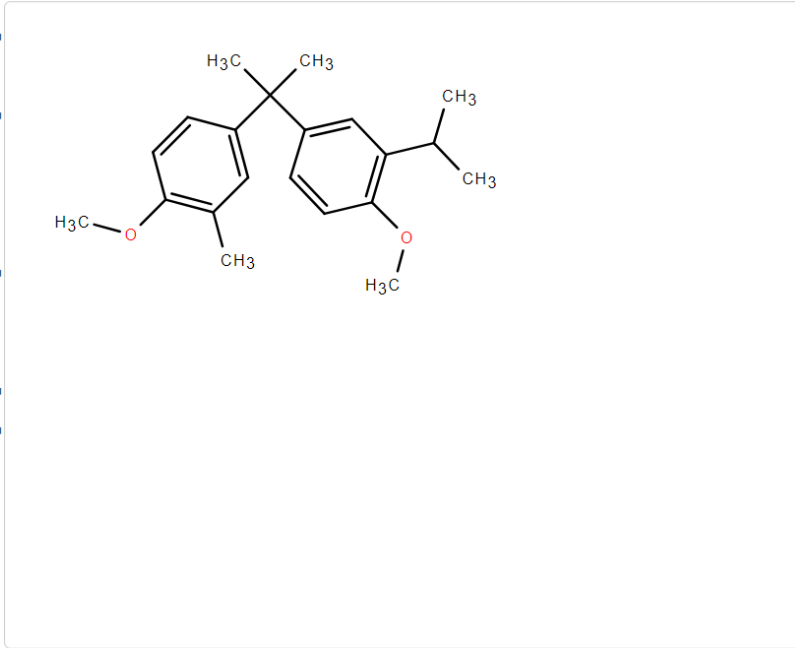
Real-Time Predictions



United States
Environmental Protection
Agency

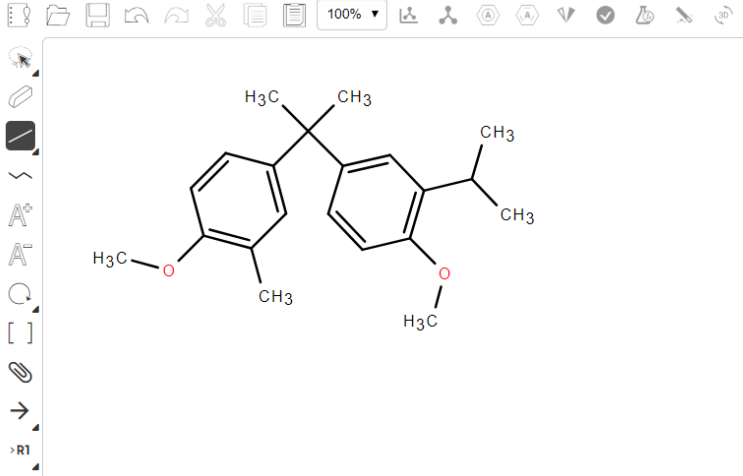
Home Advanced Search Batch Search Lists Predictions Downloads

Share Search all data



Chemical structure diagram showing a biphenyl system. The left ring has a methoxy group (H₃C-O-) at the para position and a methyl group (-CH₃) at the meta position. The right ring has a methyl group (-CH₃) at the para position, a propoxy group (-O-CH₂-CH₂-CH₃) at the meta position, and a methyl group (-CH₃) at the ortho position. The two rings are connected by a methylene group (-CH₂-) at the 1-position of the right ring.

100%



Chiral

Select properties to predict

H **C** **N** **O** **S** **P** **F** **Cl** **Br** **I** **PT**

TEST.

- ☒ **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

Calculate

ToxVal Database

- >50k chemicals
- >770k tox. values
- >30 sources of data
- ~5k journals cited
- ~70k citations

Hazard

DataType
Toxicity Value

Human Eco

Download Columns 10 Search query

More	Priority	Type	Subtype	Risk assessment class	Value	Units	Study type	Exposure route	Species	Subsource	Source
	7	cancer slope factor	-	chronic	23.5	(mg/kg-day)-1	-	dermal	-	Alaska DEC	Alaska DEC
	7	cancer unit risk	-	chronic	0.21	(mg/l)-1	-	inhalation	-	Alaska DEC	Alaska DEC
	7	cancer slope factor	-	chronic	3.08	(mg/kg-day)-1	-	inhalation	-	Alaska DEC	Alaska DEC
	7	cancer unit risk	-	chronic	0.88	(mg/m3)-1	-	inhalation	-	Alaska DEC	Alaska DEC
	7	cancer slope factor	-	chronic	7.3	(mg/kg-day)-1	-	oral	-	Alaska DEC	Alaska DEC
	7	MEG	Short-term Critical Air	short-term	80	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Short-term Marginal Air	short-term	15	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Soil Negligible Soil	chronic	12	mg/kg	-	Soil	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Long-Term, SL/d Negligible Water	chronic	0.0134	mg/L	-	oral	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Short-term Negligible Air	short-term	0.6	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD

<< < 1 2 3 4 > >>

Showing 1 to 10 of 32 records

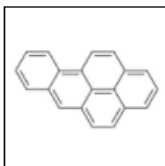
[anced_search/index](#)

Hazard Data for Copper

- 2246 rows of human hazard and ecotox data can be harvested with three clicks

1	SOURCE	SUB_SOURCE	TOXVAL_1	TOXVAL_TYPE_ORIGINAL	TOXVAL_TYPE_SUP	TOXVAL_1	TOXVAL_1	TOXVAL_1	TOXVAL_1	TOXVAL_1	TOXVAL_1	RISK_ASSE
2	ATSDR MRLs 2020	CDC	MRL	ATSDR MRL	Toxicity Value	MRL	=	0.01	0.01	mg/kg-day	mg/kg-day	acute
3	ATSDR MRLs 2020	CDC	NOAEL	NOAEL	Point of Departure	NOAEL	=	0.03	0.03	mg/kg-day	mg/kg-day	acute
4	California DPH	California	MCL	MCL California	Exposure Limit	MCL	=	1.3	1.3	mg/L	mg/L	chronic
5	California DPH	California	MCL	MCL Federal	Exposure Limit	MCL	=	1.3	1.3	mg/L	mg/L	chronic
6	California DPH	California	OEHHHA PH	OEHHHA PHG	Exposure Limit	Public Hea	=	0.3	0.3	mg/L	mg/L	chronic
7	Cal OEHHHA	California	MCL	MCL	Exposure Limit	MCL	=	1.3	1.3	mg/L	mg/L	chronic
8	Cal OEHHHA	California	REL	REL	Toxicity Value	REL	=	100	100	ug/m3	ug/m3	acute
9	Copper Manufacturers	Copper De	adequate	AI (adequate intake)			=	0.4	0.4	mg/day	mg/day	chronic
10	Copper Manufacturers	Copper De	adequate	AI (adequate intake)			=	0.7	0.7	mg/day	mg/day	chronic
11	Copper Manufacturers	Copper De	adequate	AI (adequate intake)			=	1	1	mg/day	mg/day	chronic
12	Copper Manufacturers	Copper De	adequate	AI (adequate intake)			=	1.1	1.1	mg/day	mg/day	chronic
13	Copper Manufacturers	Copper De	adequate	AI (adequate intake)			=	1.3	1.3	mg/day	mg/day	chronic
14	Copper Manufacturers	Copper De	adequate	AI (adequate intake)			=	1.5	1.5	mg/day	mg/day	chronic
15	Copper Manufacturers	Copper De	adequate	AI (adequate intake)			=	1.6	1.6	mg/day	mg/day	chronic
16	Copper Manufacturers	Copper De	drinking w	GDWQ (guideline for drinking water quality)			=	2	2	mg/L	mg/L	chronic
17	Copper Manufacturers	Copper De	LOAEL	LOAEL	Point of Departure	LOAEL	=	7	7	mg/day	mg/day	subchroni
18	Copper Manufacturers	Copper De	optimal in	Optimal intake value	Misc Information	Optimal in	=	2.6	2.6	mg/day	mg/day	chronic
19	Copper Manufacturers	Copper De	RDA	RDA (recommended dietary allowance)			=	0.2	0.2	mg/day	mg/day	chronic
20	Copper Manufacturers	Copper De	RDA	RDA (recommended dietary allowance)			=	0.34	0.34	mg/day	mg/day	chronic
21	Copper Manufacturers	Copper De	RDA	RDA (recommended dietary allowance)			=	0.7	0.7	mg/day	mg/day	chronic

Sources of Exposure to Chemicals



Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

Chemical Weight Fractions

 Download ▾

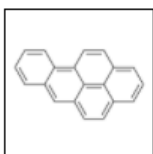
Columns ▾

10 ▾

Search query

Product Name	Product Use Category	Minimum Weight Fraction	Maximum Weight Fraction	Data Type	Source
m-525-1-5x pah mixtures 0.5 mg/ml for method 525	Not Yet Categorized:			MSDS	SIRI
mm6125 surface conditioner	Not Yet Categorized:			Health Product Declaration	Health Product Declaration Collaborative
monolithic membrane 6125 (mm6125) / monolithic membrane	Not Yet Categorized:			Health Product Declaration	Health Product Declaration Collaborative
organic potablewatr pw 32_component h:reg semi-volatile 690	Not Yet Categorized:	0.00	1.00e-3	MSDS	SIRI
polynuclear aromatic hydrocarbon mixture_ep84627	Not Yet Categorized:			MSDS	SIRI
prestone(r) power steering fluid	engine maintenance: auto fluids and additives			MSDS	CPCPdb
r-12 shield tite wet surface coating	Not Yet Categorized:	0.00	0.500	MSDS	SIRI
sea tar 1010_0028	Not Yet Categorized:			MSDS	SIRI
supelprime-hc kit pah mix_48909	Not Yet Categorized:			MSDS	SIRI
supelprime-hc pah mix 1mL_48905	Not Yet Categorized:			MSDS	SIRI

Similarity Searching



Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

Searched with a similarity threshold of 0.8

237 of 276 chemicals visible

Select all

Download

Send to Batch Search

Similarity



DTXSID

CASRN

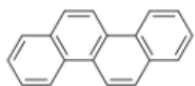
Similarity



Isotopes

Multicomponent Chemicals

Filter by Name or CASRN

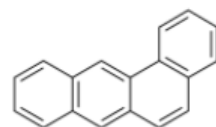


Chrysene

DTXSID:DTXSID0022432

CASRN:218-01-9

Similarity:1.00

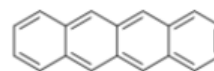


Benz(a)anthracene

DTXSID:DTXSID5023902

CASRN:56-55-3

Similarity:1.00

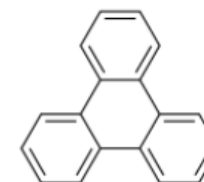


Naphthalene

DTXSID:DTXSID4059045

CASRN:92-24-0

Similarity:1.00

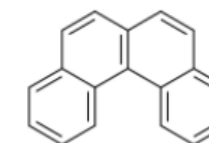


Triphenylene

DTXSID:DTXSID9059757

CASRN:217-59-4

Similarity:1.00



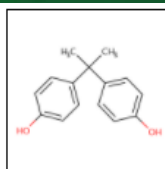
Benzo[c]phenanthrene

DTXSID:DTXSID4075459

CASRN:195-19-7

Similarity:1.00

Related Substances



Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

9 chemicals

Select all

Download

Send to Batch Search

Relationship



DTXSID

CASRN

TOXCAST

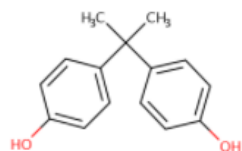


Hide chemicals that are:

Filter by Name or CASRN



Searched Chemical



[Bisphenol A](#)

DTXSID:DTXSID7020182

CASRN:80-05-7

TOXCAST:217/1152

Polymer

2 related chemical
structures with this
substance

[Formaldehyde, polymer with bisphenol A](#)

DTXSID:DTXSID3049627

CASRN:25085-75-0

TOXCAST:-

Polymer

2 related chemical
structures with this
substance

[Bisphenol A/ Epichlorohydrin resin](#)

DTXSID:DTXSID0050479

CASRN:25068-38-6

TOXCAST:-

Polymer

3 related chemical
structures with this
substance

[Bisphenol A-epichlorohydrin-polyformal...](#)

DTXSID:DTXSID9050480

CASRN:28906-96-9

TOXCAST:-

Predecessor: Component

4 related chemical
structures with this
substance

[Fatty acids, C18-unsatd., dimers, polyme...](#)

DTXSID:DTXSID40105886

CASRN:106906-26-7

TOXCAST:-

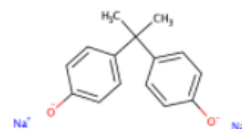
Predecessor: Component

3 related chemical
structures with this
substance

Predecessor: Component

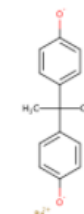
2 related chemical
structures with this
substance

Salt Form



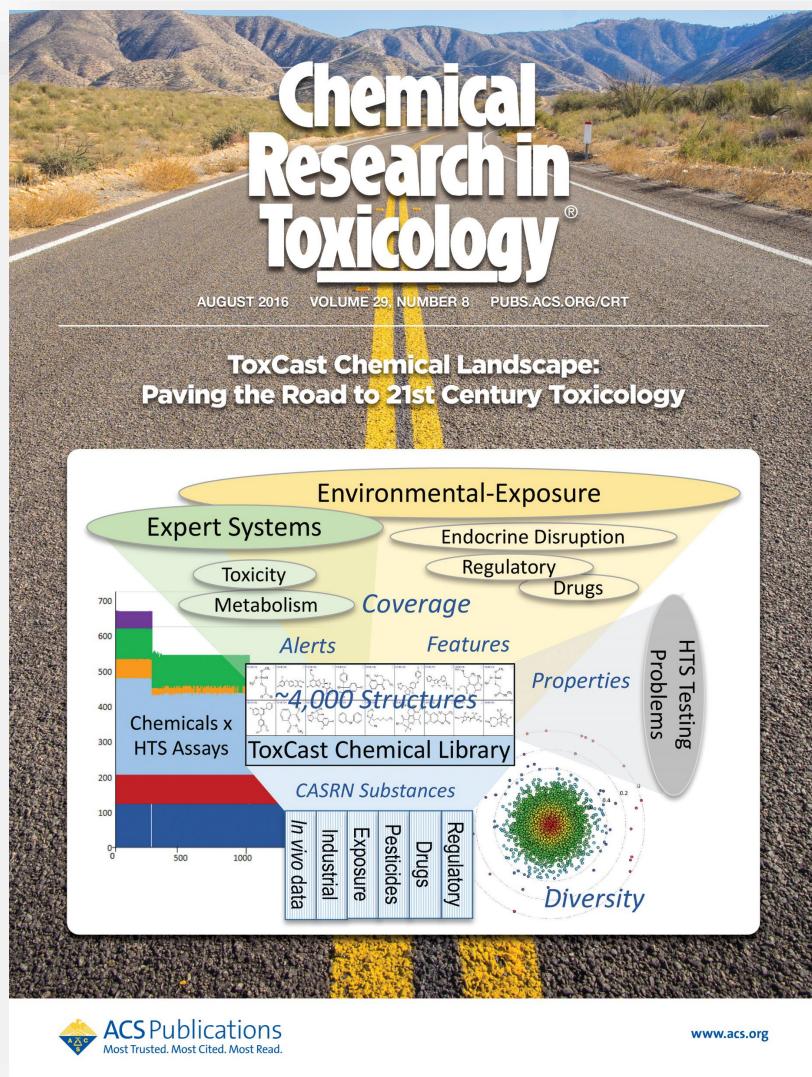
[Disodium 4,4'-isopropylidenediphenolate](#)

Salt Form



[Barium\(2+\) 4,4'-isopropylidenebispheno...](#)

Bioactivity Data



ToxCast Chemical Landscape: Paving the Road to 21st Century Toxicology

Ann M. Richard^{††}, Richard S. Judson[†], Keith A. Houck[†], Christopher M. Grulke[†], Patra Volarath[†], Inthirany Thillainadarajah[§], Chihae Yang^{||}, James Rathman^{±#}, Matthew T. Martin[†], John F. Wambaugh[†], Thomas B. Knudsen[†], Jayaram Kancherla[▽], Kamel Mansouri[▽], Grace Patlewicz[†], Antony J. Williams[†], Stephen B. Little[†], Kevin M. Crofton[†], and Russell S. Thomas[†]

View Author Information ▾

✓ **Cite this:** *Chem. Res. Toxicol.* 2016, 29, 8, 1225–1251

Publication Date: July 1, 2016 ▾

<https://doi.org/10.1021/acs.chemrestox.6b00135>

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Bioactivity Data

Summary views of >2000 Assay Endpoints

Bioactivity

ToxCast: Summary

Toxcast Conc. Response Data

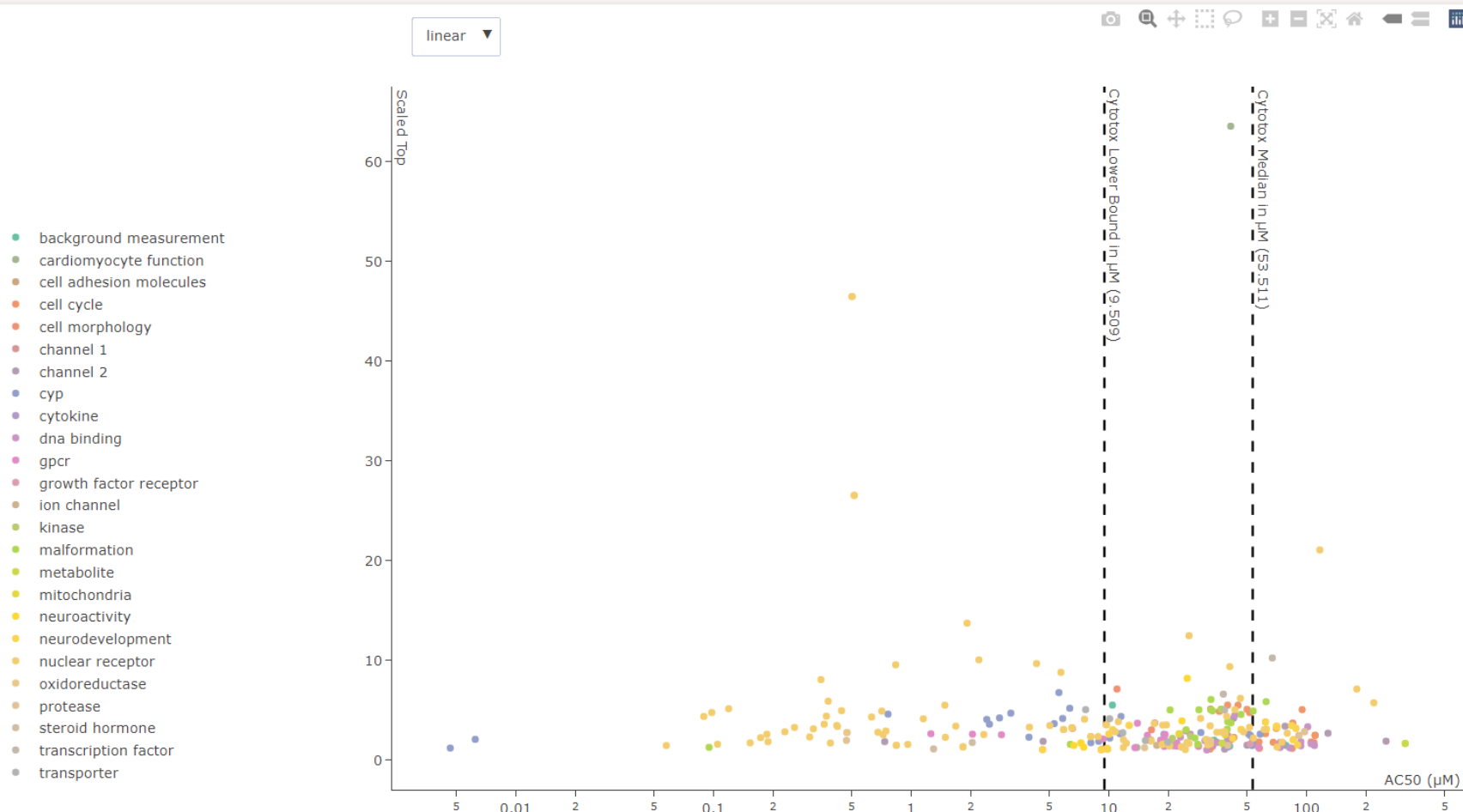
HTTr: Summary

HTPP: Summary

PubChem

ToxCast: Models

Bioactivity - TOXCAST Summary



Bioactivity Data

Full transparency of data...

Bioactivity

ToxCast: Summary

Toxcast Conc. Response Data

HTTr: Summary

HTPP: Summary














































PubChem

ToxCast: Models

Concentration Response Data

Analytical Data on Tox21 Browser [↗](#)

 EXPORT

<input type="checkbox"/>	Name ↑	Description	Endpoint Name	Active	Details	Rep. Plot	All Plots	Gene	Intended Target	Cell Line	Cell Format
<input type="checkbox"/>											
<input type="checkbox"/>	ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_agonist_80hr	Inactive				AR	steroidal	prostate	cell line
<input type="checkbox"/>	ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_agonist_AUC_viability	Active				-	cytotoxicity	prostate	cell line
<input type="checkbox"/>	ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_antagonist_80hr	Active				AR	steroidal	prostate	cell line
<input type="checkbox"/>	ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_antagonist_AUC_viability	Active				-	cytotoxicity	prostate	cell line
<input type="checkbox"/>	ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_ER_80hr	Active				ESR1	steroidal	breast	cell line
<input type="checkbox"/>	ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_ER_AUC_viability	Inactive				-	cytotoxicity	breast	cell line
<input type="checkbox"/>	ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_1h_dn	Inactive				-	proliferation	liver	cell line
<input type="checkbox"/>	ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_1h_up	Inactive				-	arrest	liver	cell line
<input type="checkbox"/>	ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_24h_dn	Inactive				-	proliferation	liver	cell line
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<input type="checkbox"/>	ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_72h_dn	Inactive				-	proliferation	liver	cell line
<input type="checkbox"/>	ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_72h_up	Inactive				-	arrest	liver	cell line
<input type="checkbox"/>	ASSAY SOURCE: APR	Apredica	APR_HepG2_CellLoss_1h_dn	Inactive				-	cytotoxicity	liver	cell line
<input type="checkbox"/>	ASSAY SOURCE: APR	Apredica	APR_HepG2_CellLoss_1h_up	Inactive				-	proliferation	liver	cell line
<input type="checkbox"/>	ASSAY SOURCE: APR	Apredica	APR_HepG2_CellLoss_24h_dn	Active				-	cytotoxicity	liver	cell line

Rows: 1,398

Total Rows: 1,398

Bioactivity Data ...including concentration-response

Bioactivity

ToxCast: Summary

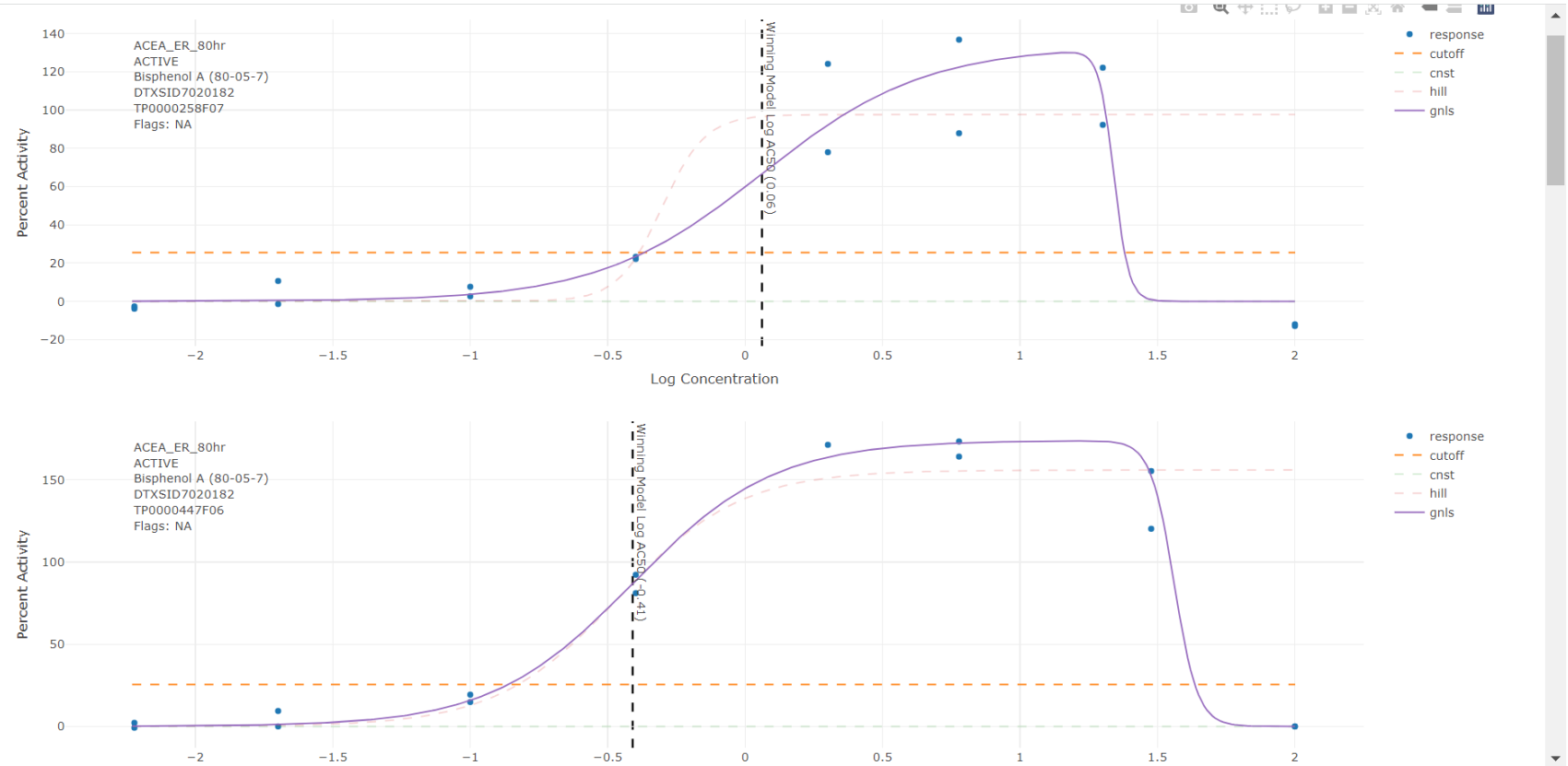
Toxcast Conc. Response Data

HTTr: Summary

HTPP: Summary

PubChem

ToxCast: Models



Bioactivity Data

NEW High-Throughput Transcriptomics

Bioactivity

ToxCast: Summary

Toxcast Conc. Response Data

HTTr: Summary

HTPP: Summary

PubChem

ToxCast: Models

Bioactivity - HTTr Summary

- Biomolecular Process
- Blood
- Cancer
- Cancer|Immune
- Cardiovascular
- Cell Cycle
- Chemical Property
- Cholinergic
- Congenital Disorder
- CYP
- Enzyme
- GPCR
- Growth Factor
- Hormone
- Immune
- Immune|Blood
- Infection
- Ion Channel
- Kinase
- Lipid
- Musculoskeletal
- NA
- Nervous System
- Nuclear Receptor
- Other
- Pesticide
- Pregnancy Complication
- Random
- Skin
- Stress
- Thyroid
- Transcription Factor
- Translation/Transcription
- Transporter

values from active signatures only (nitcat>0.9). The x-axis is concentration in μM , and the y-axis is the top value from the curve fit. Data is shown at the signature level (one dot per signature or gene set). Signatures are organized into "super targets", which can be genes, gene families or higher order biological processes, up to human diseases. The process of curve fitting is described [here](#) and the overall signature scoring process is described [here](#). <https://doi.org/10.1093/toxsci/kfab00>



Bioactivity Data

NEW High-Throughput Phenotypic Profiling

Bioactivity

ToxCast: Summary

Toxcast Conc. Response Data

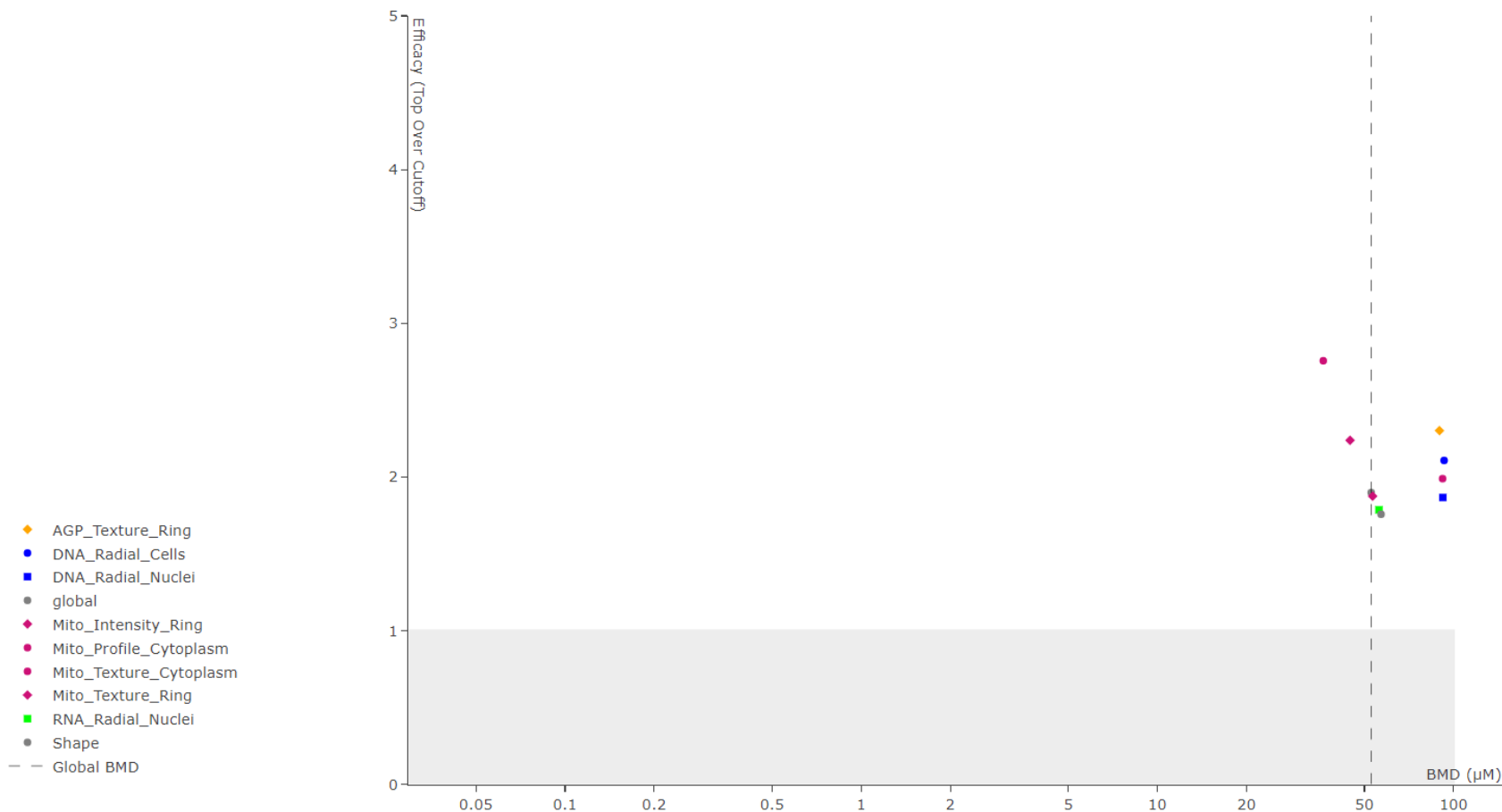
HTTr: Summary

HTPP: Summary

PubChem

ToxCast: Models

HTPP Category Plot



Bioactivity Data

Bioactivity

ToxCast: Summary

Toxcast Conc. Response Data

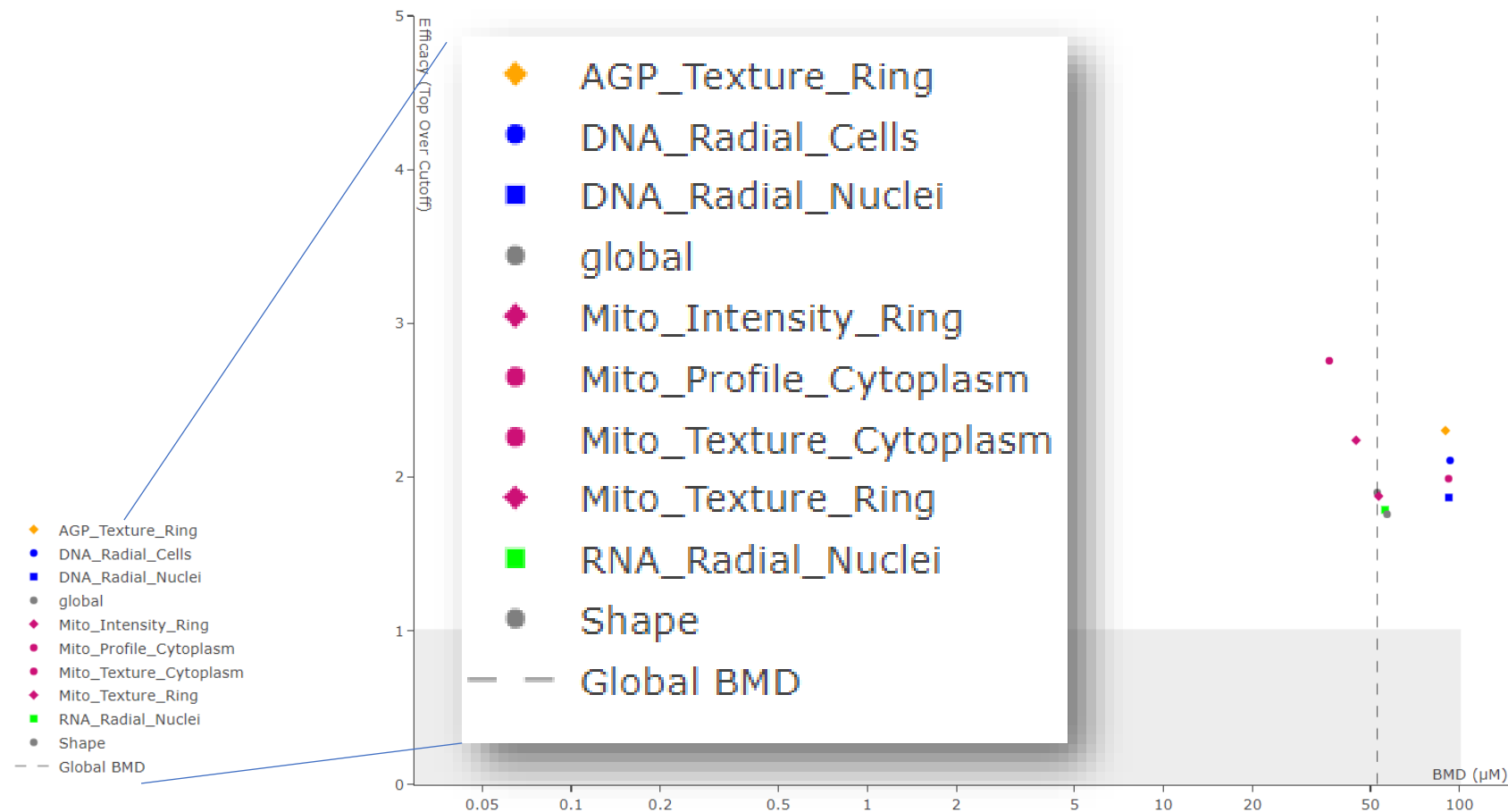
HTTr: Summary

HTPP: Summary

PubChem

ToxCast: Models

HTPP Category Plot



Use Models Derived from the Data

Screening Chemicals for Estrogen Receptor Bioactivity Using a Computational Model

Patience Browne^{*†}, Richard S. Judson[‡], Warren M. Casey[§], Nicole C. Kleinstreuer^{||}, and Russell S. Thomas[‡]

[View Author Information](#) ▾

✓ **Cite this:** *Environ. Sci. Technol.* 2015, 49, 14, 8804–8814

Publication Date: June 12, 2015 ▾

<https://doi.org/10.1021/acs.est.5b02641>

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[Vol. 124, No. 7](#) | Research

CERAPP: Collaborative Estrogen Receptor Activity Prediction Project

Kamel Mansouri, Ahmed Abdelaziz, Aleksandra Rybacka, Alessandra Roncaglioni, Alexander Tropsha, Alexandre Varnek, Alexey Zakharov, Andrew Worth, Ann M. Richard, Christopher M. Grulke, Daniela Trisciuzzi, Denis Fourches, Dragos Horvath, Emilio Benfenati, Eugene Muratov, Eva Bay Wedeby, Francesca Grisoni, Giuseppe F. Mangiatordi, ... [See all authors](#) ▾

Published: 1 July 2016 | <https://doi.org/10.1289/ehp.1510267> | Cited by: 76

CERAPP and CoMPARA available in
OPERA

Development and Validation of a Computational Model for Androgen Receptor Activity

Nicole C. Kleinstreuer^{*†} , Patricia Ceger[‡], Eric D. Watt[§] , Matthew Martin[§], Keith Houck[§], Patience Browne^{||}, Russell S. Thomas[§], Warren M. Casey[†], David J. Dix[‡], David Allen[‡], Srilatha Sakamuru[#], Menghang Xia[#], Ruili Huang[#], and Richard Judson[§]

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✓ **Cite this:** *Chem. Res. Toxicol.* 2017, 30, 4, 946–964

Publication Date: November 18, 2016 ▾

<https://doi.org/10.1021/acs.chemrestox.6b00347>

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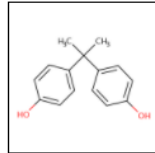
[Vol. 128, No. 2](#) | Research

CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity

Kamel Mansouri , Nicole Kleinstreuer, Ahmed M. Abdelaziz, Domenico Alberga, Vinicius M. Alves, Patrik L. Andersson, Carolina H. Andrade, Fang Bai, Ilya Balabin, Davide Ballabio, Emilio Benfenati, Barun Bhatarai, Scott Boyer, Jingwen Chen, Viviana Consonni, Sherif Farag, Denis Fourches, Alfonso T. García-Sosa, Paola Gramatica, Francesca Grisoni, ... [See all authors](#)

Published: 7 February 2020 | CID: 027002 | <https://doi.org/10.1289/EHP5580> | Cited by: 2

For Endocrine (AR and ER) better to use summary models




Bisphenol A






80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

Positive ToxCast ER pathway agonist and ToxCast AR antagonist scores.

ToxCast: Models
ToxCast Model Predictions

 Download ToxCast Model Predictions ▾

Model	Receptor	Agonist	Antagonist	Binding
 ToxCast Pathway Model (AUC)	Androgen	0.00	0.345	-
 ToxCast Pathway Model (AUC)	Estrogen	0.450	0.00	-
 COMPARA (Consensus)	Androgen	Inactive	Active	Active
 CERAPP Potency Level (From Literature)	Estrogen	Active (Weak)	-	Active (Weak)
 CERAPP Potency Level (Consensus)	Estrogen	Active (Weak)	Active (Strong)	Active (Weak)

CERAPP = consensus ER QSAR (from 17 groups)

COMPARA = consensus AR QSAR

ToxCast Pathway Model AUC ER = full ER model (18 assays)

ToxCast Pathway Model AUC AR = full AR model (11 assays)

DETAILS

EXECUTIVE SUMMARY

PROPERTIES

ENV. FATE/TRANSPORT

HAZARD

► SAFETY

► ADME

► EXPOSURE

▼ BIOACTIVITY

TOXCAST: SUMMARY

EDSP21

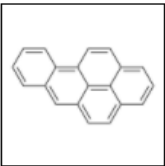
TOXCAST/TOX21

PUBCHEM

TOXCAST: MODELS

Searching Literature and the Internet

Identifiers Support Searches in other systems



Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

Synonyms

Download

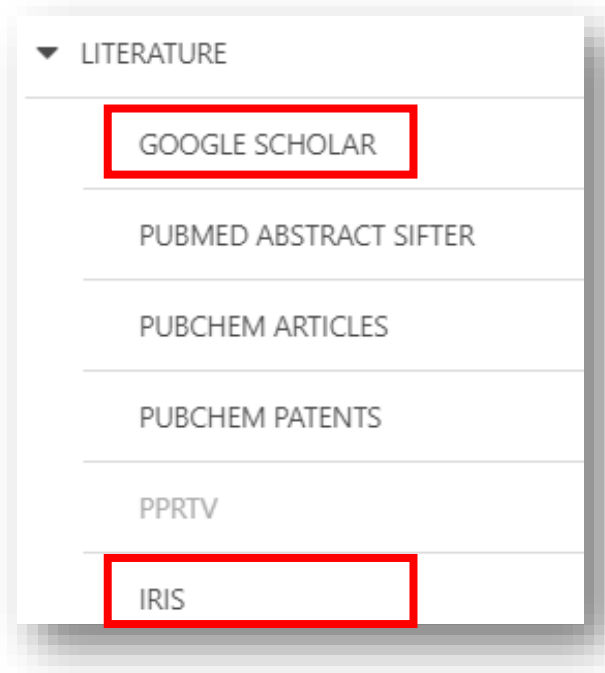
25

Search query

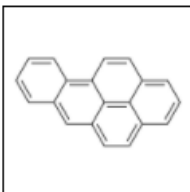
Synonym	Quality
Benzo(a)pyrene	Valid
Benzo[pqr]tetraphene	Valid
Benzo[a]pyrene	Valid
50-32-8 Active CAS-RN	Valid
BaP	Valid
Benzo[a]pyrene	Good
3,4-Benz[a]pyrene	Good
3,4-Benzopyrene	Good
3,4-Benzpyrene	Good
6,7-Benzopyrene	Good
BENZ(A)PYREN	Good
Benz(a)pyrene	Good
Benz[a]pyrene	Good

Identifiers are used in the app

- Identifiers are used to feed and link into “Literature”



A screenshot of the EPA IRIS website. The header features the EPA logo and navigation links: "Environmental Topics", "Laws & Regulations", and "About EPA". A search bar is located on the right. The main content area is titled "IRIS" and includes a sidebar with links: "IRIS Home", "About IRIS", "IRIS Recent Additions", "IRIS Calendar", "IRIS Assessments" (highlighted), "Advanced Search", "IRIS Program Materials", and "Contact Us". The main content area displays the title "Benzo[a]pyrene (BaP)" and its CASRN (50-32-8) and DTXSID (2020139). It lists three documents: "Toxicological Review (PDF)", "IRIS Executive Summary (PDF)", and "Supplemental Information on the IRIS Toxicological Review of Benzo[a]pyrene". Below this, there are tabs for "Key IRIS Values", "Organ/System Specific Values", "Chemical Documents", and "Other EPA Information". The "Noncancer Assessment" section is visible, showing the "Reference Dose for Oral Exposure (RfD) (PDF)" and its last updated date (01/19/2017). A table with columns "System", "RfD (mg/kg-day)", "Basis", and "PoD" is partially visible. On the right, a "Related Links" section contains a link to the "EPA Chemicals Dashboard - Benzo[a]pyrene (BaP)".




Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

Abstract Sifter

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

Hazard 

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.



("50-32-8" OR "Benzo(a)pyrene") AND (NOAEL OR NOEL OR LOEL OR Rfd OR "reference dose" OR "reference concentration" OR "adverse effect level"[tiab] OR "cancer slope factor"[tiab])

- Real-time retrieval of data from PubMed (~30 million abstracts and growing)
- Choose from set of pre-defined queries
- Adjust and fine tune queries based on interests

Literature Searching

- “Sifting” of results using multiple terms
- Frequency counting terms
- Color highlighting of terms
- Download list to Excel
- Send list to PubMed for downloading ref. file
- Direct link via PubMed ID

To find articles quickly, enter terms to sift abstracts. 

dermal cancer pyrene  

<input type="checkbox"/>	dermal	cancer ↓	pyrene	Total	PMID	Year	Title	Authors	Journal	Rev
<input type="checkbox"/>	0	7	1	8	23922326	2013	Using immunotoxicity information to improve cancer risk a...	Zaccaria, McClure	International journal of toxicology	✓
<input type="checkbox"/>	8	7	2	17	16632147	2006	Development of a dermal cancer slope factor for benzo[a]...	Knafila, Philipps, Brecher, Petrovic, Richardson	Regulatory toxicology and pharmacology : RTP	✓
<input type="checkbox"/>	4	6	2	12	33359623	2020	Testing the validity of a proposed dermal cancer slope fac...	Magee; Forsberg	Regulatory toxicology and pharmacology : RTP	✓
<input type="checkbox"/>	0	5	1	6	28477805	2017	Pollution characteristics, sources and lung cancer risk of ...	Wang; Xia; Wu; Zhang; Sun; Yin; Zhou; Yang	Journal of environmental sciences (China)	
<input type="checkbox"/>	4	4	2	10	20888881	2010	Development and application of a skin cancer slope factor...	Knafila; Petrovic; Richardson; Campbell; Rowat	Regulatory toxicology and pharmacology : RTP	
<input type="checkbox"/>	4	4	1	9	16307791	2005	Health risk assessment on human exposed to environme...	Chen; Liao	The Science of the total environment	
<input type="checkbox"/>	2	4	1	7	11807932	2002	Cancer risk assessment for oral exposure to PAH mixtures.	Schneider; Roller; Kalberlah; Schuhmacher-Wolz	Journal of applied toxicology : JAT	
<input type="checkbox"/>	2	3	1	6	32460055	2020	PAHs in Chinese atmosphere Part II: Health risk assessm...	Ma; Zhu; Liu; Jia; Yang; Li	Ecotoxicology and environmental safety	
<input type="checkbox"/>	0	3	1	4	23379661	2013	Parent and halogenated polycyclic aromatic hydrocarbon...	Ni; Guo	Journal of agricultural and food chemistry	
<input type="checkbox"/>	0	3	1	4	20800879	2010	Health risk assessment on dietary exposure to polycyclic ...	Xia; Duan; Qiu; Liu; Wang; Tao; Jiang; Lu; Song; Hu	The Science of the total environment	
<input type="checkbox"/>	2	3	1	6	16293284	2005	Probabilistic risk assessment for personal exposure to car...	Liao; Chiang	Chemosphere	
<input type="checkbox"/>	0	2	1	3	17544483	2007	Health risk assessment for traffic policemen exposed to p...	Hu; Bai; Zhang; Wang; Zhang; Yu; Zhu	The Science of the total environment	
<input type="checkbox"/>	0	1	1	2	28795279	2017	Human health risk assessment and PAHs in a stretch of ri...	Srivastava; Sreekrishnan; Nema	Environmental monitoring and assessment	
<input type="checkbox"/>	0	1	1	2	12634119	2003	Deviation from additivity in mixture toxicity: relevance of n...	Lutz; Vamvakas; Kopp-Schneider; Schlatter; Stopper	Environmental health perspectives	
<input type="checkbox"/>	0	1	2	3	3709501	1986	The adsorption of polyaromatic hydrocarbons on natural a...	Menard; Noel; Khorami; Jouve; Dunnigan	Environmental research	
<input type="checkbox"/>	0	0	1	1	33136306	2020	Effects on Animal Outcomes of Regulatory Relevance of F...	Crumo; Boulanger; Farhat; Williams; Basu; Hecker	Environmental toxicology and chemistry	

Development of a dermal cancer slope factor for benzo[a]pyrene.
Polycyclic aromatic hydrocarbons (PAHs) are commonly found at environmentally impacted sites in both Canada and the United States, and also occur naturally. Typically, benzo[a]pyrene (B[a]P) is selected as a standard to which the cancer potencies of other carcinogenic PAHs are compared. Cancer potency estimates for B[a]P have been published for the oral and inhalation routes of exposure, however, no such estimate has been established by a regulatory agency for dermal exposure. The main objectives of the current investigation were to: evaluate approaches used to examine the relative carcinogenicity of PAHs; to conduct a review of mammalian dermal carcinogenicity studies for B[a]P; and derive a cancer slope factor for dermal exposure to PAHs using B[a]P as a surrogate for other PAHs. The toxicological database of dermal B[a]P studies was examined for relevant animal bioassays. Seven relevant studies were identified. A cancer slope factor for B[a]P was developed using the benchmark dose approach and the linearized multistage model. The upper 95th CI at the 5% effect level above background incidence was used as the point of departure for low-dose linear extrapolation. An average slope factor of 0.55 (microg/animal day)⁻¹ was calculated for mice, which was converted to a dose-equivalent slope factor of 25 (mg/kg day)⁻¹. This latter slope factor is proposed for application to human health risk assessment with no scaling adjustment. Dermal potency equivalency factor values were identified which may be used with other carcinogenic PAH in the calculation of total B[a]P equivalent dermal cancer risk estimates. An identified area for further investigation is the consideration of scaling in extrapolating the calculated dermal cancer slope factor from mice to humans.

What's the best way to search the internet for chemical data?

- We know how complex chemicals identifiers are...
 - CASRN(s)
 - Hundreds of names (maybe)
 - SMILES
 - InChIs
 - EINECS, EC numbers
- What can WE do to help you navigate the internet?

External Links – Also use Identifiers Names, CASRN, PubChem IDs, InChIs...























Benzo(a)pyrene




















50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.




















General

-  EPA Substance Registry Service
-  PubChem
-  ChempSpider
-  CPCat
-  DrugBank
-  Wikipedia
-  MSDS Lookup
-  ChEMBL
-  ToxPlanet
-  ACS Reagent Chemicals
-  Wolfram Alpha
-  ECHA Infocard
-  ChemAgora
-  Consumer Product Information Database
-  ChEBI
-  NIST Chemistry Webbook
-  WEBWISER
-  PubChem Safety Sheet
-  Consumer Product Information Database
-  PubChem: Chemical Vendors













Toxicology

-  ACToR
-  DrugPortal
-  CCRIS
-  ChemView
-  CTD
-  eChemPortal
-  Gene-Tox
-  HSDB
-  ACToR PDF Report
-  CREST
-  National Air Toxics Assessment
-  ECOTOX
-  ChemView
-  Chemical Checker
-  BindingDB
-  CalEPA OEHHHA
-  NIOSH IDLH Values
-  LactMed
-  ECOTOX






Publications

-  Toxline
-  PPRTVWEB
-  PubMed
-  IRIS Assessments
-  EPA HERO
-  NIOSH Skin Notation Profiles
-  NIOSH Pocket Guide
-  RSC Publications
-  BioCaddie DataMed
-  Springer Materials
-  Bielefeld Academic Search Engine
-  CORE Literature Search
-  Google Books (Text Search)
-  Google Patents (Text search)
-  Google Scholar (Text search)
-  Google Patents (Structure search)
-  Google Books (Structure Search)
-  Google Scholar (Structure search)
-  Federal Register

Analytical

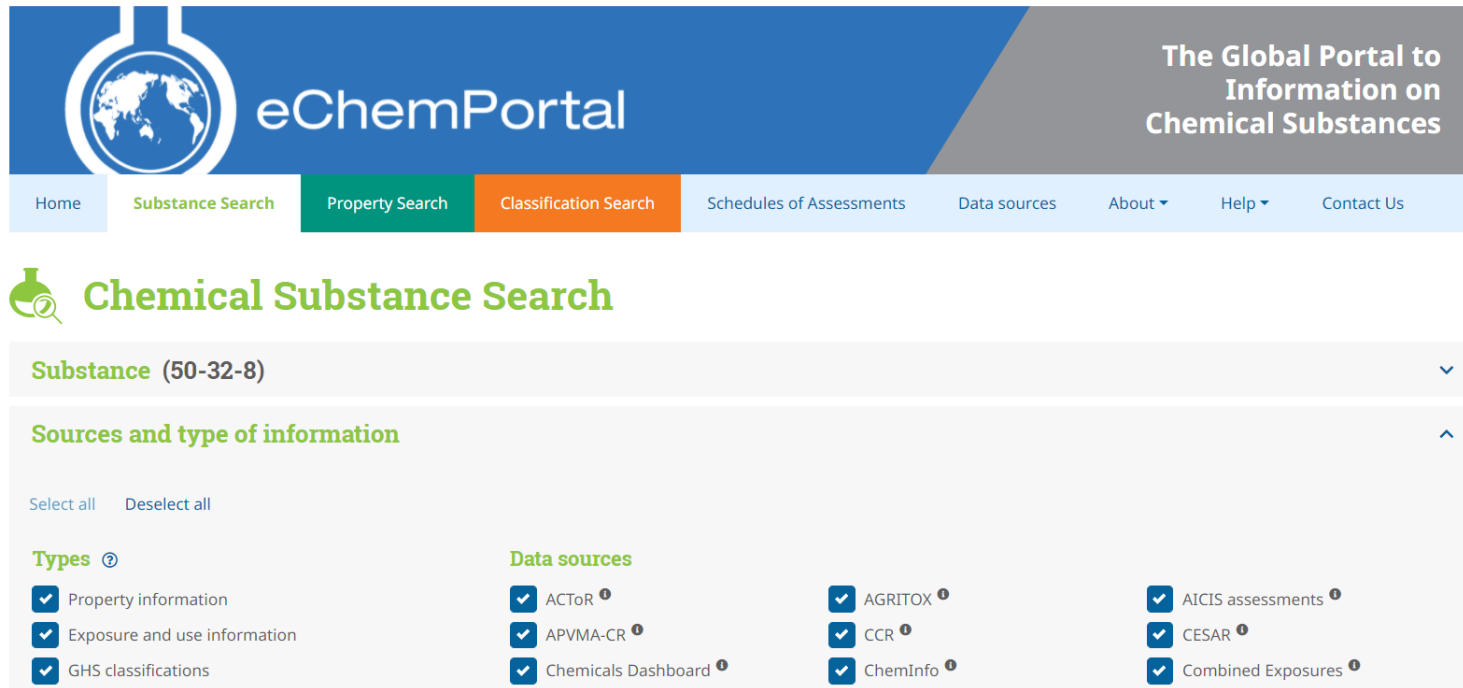
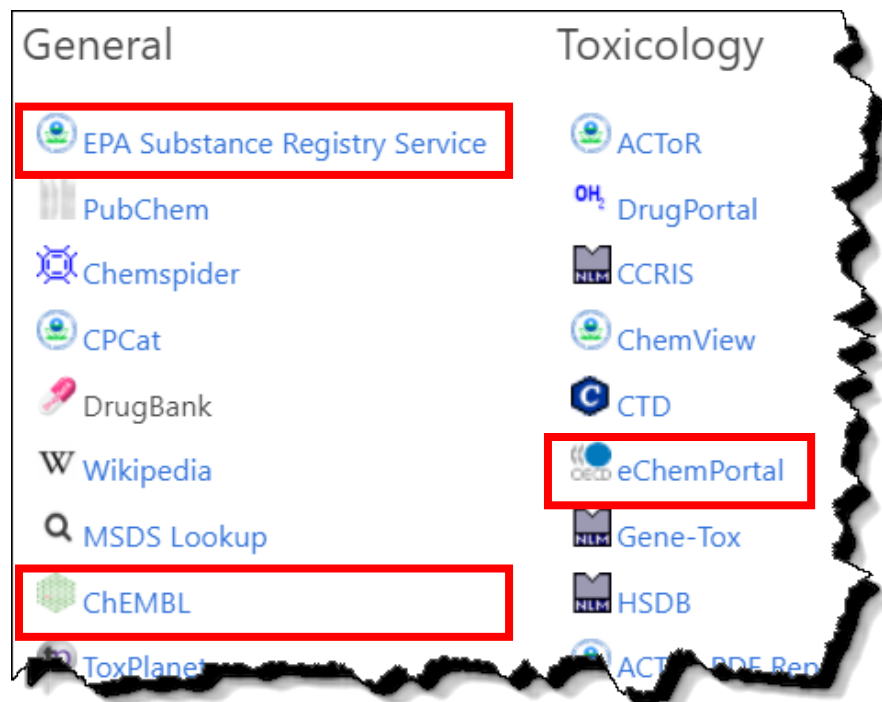
-  RSC Analytical Abstracts
-  Tox21 Analytical Data
-  MONA: MassBank North America
-  mzCloud
-  NIST IR Spectrum
-  NIST MS Spectrum
-  MassBank
-  NIST Antoine Constants
-  IR Spectra on PubChem
-  NIST Kovats Index values
-  Protein DataBank
-  National Environmental Methods Index

Prediction

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

External Links

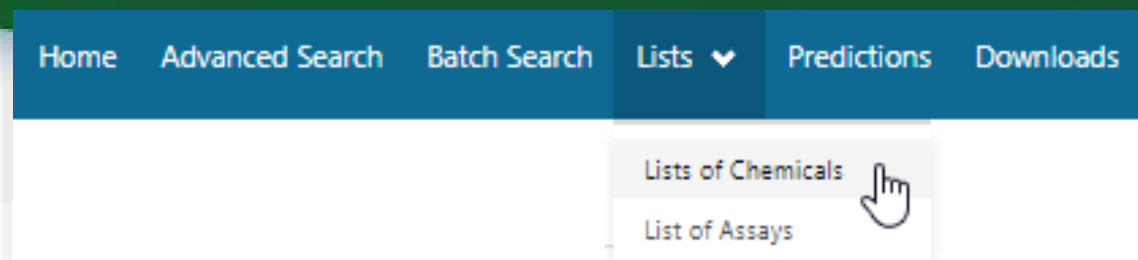
- Links to ~90 websites providing access to additional data on the chemical of interest



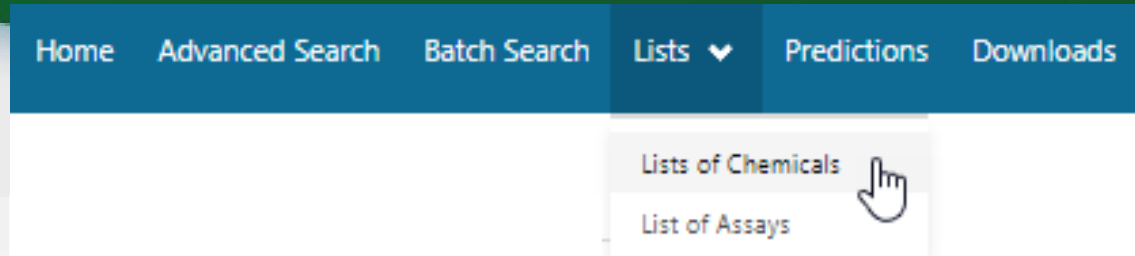
The screenshot shows the eChemPortal website. The header features the OECD logo and the text 'The Global Portal to Information on Chemical Substances'. The navigation bar includes links for Home, Substance Search (highlighted), Property Search, Classification Search, Schedules of Assessments, Data sources, About, Help, and Contact Us. The main content area is titled 'Chemical Substance Search' and shows a search for 'Substance (50-32-8)'. Below this, there is a section for 'Sources and type of information' with a 'Select all' / 'Deselect all' toggle. The 'Types' section has checkboxes for Property information, Exposure and use information, and GHS classifications, all of which are checked. The 'Data sources' section has checkboxes for ACToR, APVMA-CR, Chemicals Dashboard, AGRITOX, CCR, ChemInfo, AICIS assessments, CESAR, and Combined Exposures, all of which are checked.

Chemical Lists and Categories

Example: PFAS Structure Lists



Example: PFAS Structure Lists



Assembly and Curation of Lists of Per- and Polyfluoroalkyl Substances (PFAS) to Support Environmental Science Research

OPEN ACCESS

Antony J. Williams^{1*}, Linda G. T. Gaines², Christopher M. Grulke^{1†}, Charles N. Lowe¹, Gabriel F. B. Sinclair³, Vicente Samano⁴, Inthirany Thillainadarajah⁴, Bryan Meyer⁴, Grace Patlewicz¹ and Ann M. Richard¹

Example: PFAS Structure Lists

[Home](#) [Advanced Search](#) [Batch Search](#) [Lists](#) [Predictions](#) [Downloads](#)

[Lists of Chemicals](#) [List of Assays](#)

PFAS|EPA: PFAS structures in DSSTox (update August 2022)

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

Start typing to search.



☐ Identifier substring search

List Details

Description: List consists of all records with a structure assigned, and using a combination of a set of substructural filters and percent of fluorine in the molecular formula ignoring all hydrogen atoms. For example, for a compound with the molecular formula $C_6HF_9O_6$, the percent of fluorine excluding hydrogen contained in the formula would be $9F/(6C + 9F + 6O) = 42\%$. A threshold of 30% fluorine without hydrogen allows for inclusion of some of the complex highly fluorinated structures. The combination of the set of substructural filters ([visible here](#)) are designed to be simple, reproducible and transparent, yet general enough to encompass the largest set of structures having sufficient levels of fluorination to potentially impart PFAS-type properties. The combination of substructural filters and threshold of percentage of fluorination were identified in the development of the manuscript "A Proposed approach to defining per- and polyfluoroalkyl substances (PFAS) based on molecular structure and formula" by Gaines et al.

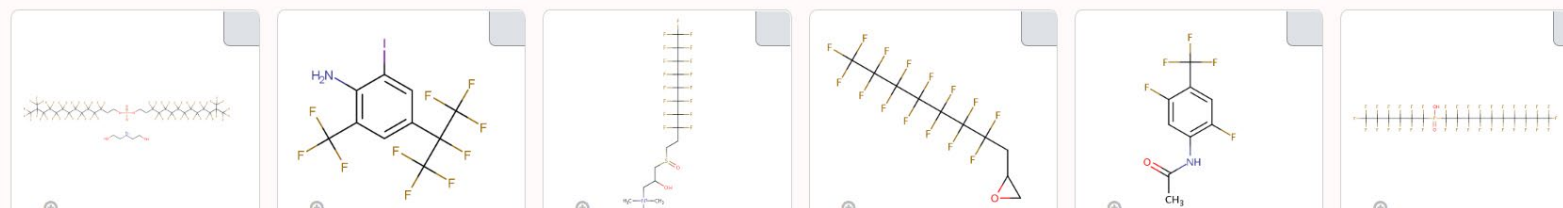
Number of Chemicals: 14735

OPEN ACCESS

  Search Results


[SEND 14735 TO BATCH SEARCH](#) [TITLE INFO](#) [FILTER](#) [EXPORT](#) [PREFERRED VIEW](#)

Showing 14735 of 14735 chemicals



PFAS lists of Chemicals

Select List

 Download ▼

Columns ▼

PFAS

 Copy Filtered Lists URL

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

Batch Searching

- Singleton searches are great but...
- ...we generally want data on LOTS of chemicals!
- Typical questions
 - What are the structures for a set of chemical names? Set of CASRN's?
 - Can I get chemical lists in Excel files? As a list of SMILES strings?
Can I get an SDF file?
 - Can I include predicted properties? OPERA? TEST?
 - Are “these chemicals” screened in Toxcast?
 - I need masses and formulae for a list of chemicals

Batch Search CASRN

Batch Search

Step 1

Step 2

Step 3







Step 4

Step 5






Step Four: Select Data Output Format and Choose Data Fields to Download

Please enter one identifier per line






Chemical Identifiers

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







Structures

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

Intrinsic And Predicted Properties

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

Metadata

- ☐ Curation Level Details 
- ☐ NHANES/Predicted Exposure 
- ☐ Data Sources 
- ☒ Include ToxVal Data Availability 
- ☒ Assay Hit Count 
- ☒ Number of PubMed Articles 

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P	Q
1	INPUT	FOUND_BY	DTXSID	PREFERRED	CASRN	INCHIKEY	IUPAC NAME	MOLECULAR	TOXVAL_D	TOXCAST	TOXCAST	MS_READY	NUMBER_CIRIS	LINK	PPRTV_LIN	ATMOSPHE	BIOCONCE
2	534-52-1	CAS-RN	DTXSID10	2-Methyl-4,6	534-52-1	ZXVONLUN	2-Methyl-4,6	C7H6N2O5	Y	27.56	261/947	CC1=C(O)C	179	-	Y	1.571E-12	2.88959
3	115-21-9	CAS-RN	DTXSID70	Ethyl silicon	115-21-9	ZOYFEXPF	Trichloro(ethyl)	C2H5Cl3Si	Y	-	-	-	-	-	-	8.289E-12	13.9658
4	111-44-4	CAS-RN	DTXSID90	Bis(2-chloro	111-44-4	ZNSMNVML	1-Chloro-2-(C4H8Cl2O	Y	1.12	10/891	CICCOCCC	12	Y	-	2.647E-12	9.99608
5	2763-96-4	CAS-RN	DTXSID50	Muscimol	2763-96-4	ZJQHPWUV	5-(Aminome	C4H6N2O2	Y	-	-	NCC1=CC(C	4308	-	-	1.179E-10	5.05695
6	1464-53-5	CAS-RN	DTXSID00	2,2'-Bioxiran	1464-53-5	ZFIVKAOQ	2,2'-Bioxiran	C4H6O2	Y	-	-	C1OC1C1C	363	-	-	4.383E-12	1.27107
7	22224-92-6	CAS-RN	DTXSID30	Fenamiphos	22224-92-6	ZCJPOPBZ	Ethyl 3-methyl	C13H22NO3	Y	10.8	105/972	CCOP(=O)(C	58	Y	-	1.66E-11	2.3394
8	359-06-8	CAS-RN	DTXSID40	Fluoroacetyl	359-06-8	ZBHDYQJ	Fluoroacetyl	C2H2ClFO	Y	-	-	FCC(Cl)=O	-	-	-	3.513E-13	4.49379
9	5344-82-1	CAS-RN	DTXSID40	1-(o-Chloro	5344-82-1	YZUKKTCD	N-(2-Chloro	C7H7ClN2S	Y	-	-	NC(=S)NC1	-	-	-	2.482E-11	9.95206
10	7446-18-6	CAS-RN	DTXSID10	Thallium (I)	7446-18-6	YTQVHRVI	Dithallium(1-	O4STI2	Y	-	-	-	34	Y	Y	-	-
11	62207-76-5	CAS-RN	DTXSID40	Bis(3-fluoro	62207-76-5	YRZXYIHD	-	C16H14CoF	Y	-	-	-	-	-	-	-	-
12	66-81-9	CAS-RN	DTXSID60	Cycloheximi	66-81-9	YPHMISFO	4-[(2R)-2-[(C15H23NO4	Y	32.27	294/911	CC1CC(C)C	18709	-	-	1.756E-11	2.81761
13	106-96-7	CAS-RN	DTXSID30	Propargyl bi	106-96-7	YORCIIVHU	3-Bromopro	C3H3Br	Y	-	-	BrCC#C	-	-	-	1.069E-11	10.4968
14	315-18-4	CAS-RN	DTXSID70	Mexacarbat	315-18-4	YNEVBPNZ	4-(Dimethyl	C12H18N2C	Y	5.11	12/235	CNC(=O)OC	27	-	-	1.447E-11	26.2914
15	110-00-9	CAS-RN	DTXSID60	Furan	110-00-9	YLQBMQCI	Furan	C4H4O	Y	0.0	0/235	O1C=CC=C	919	Y	-	4.019E-11	5.01648
16	3037-72-7	CAS-RN	DTXSID20	4-(diethoxy	3037-72-7	YHFFINXFN	4-[Diethoxy	C9H23NO2	Y	-	-	-	-	-	-	5.95E-12	6.71292
17	75-44-5	CAS-RN	DTXSID00	Phosgene	75-44-5	YGYAWVD	Carbonyl dic	CCl2O	Y	-	-	ClC(Cl)=O	489	Y	-	9.994E-16	13.0711
18	2032-65-7	CAS-RN	DTXSID30	Methiocarb	2032-65-7	YFBPRJGD	3,5-Dimethy	C11H15NO2	Y	18.14	88/485	CNC(=O)OC	65	-	-	1.446E-11	34.1692
19	2778-04-3	CAS-RN	DTXSID20	Endothion	2778-04-3	YCAGGFXS	[(5-Metho	C9H13O6P	Y	-	-	COC1=COC	-	-	-	4.355E-11	1.18341
20	12108-13-3	CAS-RN	DTXSID90	(Methylcyc	12108-13-3	YASXMYPV	Tricarbonyl	C9H7MnO3	Y	2.56	11/430	-	68	-	-	-	-
21	7803-51-2	CAS-RN	DTXSID20	Phosphine	7803-51-2	XYFCBTPG	Phosphane	H3P	Y	-	-	-	928	Y	-	-	-
22	107-18-6	CAS-RN	DTXSID80	Allyl alcohol	107-18-6	XXROGKLT	Prop-2-en-1	C3H6O	Y	3.99	17/426	OCC=C	627	Y	Y	2.592E-11	4.03901
23	108-05-4	CAS-RN	DTXSID30	Vinyl acetat	108-05-4	XTXRWKR	Ethethyl acet	C4H6O2	Y	1.7	4/235	CC(=O)OC	206	Y	-	2.5E-11	5.52157
24	19624-22-7	CAS-RN	DTXSID10	Pentaborane	19624-22-7	XPIBKKWN	-	B5H9	Y	-	-	-	-	-	-	-	-
25	75-74-1	CAS-RN	DTXSID00	Tetramethyl	75-74-1	XOOGZRUE	Tetramethyl	C4H12Pb	Y	-	-	C[Pb](C)(C)	24	-	-	-	-

Worksheet1

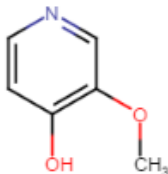
Underneath the Dashboard

View/Edit a Single Record Structure Search Browse/Curate Records Export DSSTox Chemotypes Manage Chemical Lists Manage Property Data Add Deleted Casms

Preferred Name matched null
You are viewing the record associated with
DTXSID80198757
CASRN: 62885-41-0

4-Hydroxy-3-methoxy

Valid license cannot be found



Chemical structure of 4-Hydroxy-3-methoxypyridine is displayed. The structure shows a pyridine ring with a hydroxyl group (-OH) at the 4-position and a methoxy group (-OCH₃) at the 3-position.

Calculate from Structure

Substance_ID:	DTXSID80198757	Compound_ID:	DTXCID40121248
CAS:	62885-41-0	Chemical Shown:	Tested Chemical
Name:	4-Hydroxy-3-methoxypyridine	Private Notes:	
Substance Type:	Single Compound	Source of CAS-Compound:	STN(DSSTox)
QC Level:	DSSTox_High	Double Stereo:	None
Data Source:	STN(DSSTox)	Chiral Stereo:	None
QC Notes:	CAS [50700-60-2] assigned by DSSTox to pyridin-one tautomer form, which resolves to hydroxy form thru InChI	Chemical Form:	Organic
		Organic Form:	Parent

A little more about our data quality

Computational Toxicology 12 (2019) 100096



ELSEVIER

Contents lists available at ScienceDirect

Computational Toxicology

journal homepage: www.elsevier.com/locate/comtox

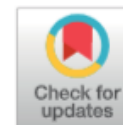


EPA's DSSTox database: History of development of a curated chemistry resource supporting computational toxicology research

Christopher M. Grulke^a, Antony J. Williams^a, Inthirany Thillanadarajah^b, Ann M. Richard^{a,*}

^a National Center for Computational Toxicology, Office of Research & Development, US Environmental Protection Agency, Mail Drop D143-02, Research Triangle Park, NC 27711, USA

^b Senior Environmental Employment Program, US Environmental Protection Agency, Research Triangle Park, NC 27711, USA



Generalized Read-Across

Search for a chemical of interest (target) using the search box

Radial plot with target in the centre and 10 (default) source analogues (similar) ordered clockwise by decreasing similarity (Jaccard) on the basis of Morgan FP (default FP)

Proof-of-Concept Apps

- Structure-substructure-similarity searching of Dashboard
- Batch prediction of physicochemical properties and toxicity
- “Hazard Comparison Dashboard” for comparing hazard profiles for chemicals

Hazard Comparison Dashboard

version: DEV, build: 2021-10-14 13:20:48 UTC

HAZARD

PREDICT

SEARCH

STANDARDIZE

TOXPRINT

Full

Skipped (9)

Unlikely (0)

Filters (0)

Sorting (0)

Structure

CAS Name

107-02-8

AHIGB

Acrolein

107-13-1

AIGBT

Acrylonitrile

309-00-2

IGBTP

Aldrin

107-18-6

IGBTP

Allyl alcohol

12125-02-9

GBTS

Ammonium chlori...

3012-65-5

Diammonium citra...

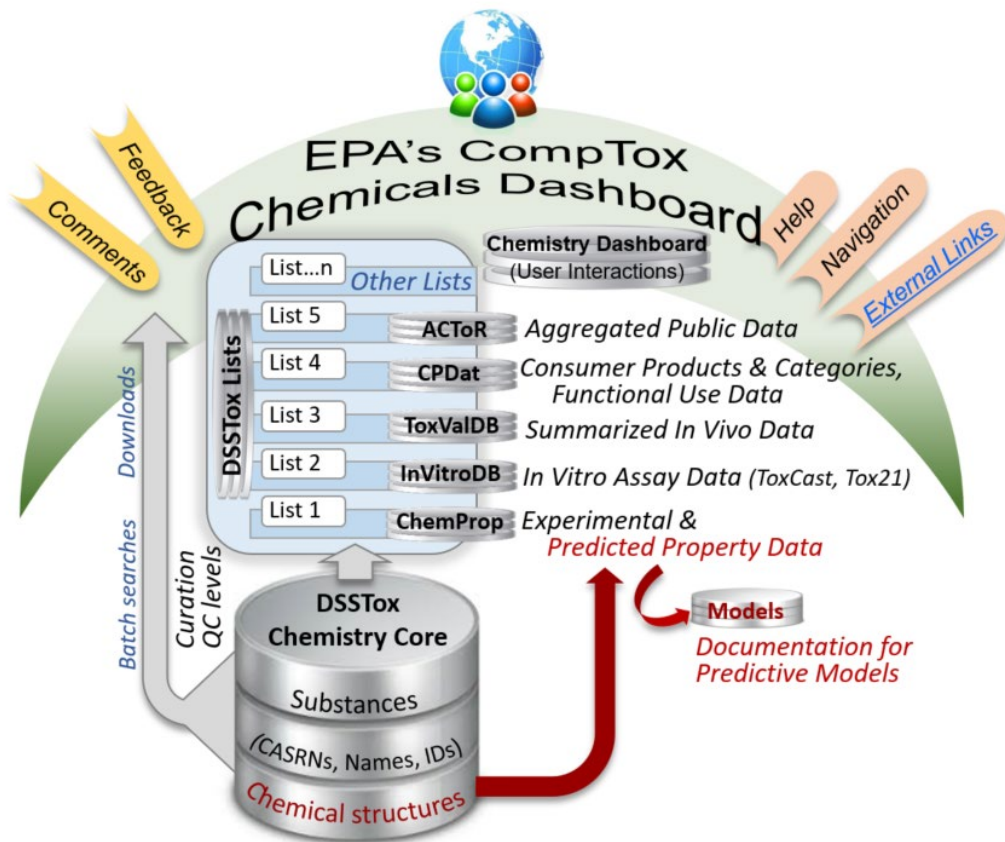
Human Health Effects

Ecotoxicity

Fate

Acute Mammalian Toxicity

Summary and Conclusion



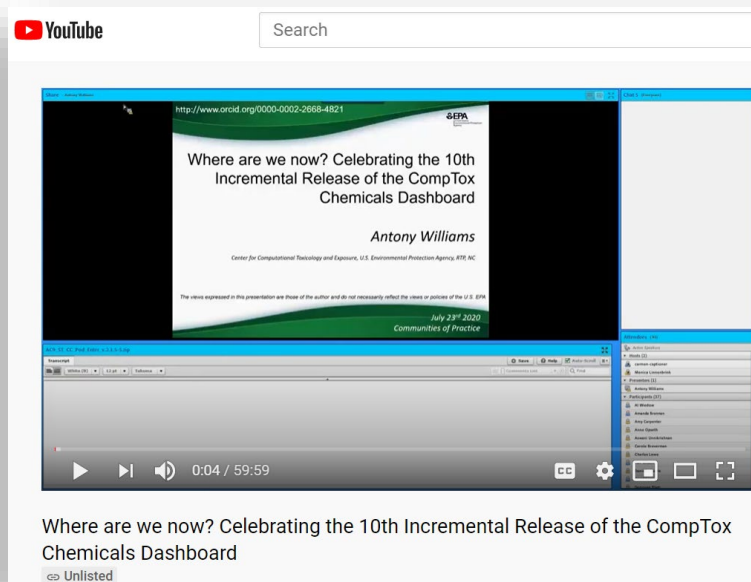
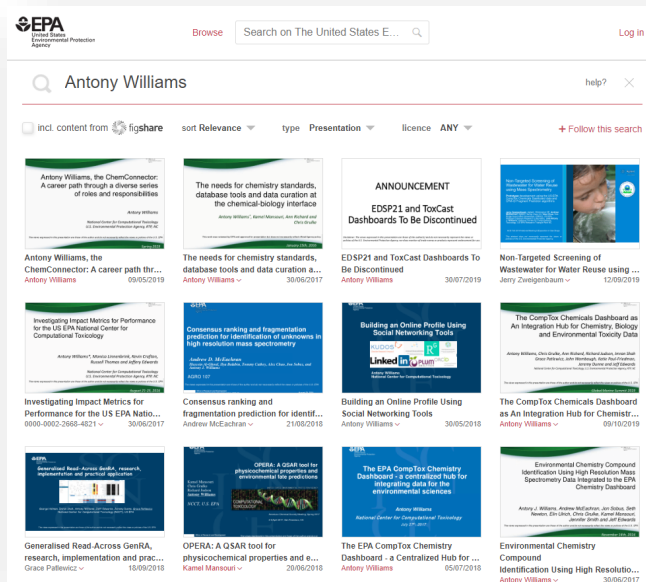
- CompTox Chemicals Dashboard - a central hub for environmental data
 - ~1.2M chemical substances
 - Integrating property data, hazard data, exposure data, *in vitro* bioactivity data
 - Interrogation of bioactivity data -
 - Multiple types of searches



- Batch search for thousands of chemicals
- Real-time property and toxicity predictions
- Downloadable files – CSV, TSV and Excel

You want to know more...

- Lots of resources available
 - Presentations: <https://tinyurl.com/w5hq55>
 - Communities of Practice Videos: <https://rb.gy/qsbn01>
 - Manual: <https://rb.gy/4fgydc>
 - Latest News: https://comptox.epa.gov/dashboard/news_info



CompTox Chemicals Dashboard primer videos

The CompTox Chemicals Dashboard is a one-stop-shop for chemistry, toxicity and exposure information for over 875,000 chemicals. Data and models within the Dashboard also help with efforts to identify chemicals of most need of further testing and reducing the use of animals in chemical testing.

Explore the wealth of data and features available in the CompTox Chemicals Dashboard with these instructional videos narrated by EPA scientists.

General Chemistry and Search Capabilities

