United States Environmental Protection Agency

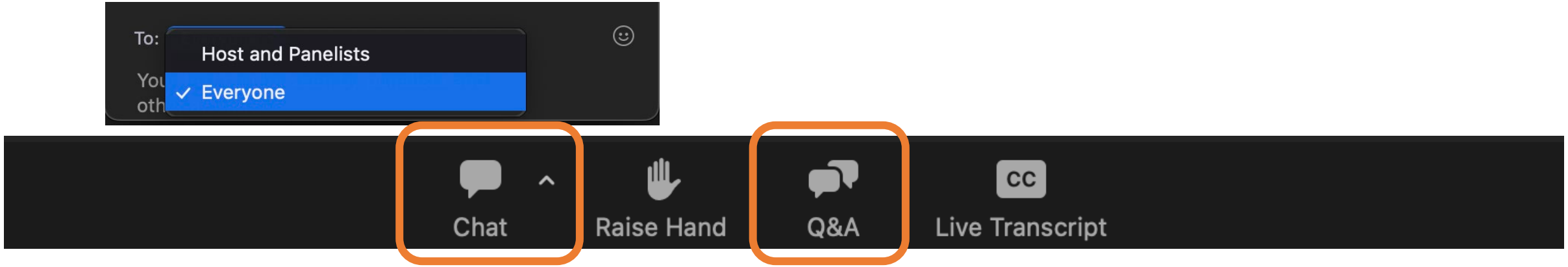
EPA Center for Computational Toxicology and Exposure:

CompTox Chemicals Dashboard Virtual Training

Nisha Sipes
US EPA Office of Research and Development

October 18, 2022

The views expressed in this presentation are those of the authors and do not necessarily reflect the views or policies of the US EPA.


To:
Host and Panelists
Everyone
Chat
Raise Hand
Q&A
Live Transcript

EPA NAMs Pilot Training Program

- The New Approach Methodologies (NAMs) Training Program is a deliverable in the Agency's NAMs Work Plan.
  *first released in 2019 and updated in 2021
  1. ECOTOX Knowledgebase training
  2. Today's CompTox Chemicals Dashboard training
- **Goal: Develop, implement and maintain an engaging training program.**
  - Interactive case studies to encourage active learning
  - Train the trainer
  - Obtain feedback
- Additional trainings (virtual and in-person) are being planned.
- The EPA NAMs training website includes existing training resources, such as recordings and guidance documents.

EPA NAMs Training: www.epa.gov/chemical-research/new-approach-methods-nams-training

EPA NAMs Work Plan: www.epa.gov/chemical-research/epa-new-approach-methods-work-plan-reducing-use-vertebrate-animals-chemical

Agenda

- Welcome and Introductions
- Intro to Computational Toxicology
- Vision of the CompTox Chemicals Dashboard
- Dashboard Navigation
- Summary
- Breakout Exercises (separate Zoom meeting)

United States Environmental Protection Agency

Dr. Nisha Sipes

US EPA Office of Research and Development
Center for Computational Toxicology and Exposure

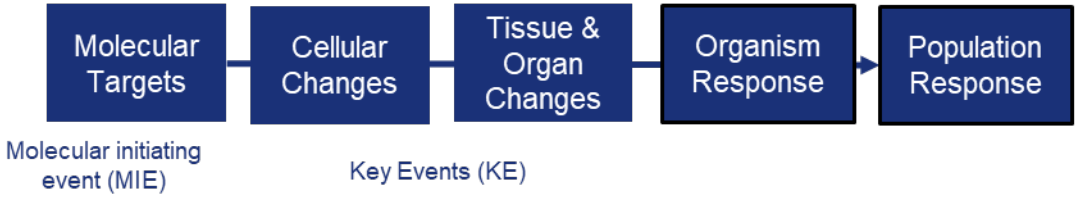
Computational Toxicology

Developing, gathering, integrating and evaluating data and information using mathematical and computer-based approaches to better understand chemical hazards and risks to human health and the environment

- Hazard + exposure
- New Approach Methodologies (NAMs)

New Approach Methodologies (NAMs)

- **Adverse outcome pathways (AOPs)**
  Pathway identification and knowledge integration



- **Databases of existing toxicology data**
  Enables training and evaluation of NAM models

- ***In vitro* assays**
  - Broad / screening (transcriptomics, cell painting)
  - Targeted (receptors, enzymes)
  - *In vitro* PODs, modes/mechanisms of action
- ***In vitro* toxicokinetics**
  Allow conversion of an *in vitro* POD to *in vivo* (IVIVE)

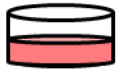


Image: https://ncats.nih.gov/news/releases/2018/tox21-strategic-plan

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

- ***In silico* (e.g., QSAR and read-across)**
  Estimate effects and doses
- **Computer models**
  Integrate multiple *in silico* and *in vitro* data streams

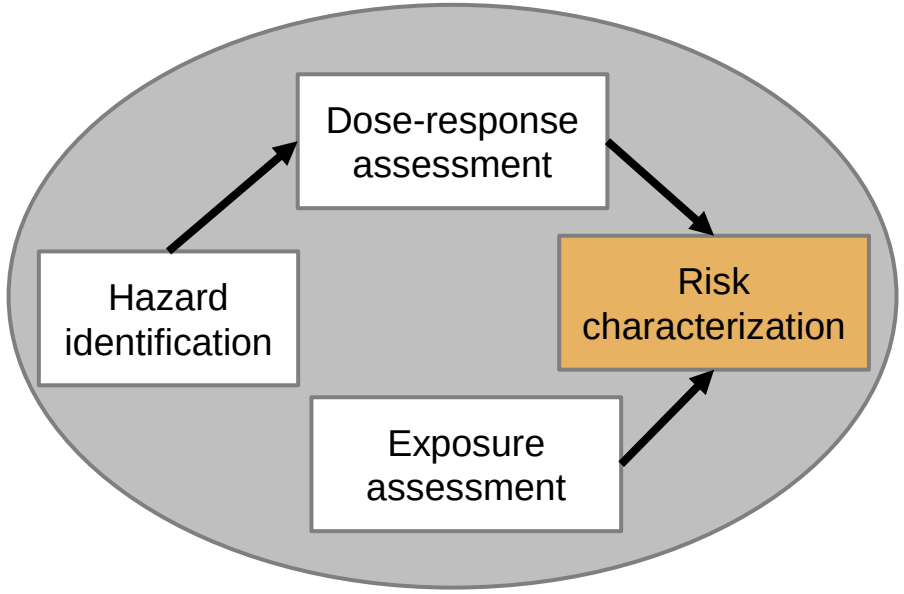
CompTox Chemicals Dashboard

- **Centralized location** for publicly available chemical toxicity data
  - Chemistry, exposure, hazard, bioactivity and dosimetry
  - Combination of existing data and predictive models
  - Periodically updated and curated
- Publicly accessible
- Supports EPA and partner decision making

➢ Easy access to data improves efficiency and ultimately accelerates chemical risk assessment.

Dashboard Data Contents

- Chemical characterization
- Hazard/Bioactivity: safety classifications, human health and ecological data, *in vivo* animal data, biological targets (effect), dose-response characterization (dose)
- Toxicokinetics
- Exposure: exposure levels



+ online EPA web applications:
  - webTEST (hazard and physchem QSAR predictions)
  - GenRA (read-across)
  - Abstract Sifter (literature search)

CCD Information That Stakeholders Use

United States Environmental Protection Agency

Examples

- Physico-chemical property predictions for data-poor substances
- Bioactivity data for use in endocrine hazard assessments and weight of evidence
- Chemical synonyms, bioconcentration and toxicity factors for Clean Water Act programs

Dashboard Overview

EPA United States Environmental Protection Agency

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

Identifier substring search

Latest News

Read More News

The new Dashboard is a complete rebuild and is replacing the CompTox Chemicals Dashboard released on July 12th 2020.

Updated at December 8, 2021

Check out the new CCD Dashboard About Page for details about the CCD Dashboard. The CCD Users Manual can help get you started.
Please log issues or questions using the Submit Comments function/button in the Menu bar.

Known Issues

1. Browser Cache: In order to properly load the new Comptox Chemical Dashboard and data, please clear the browser cache. We are observing issues caused by browser cache. Refer to the specific instructions on how to clear the cache for the various browsers.
2. Chemical Lists:
    1. Issue: Some hyperlinks for the list acronyms (e.g. toxcast_phaseI, etc.) in the chemical list description are not functional i.e. all chemicals in the list are not displayed.
    2. Workaround: To select a particular list in the chemical list, perform the following steps:
        - Select Chemical Lists from the Comptox Dashboard home page

Release Notes

EPA United States Environmental Protection Agency

CompTox Chemicals Dashboard | Home | Search | Lists | About | Tools | Submit Comments | Search all data

Release Notes

Version 2.1 - Fall 2022

Version 2.1 - Fall 2022

Feature Updates

- Added HTTr and HTPP data and visualizations - data from EPA's High Throughput Transcriptomics (HTTr) and High Throughput Phenotypic Profiling (HTPP) have been added in separate "HTTr: Summary" and "HTTP: Summary" tabs, under the "Bioactivity" main tab. Data can be visualized in plots, searched, and downloaded.
- Extended ToxVal download available in batch search - A new "Enhanced Data Sheet->ToxVal Details" in the batch search allows the user to download the ToxVal data values. The ability to populate a Yes/No column for ToxVal data from the batch search "Metadata->Include ToxVal Data Availability" is still available.
- Extended chemical property download … gether.
- Updated demographics exposure predi … SETox), and new generic predictions data table for predicted production volume, presence
- Updated "More" column in the Hazard c
- Updated ADME>IVIVE data table to incl
- Streamlined the About dropdown menu

Data

- **Data update**
  - DSSTOX (prod_dsstox_202202), in
  - invitroDBv3.5 (prod_internal_invitr
  - ChemExpoDB (prod_factotum_20
- **New data**
  - HTTr (ro_httr_20220120) and HTP
  - Please note, this initial release of t
- Note, new chemicals have been added … chemical predictions (TEST, OPERA, Percepta/ACD Labs, EPISuite) have not been included
- Note, analytical QC data have not yet be … re.

Resolved Issues

- Executive summary links work properly
- Chemical list SDF download works
- Chemicals with only DTXCID values are now visible
- Broken image in chemical tile view is fixed
- ToxPrint fingerprints (ChemoTyper) are now downloadable in standard CSV format
- Link in downloadable data from the batch search using ToxVal Data Availability now works
- Updated NIH NCATS Tox21 analytical QC link

…If you are having trouble seeing the new updates or are experiencing issues, please first try to **clear your browser cache.**

<u>Example steps in Google Chrome</u>

- Settings
- Privacy and security
- Clear browsing data.
- Ensure "Cached images and files" are selected in the time range "All time."
- Select the "Clear data" button.

Basic Search – Three Ways

EPA United States Environmental Protection Agency

CompTox Chemicals Dashboard | Home | Search | Lists | About | Tools | Submit Comments

CompTox Chemicals Dashboard

Search 1,200,059 Chemicals

Chemicals | Products/Use Categories | Assay/Gene

bisphenol a

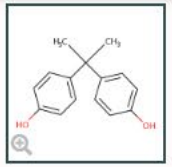
- Bisphenol A
  DTXSID7020182
- Bisphenol A-13C12 beta-D-Glucuronide
  DTXSID601017638
- Bisphenol A-4,4'-dihydroxydiphenyl sulfone copolymer
  DTXSID901094150
- Bisphenol A bis(2-hydroxyethyl ether) diacrylate
  DTXSID6066991
- Bisphenol A bis(2-hydroxypropyl) ether
  DTXSID8051592
- Bisphenol A-bis(4-chlorophenyl) sulfone copolymer
  DTXSID00948014
- Bisphenol A-Bisphenol A diglycidyl ether polymer

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

Details Tab – Chemical Landing Page

EPA United States Environmental Protection Agency

CompTox Chemicals Dashboard | Home | Search | Lists | About | Tools | Submit Comments | Search all data



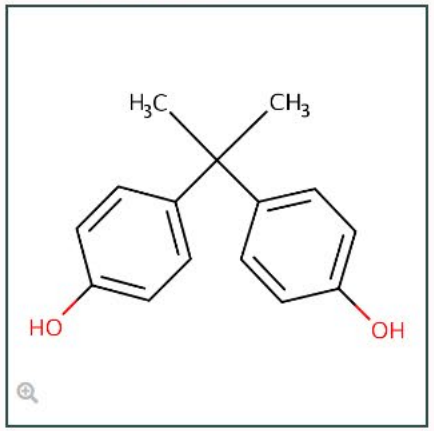
Bisphenol A

80-05-7 | DTXSID7020182

Searched by Approved Name.

- Details
- Executive Summary
- Properties
- Env. Fate/Transport
- Hazard
- Safety > GHS Data
- ADME > IVIVE
- Exposure
- Bioactivity
- Similar Compounds
- GenRA
- Related Substances
- Synonyms
- Literature
- Links
- Comments

Chemical Details



Wikipedia

Bisphenol A (**BPA**) is a chemical compound primarily used in the manufacturing of various plastics. It is a colourless solid which is soluble in most common organic solvents, but has very poor solubility in water. BPA is produced on an industrial scale by the condensation of phenol and acetone, and has a global production scale which is expected to reach 10 million tonnes in 2022.

BPA's largest single application is as a co-monomer in the

Read more

Quality Control Notes

Intrinsic Properties

Molecular Formula: $C_{15}H_{16}O_2$ | MOL FILE | FIND ALL CHEMICALS

Average Mass: 228.291 g/mol | ISOTOPE MASS DISTRIBUTION

Monoisotopic Mass: 228.11503 g/mol

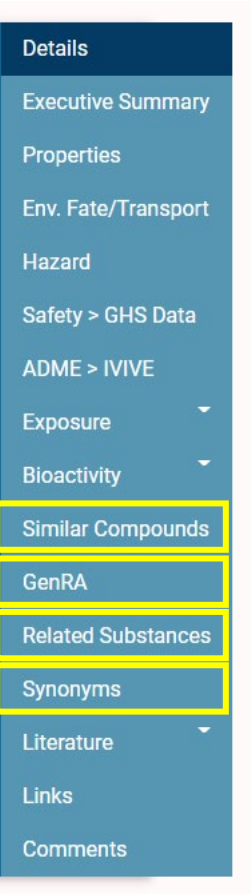
Structural Identifiers

Linked Substances

Presence in Lists

Record Information

Additional Chemistry-Related Tabs

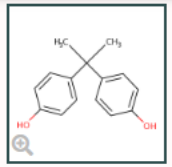


- **Similar Compounds:** Provides a list of similar chemicals based on similarity of molecular fingerprints
- **GenRA:** Generalized Read-Across application
- **Related Substances:** Provides a list of related substances based on—
  - Salt Form
  - Monomer
  - Polymer
  - Predecessor: Component
  - Component
  - Markush Parent
  - Markush Child
  - Transformation Parent
  - Transformation Product
- **Synonyms**

Executive Summary Tab

EPA United States Environmental Protection Agency

CompTox Chemicals Dashboard | Home | Search | Lists | About | Tools



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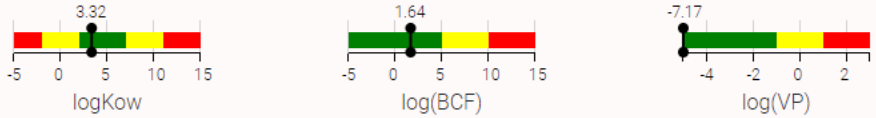
Executive Summary

- **Quantitative Risk Assessment Values**
  - IRIS values available
  - No PPRTV values
  - EPA RSL values available
  - Minimum RfD:0.05 mg/kg-day (chronic,)
  - No RfC calculated
  - IVIVE POD not calculated
- **Quantitative Hazard Values**
  - Minimum oral POD:0.003 mg/kg-day (immunotoxicity, oral)
  - Inhalation POD values:10 mg/m3 (subchronic, inhalation)
  - Lowest Observed Bioactivity Equivalent Level: CYP1A1, CYP1A2, ESR1, NR1I3, NA, ESR1, PPARA, ESR1, ESR1, ESR1
- **Cancer Information**
  - No cancer slope factor
  - No cancer unit risk values
  - No cancer data
  - Genotoxicity Data:predicted to be clastogenic
- **Reproductive Toxicology**
  - Reproductive toxicity PODs available
- **Chronic Toxicology**
  - Chronic toxicity PODs available
- **Subchronic Toxicology**
  - Subchronic toxicity PODs available
- **Developmental Toxicology**
  - Developmental toxicity PODs available
- **Acute Toxicology**

Regional Screening

Class		
RFDo (mg/kg-day)		
risk-based SSL (mg/kg soil)		
screening level (tap water) (ug/L)		
screening level (residential soil) (mg/kg soil)		
screening level (industrial soil) (mg/kg soil)	THQ = 0.1	4.10e+3
risk-based SSL (mg/kg soil)	THQ = 1	58.0
screening level (tap water) (ug/L)	THQ = 1	770
screening level (residential soil) (mg/kg soil)	THQ = 1	3.20e+3
screening level (industrial soil) (mg/kg soil)	THQ = 1	4.10e+4

PhysChem Parameters



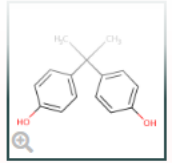
Scroll to see more

Point-of-Departure Plots

Overview of data

- Quantitative toxicity values
- ADME-IVIVE (high throughput toxicokinetics)
- Exposure
- Adverse outcome pathway (AOP) links
- Physchem, fate, transport
- Plots: hazard point-of-departure (POD) oral/inhalation and *in vitro* bioactivity summary

Properties Tab



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- Comments

Properties: Summary

Summary | Search Chemical Properties

EXPORT

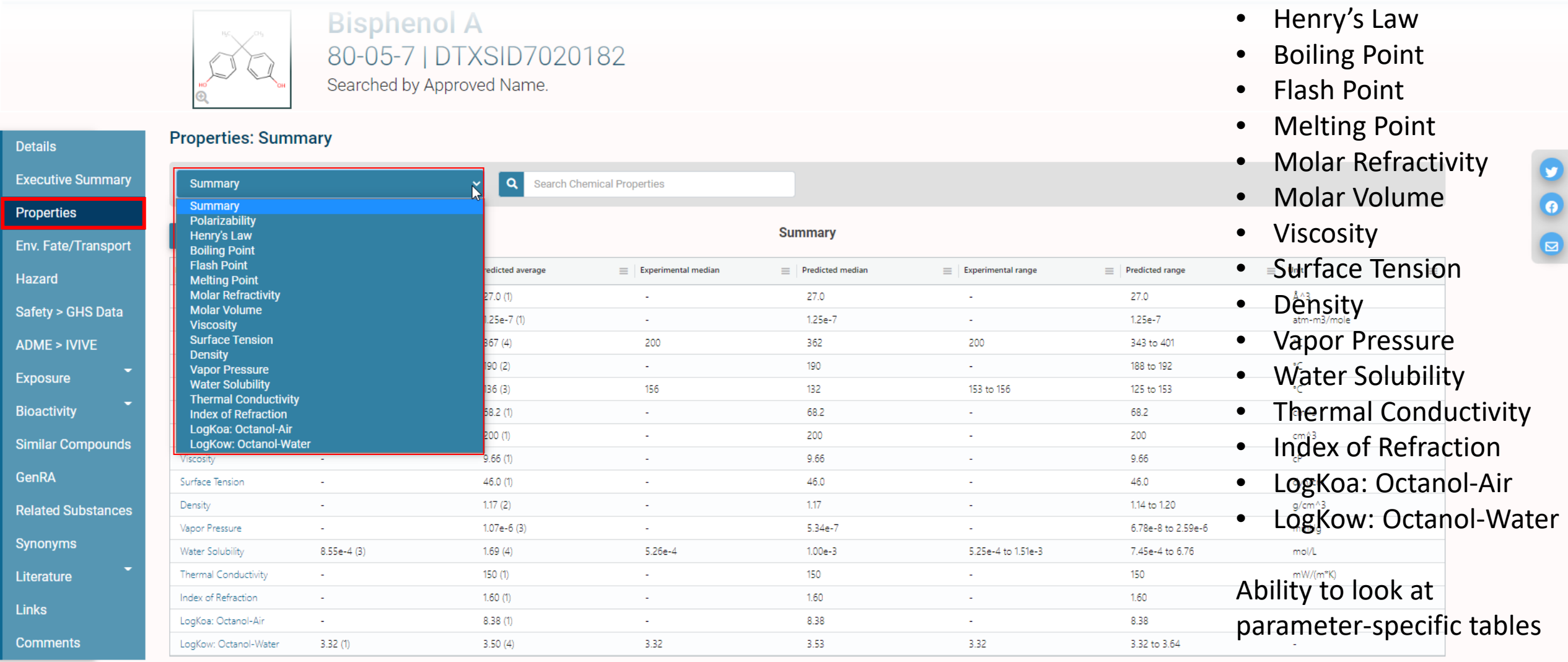
Summary

Property	Experimental average	Predicted average	Experimental median	Predicted median	Experimental range	Predicted range	Unit
Polarizability	-	27.0 (1)	-	27.0	-	27.0	Å^3
Henry's Law	-	1.25e-7 (1)	-	1.25e-7	-	1.25e-7	atm-m3/mole
Boiling Point	200 (1)	367 (4)	200	362	200	343 to 401	°C
Flash Point	-	190 (2)	-	190	-	188 to 192	°C
Melting Point	155 (7)	136 (3)	156	132	153 to 156	125 to 153	°C
Molar Refractivity	-	68.2 (1)	-	68.2	-	68.2	cm^3
Molar Volume	-	200 (1)	-	200	-	200	cm^3
Viscosity	-	9.66 (1)	-	9.66	-	9.66	cP
Surface Tension	-	46.0 (1)	-	46.0	-	46.0	mN/m
Density	-	1.17 (2)	-	1.17	-	1.14 to 1.20	g/cm^3
Vapor Pressure	-	1.07e-6 (3)	-	5.34e-7	-	6.78e-8 to 2.59e-6	mmHg
Water Solubility	8.55e-4 (3)	1.69 (4)	5.26e-4	1.00e-3	5.25e-4 to 1.51e-3	7.45e-4 to 6.76	mol/L
Thermal Conductivity	-	150 (1)	-	150	-	150	mW/(m*K)
Index of Refraction	-	1.60 (1)	-	1.60	-	1.60	-
LogKoa: Octanol-Air	-	8.38 (1)	-	8.38	-	8.38	-
LogKow: Octanol-Water	3.32 (1)	3.50 (4)	3.32	3.53	3.32	3.32 to 3.64	-

- Polarizability
- Henry's Law
- Boiling Point
- Flash Point
- Melting Point
- Molar Refractivity
- Molar Volume
- Viscosity
- Surface Tension
- Density
- Vapor Pressure
- Water Solubility
- Thermal Conductivity
- Index of Refraction
- LogKoa: Octanol-Air
- LogKow: Octanol-Water

Ability to look at parameter-specific tables

Properties Tab



- Polarizability
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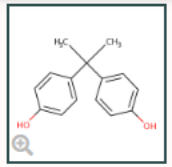
- LogKow: Octanol-Water

Ability to look at parameter-specific tables

Properties Tab

EPA United States Environmental Protection Agency

CompTox Chemicals Dashboard | Home | Search | Lists | About | Tools | Submit Comments | Search all data



Bisphenol A

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- Details
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- Comments

Properties: Boiling Point

Boiling Point | Search Chemical Properties

EXPORT

Summary

Type	Average	Median	Range	Unit
Experimental	200	200	200	°C
Predicted	367	362	343 to 401	°C

EXPORT

Experimental

Source	Result	Experimental Details
Alfa Aesar (Chemical company)	200	-

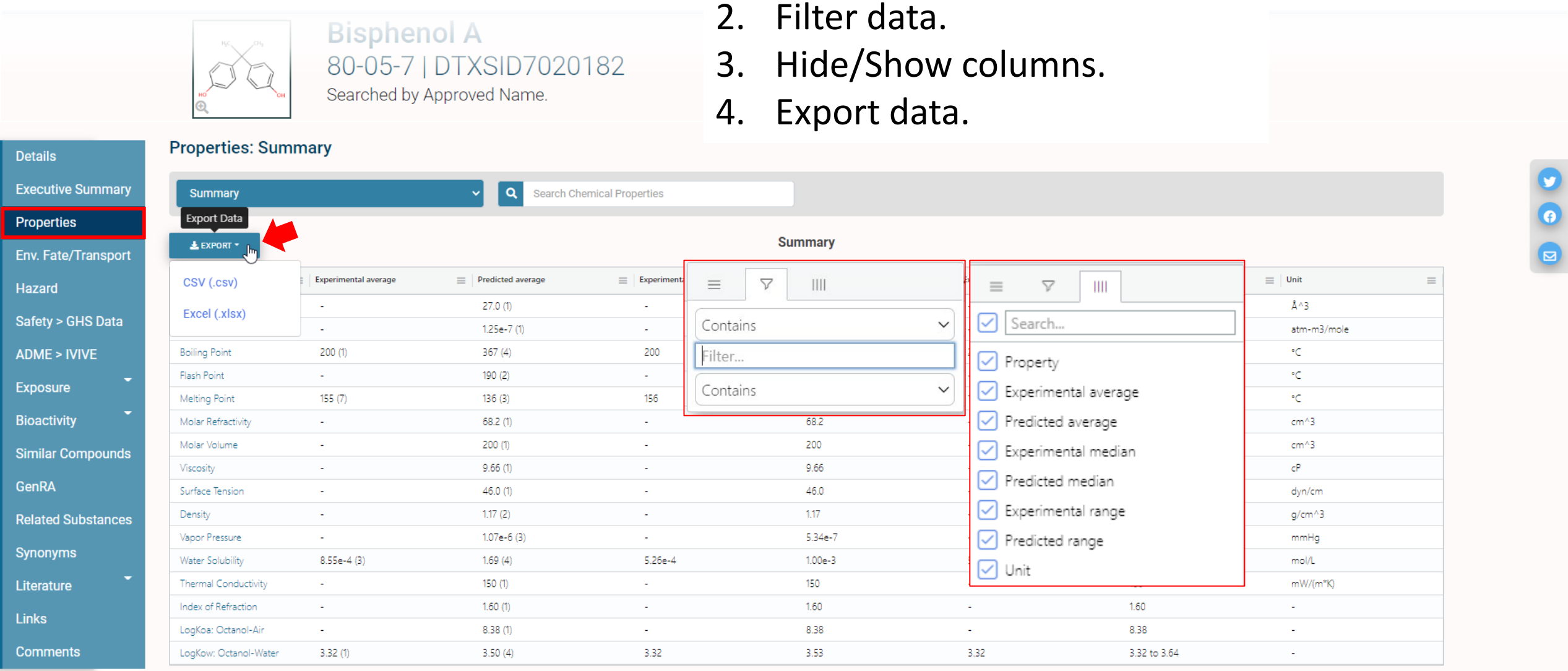
EXPORT

Predicted

Source	Result	Calculation Details	QMRF
OPERA	343	OPERA Calculation Report [Inside AD]	Available
TEST	360	Available	Not Available
EPISUITE	364	Not Available	Not Available
ACD/Labs	401	Not Available	Not Available

Properties Tab

1. Click on column name to sort.
2. Filter data.
3. Hide/Show columns.
4. Export data.



	Experimental average	Predicted average	Experimental median	Predicted median	Experimental range	Predicted range	Unit
	-	27.0 (1)	-				Å^3
	-	1.25e-7 (1)	-				atm-m3/mole
Boiling Point	200 (1)	367 (4)	200				°C
Flash Point	-	190 (2)	-				°C
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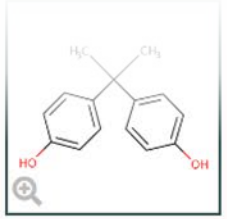
Index of Refraction	-	1.60 (1)	-	1.60	-	1.60	-
LogKoa: Octanol-Air	-	8.38 (1)	-	8.38	-	8.38	-
LogKow: Octanol-Water	3.32 (1)	3.50 (4)	3.32	3.53	3.32	3.32 to 3.64	-

Environmental Fate/Transport Tab

- Atoms. Hydroxylation Rate
- Biodeg. Half-Life (Km)
- Soil Adsorp. Coeff (Koc)
- Bioaccumulation Factor
- Bioconcentration Factor

Ability to look at parameter-specific tables



Bisphenol A

80-05-7 | DTXSID7020182

Searched by Expert Validated Synonym.

- Details
- Executive Summary
- Properties
- Env. Fate/Transport
- Hazard
- Safety > GHS Data
- ADME > IVIVE
- Exposure
- Bioactivity
- Similar Compounds
- GenRA
- Related Substances

Env. Fate/Transport: Summary

Summary | Search Fate/Transport

EXPORT

Summary

Property	Experimental average	Predicted average	Experimental median	Predicted median	Experimental range	Predicted range	Unit
Atmos. Hydroxylation Rate		1.64e-11 (1)		1.64e-11	-	1.64e-11	cm3/molecule*sec
Biodeg. Half-Life		15.1 (1)		15.1	-	15.1	days
Fish Biotrans. Half-Life (Km)	1.86 (1)	1.86 (1)	1.86	1.86	1.86	1.86	days
Soil Adsorp. Coeff. (Koc)		1.34e+3 (2)		1.34e+3	-	1.24e+3 to 1.44e+3	L/kg
Bioaccumulation Factor		173 (1)		173	-	173	
Bioconcentration Factor	54.7 (13)	101 (4)	23.5	94.6	1.70 to 250	43.7 to 173	

Note: Predictions Tool

webTEST is the web version of the EPA's Toxicity Estimation Software Tool that runs QSAR models for toxicological and physchem properties.

United States Environmental Protection Agency

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GenRA
Predictions
Abstract Sifter

Predictions

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

100%

H C N O S P F Cl Br I PT [abs]

Select properties to predict

- Toxicological properties
  - 96 hour fathead minnow LC50
  - 48 hour D. magna LC50
  - 48 hour T. pyriformis IGC50
  - Oral rat LD50
  - Bioconcentration 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

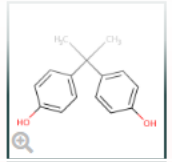
https://comptox.epa.gov/dashboard/predictions

Hazard Tab

Traditional animal studies toward human toxicity and ecotoxicology

ToxValDB Database – 30 worldwide sources

- e.g., EPA, HESS, Health Canada, EU…
- + ECOTOXicology Knowledgebase (ECOTOX) – aquatic life, terrestrial plants and wildlife



Bisphenol A

80-05-7 | DTXSID702018

Searched by Approved Name.

Hazard: Point of Departure

Point of Departure | Search Hazar | human | eco

- Details
- Executive Summary
- Properties
- Env. Fate/Transport
- Hazard
- Safety > GHS Data
- ADME > IVIVE
- Exposure
- Bioactivity
- Similar Compounds
- GenRA
- Related Substances
- Synonyms
- Literature
- Links
- Comments

EXPORT

More	Priority	Source	Type	Subtype	Risk Assessment	Qualifier	Value	Units	Study Type	Exposure Route	Critical effect	Species	Year
	1	IRIS	LOAEL	-	chronic	=	50.0	mg/kg-day	-	oral	reduced mean body weight	-	2020
	3	ECHA eChemPor...	NOAEL	-	developmental	=	0.200	mg/kg-day	developmental	oral	-	rat	2001
	3	ECHA eChemPor...	NOAEL	-	developmental	=	0.200	mg/kg-day	developmental	oral	-	rat	2001
	3	ECHA eChemPor...	NOAEL	-	reproduction	=	0.200	mg/kg-day	reproduction	oral	f1	rat	2001
	3	ECHA eChemPor...	NOAEL	-	reproduction	=	0.200	mg/kg-day	reproduction	oral	-	rat	2001
	3	ECHA eChemPor...	NOAEL	-	reproduction	=	0.200	mg/kg-day	reproduction	oral	-	rat	2001
	3	ECHA eChemPor...	LOAEL	-	short-term	=	600	mg/kg-day	short-term	oral	-	rat	2002
	3	ECHA eChemPor...	NOEL	-	repeat dose	=	30.0	ppm	repeat dose	oral	systemic	mouse	2007
	3	ECHA eChemPor...	NOAEL	-	repeat dose	=	300	ppm	repeat dose	oral	systemic	mouse	2007
	3	ECHA eChemPor...	NOEL	-	repeat dose	=	75.0	ppm	repeat dose	oral	systemic	rat	2000
	3	ECHA eChemPor...	NOAEL	-	repeat dose	=	750	ppm	repeat dose	oral	systemic	rat	2000
											centrilobular		

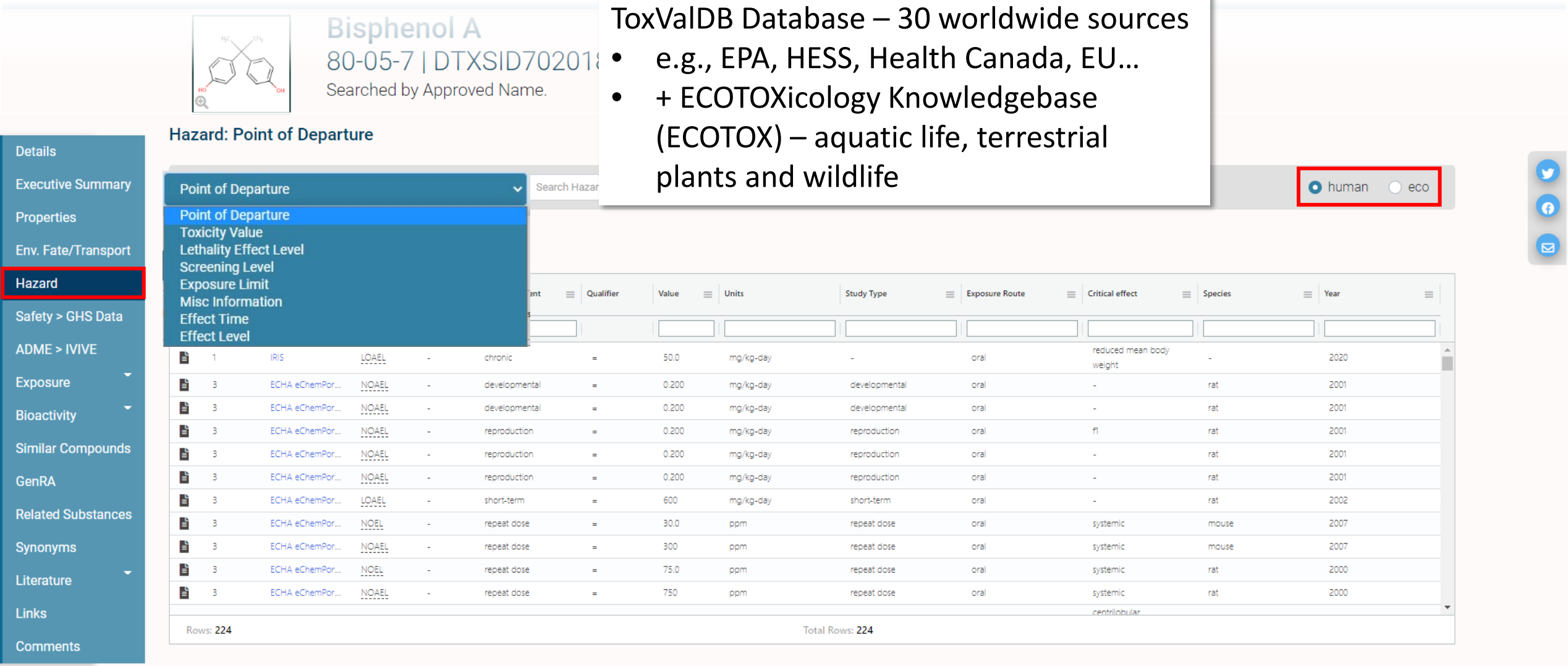
Rows: 224 Total Rows: 224

Hazard Tab

Traditional animal studies toward human toxicity and ecotoxicology

ToxValDB Database – 30 worldwide sources

- e.g., EPA, HESS, Health Canada, EU…
- + ECOTOXicology Knowledgebase (ECOTOX) – aquatic life, terrestrial plants and wildlife



						Qualifier	Value	Units	Study Type	Exposure Route	Critical effect	Species	Year
1	IRIS	LOAEL	-	chronic	=		50.0	mg/kg-day	-	oral	reduced mean body weight	-	2020
3	ECHA eChemPor...	NOAEL	-	developmental	=		0.200	mg/kg-day	developmental	oral	-	rat	2001
3	ECHA eChemPor...	NOAEL	-	developmental	=		0.200	mg/kg-day	developmental	oral	-	rat	2001
3	ECHA eChemPor...	NOAEL	-	reproduction	=		0.200	mg/kg-day	reproduction	oral	f1	rat	2001
3	ECHA eChemPor...	NOAEL	-	reproduction	=		0.200	mg/kg-day	reproduction	oral	-	rat	2001
3	ECHA eChemPor...	NOAEL	-	reproduction	=		0.200	mg/kg-day	reproduction	oral	-	rat	2001
3	ECHA eChemPor...	LOAEL	-	short-term	=		600	mg/kg-day	short-term	oral	-	rat	2002
3	ECHA eChemPor...	NOEL	-	repeat dose	=		30.0	ppm	repeat dose	oral	systemic	mouse	2007
3	ECHA eChemPor...	NOAEL	-	repeat dose	=		300	ppm	repeat dose	oral	systemic	mouse	2007
3	ECHA eChemPor...	NOEL	-	repeat dose	=		75.0	ppm	repeat dose	oral	systemic	rat	2000
3	ECHA eChemPor...	NOAEL	-	repeat dose	=		750	ppm	repeat dose	oral	systemic	rat	2000
											centrilobular		

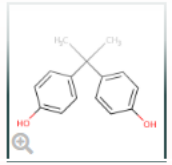
Hazard Tab

EPA United States Environmental Protection Agency

Exposure limits

Water quality, air quality, occupational and estimated exposure values

e.g., EPA's OW, OSHA, FDA, DOD, EFSA, state-specific values



Bisphenol A

80-05-7 | DTXSID7020182

Searched by Approved Name.

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- Safety > GHS Data
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- Exposure
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Hazard: Exposure Limit

Exposure Limit | Search Hazard

EXPORT

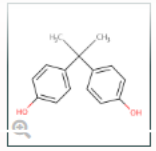
More	Priority	Source	Type	Subtype	Risk Assessment	Qualifier	Value	Units	Study Type	Exposure Route	Critical effect	Species	Year
	2	FDA CEDI	cumulative e	-	chronic	=	1.85e-4	mg/kg-day	-	oral	-	-	-
	2	FDA CEDI	cumulative c	-	chronic	=	3.70	ppb	-	oral	-	-	-
	5	EFSA	TDI	-	chronic	=	5.00e-2	mg/kg-day	-	oral	-	-	2008
	5	EFSA	TDI	-	chronic	=	4.00	ug/kg-day	-	oral	-	-	2008
	7	DOE Protective ...	PAC-1	PAC 1	acute	=	15.0	mg/m3	acute	inhalation	-	-	2018
	7	DOE Protective ...	PAC-2	PAC 2	acute	=	110	mg/m3	acute	inhalation	-	-	2018
	7	DOE Protective ...	PAC-3	PAC 3	acute	=	650	mg/m3	acute	inhalation	-	-	2018

Rows: 7 Total Rows: 7

Safety > GHS Data Tab

GHS (Globally Harmonized System of Classification and Labelling of Chemicals) is a United Nations system to identify hazardous chemicals and to inform users about these hazards.

EPA United States Environmental Protection Agency



Bisphenol A

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Searched by Expert Validated Synonym.

Safety - GHS Data

PRINT PAGE

Links out to external source (PubChem)

- Details
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PUBCHEM > BISPHENOL A > LABORATORY CHEMICAL SAFETY SUMMARY (LCSS) > GHS CLASSIFICATION

CID 6623

Bisphenol A

GHS Classification

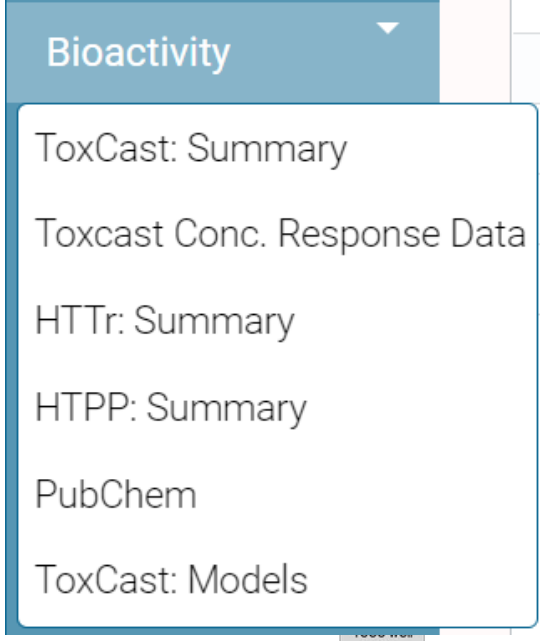
Showing 6 of 6

Pictogram(s)	Corrosive, Irritant, Health Hazard
Signal	Danger
GHS Hazard Statements	H317: May cause an allergic skin reaction [Warning Sensitization, Skin] H318: Causes serious eye damage [Danger Serious eye damage/eye irritation] H335: May cause respiratory irritation [Warning Specific target organ toxicity, single exposure; Respiratory tract irritation] H360F: May damage fertility [Danger Reproductive toxicity]
Precautionary Statement Codes	P203, P261, P264+P265, P271, P272, P280, P302+P352, P304+P340, P305+P354+P338, P317, P318, P319, P321, P333+P313, P362+P364, P403+P233, P405, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)

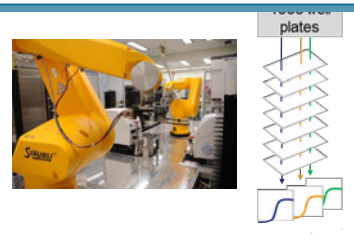
EU REGULATION (EC) No 1272/2008

Pictogram(s)	Corrosive, Irritant, Health Hazard, Environmental Hazard
Signal	Danger

Bioactivity Tab (*in vitro*)

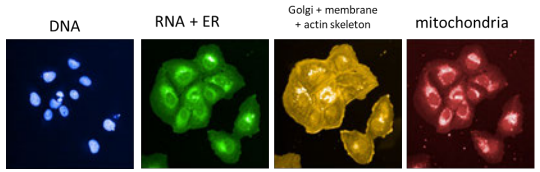


- High-throughput chemical screens to generate biological data on hundreds to thousands of chemicals
  - US EPA's Toxicity Forecasting (ToxCast) Program www.epa.gov/chemical-research/toxicity-forecasting
  - e.g., chemical-biological receptor interaction, metabolomics changes, functional cellular changes (neural network function), zebrafish development
  - Tox21 – intergovernmental US collaboration
  - invitroDB database (v3.5) www.epa.gov/chemical-research/exploring-toxcast-data-downloadable-data

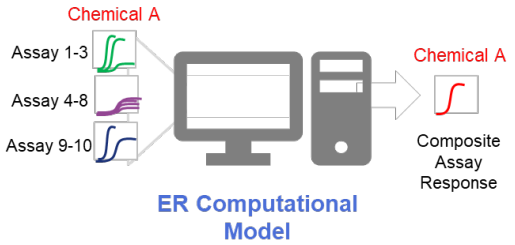


- High-throughput transcriptomics (HTTr)

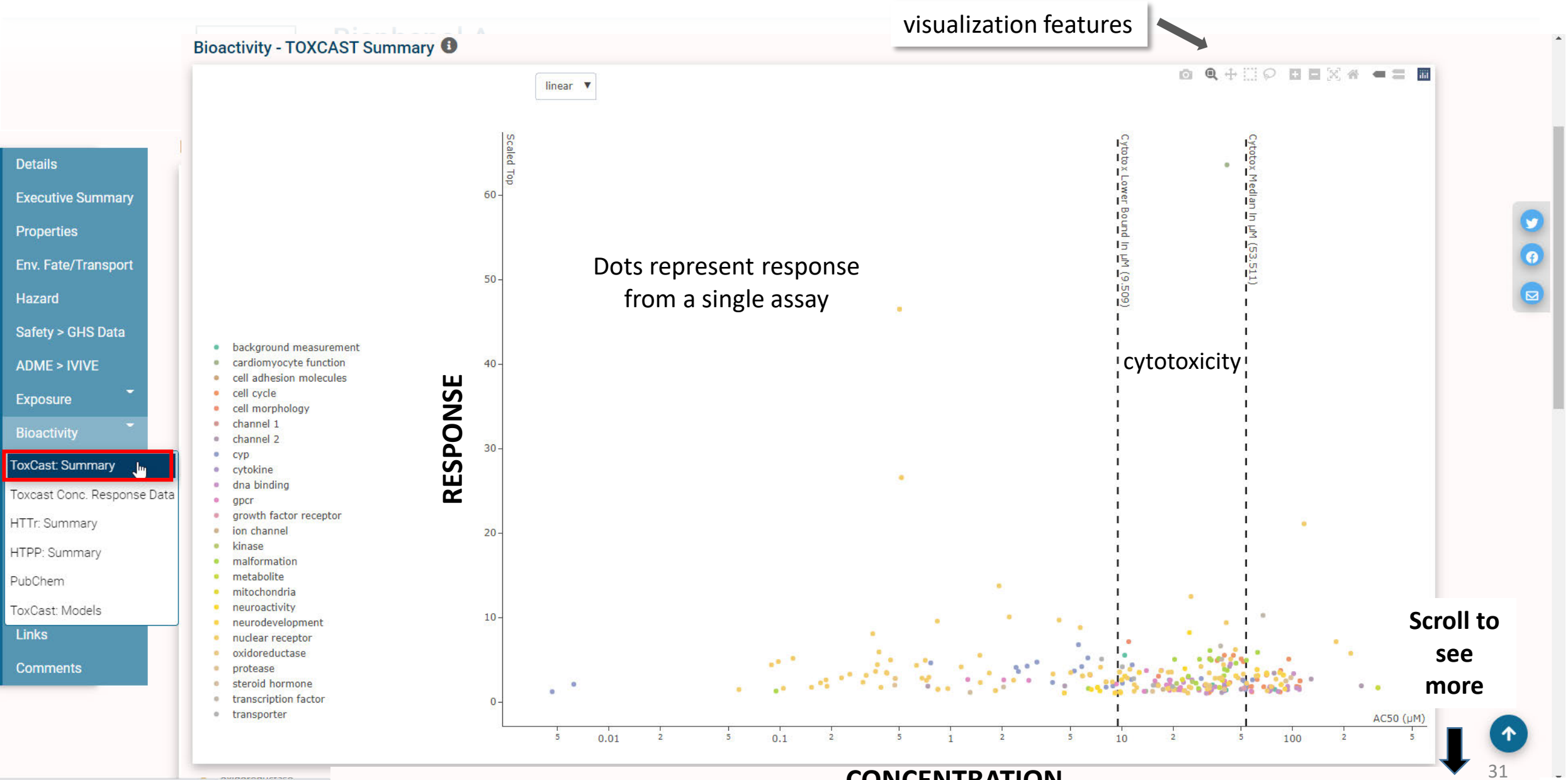
- High-throughput phenotypic profiling (HTPP)



- Development of predictive models utilizing individual assay data (e.g., estrogen receptor [ER] model)



Bioactivity Tab: ToxCast Summary



Bioactivity Tab: ToxCast Summary

Ecology linkage: Sequence Alignment to Predict Across Species Susceptibility (SeqAPASS)

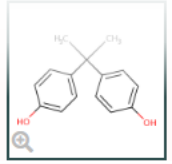
EXPORT

Filter out 'background' from Intended Target Family

Name	Details	SeqAPASS	Gene Symbol	AOP	Event	Hit Call	Top	AC50	logAC50	Max Med	Cutoff	Modl Acc	Intended Target Family
						(1) Active							background
ACEA_AR_agonist_AUC_viabilit				-	-	Active	148	40.0	1.60	123.326 - percent_activity	26.9	1.14	cell cycle
ACEA_AR_antagonist_80hr			AR |	-	-	Active	3.43	41.0	1.61	2.860 - log2_fold_induction	0.366	1.07	nuclear receptor
ACEA_AR_antagonist_AUC_vial				-	-	Active	141	36.3	1.56	116.273 - percent_activity	29.0	1.10	cell cycle
ACEA_ER_80hr		NP_000116.2	ESR1 |	-	-	Active	112	0.373	-0.428	112.502 - percent_activity	25.5	-0.701	nuclear receptor
APR_HepG2_CellLoss_24h_dn				-	-	Active	1.20	106	2.02	1.197 - log2_fold_induction	0.662	2.03	cell cycle
APR_HepG2_CellLoss_72h_dn				-	-	Active	4.49	95.2	1.98	4.435 - log2_fold_induction	0.887	1.75	cell cycle
APR_HepG2_MitoMass_24h_dr				-	-	Active	0.874	109	2.04	0.867 - log2_fold_induction	0.498	2.05	cell morphology
APR_HepG2_MitoMembPot_24				-	-	Active	5.92	11.0	1.04	6.453 - log2_fold_induction	0.831	0.811	cell morphology
APR_HepG2_MitoMembPot_72				-	-	Active	2.71	85.3	1.93	2.255 - log2_fold_induction	0.729	1.70	cell morphology
APR_HepG2_MitoticArrest_72h			H3F3A |	-	-	Active	1.66	84.7	1.93	1.443 - log2_fold_induction	1.42	2.29	cell cycle
APR_HepG2_P-H2AX_24h_up		NP_002096.1	H2AFX |	-	-	Active	1.20	110	2.04	1.192 - log2_fold_induction	0.821	2.08	dna binding
APR_HepG2_P-H2AX_72h_up		NP_002096.1	H2AFX |	-	-	Active	1.80	106	2.02	1.596 - log2_fold_induction	1.10	2.08	dna binding
ATG_Ahr_CIS_up		NP_001612.1	AHR |	131 | 21 | 57 | 310 | 41 | 150 | 57 | 131 | 21 | 41 | 150 | 310	165	Active	1.31	23.4	1.37	1.281 - log2_fold_induction	0.991	1.55	dna binding
ATG_AP_1_CIS_up		NP_005243.1 NP_002219.1	FOS | JUN |	-	-	Active	0.895	33.7	1.53	0.746 - log2_fold_induction	0.600	1.67	dna binding

Rows: 304 of 1,517 Total Rows: 1,517 Filtered: 304

Bioactivity Tab: Conc. Response Data



Bisphenol A

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  - HTPP: Summary
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  - ToxCast: Models
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- Comments

Concentration Response Data

Analytical Data on Tox21 Browser

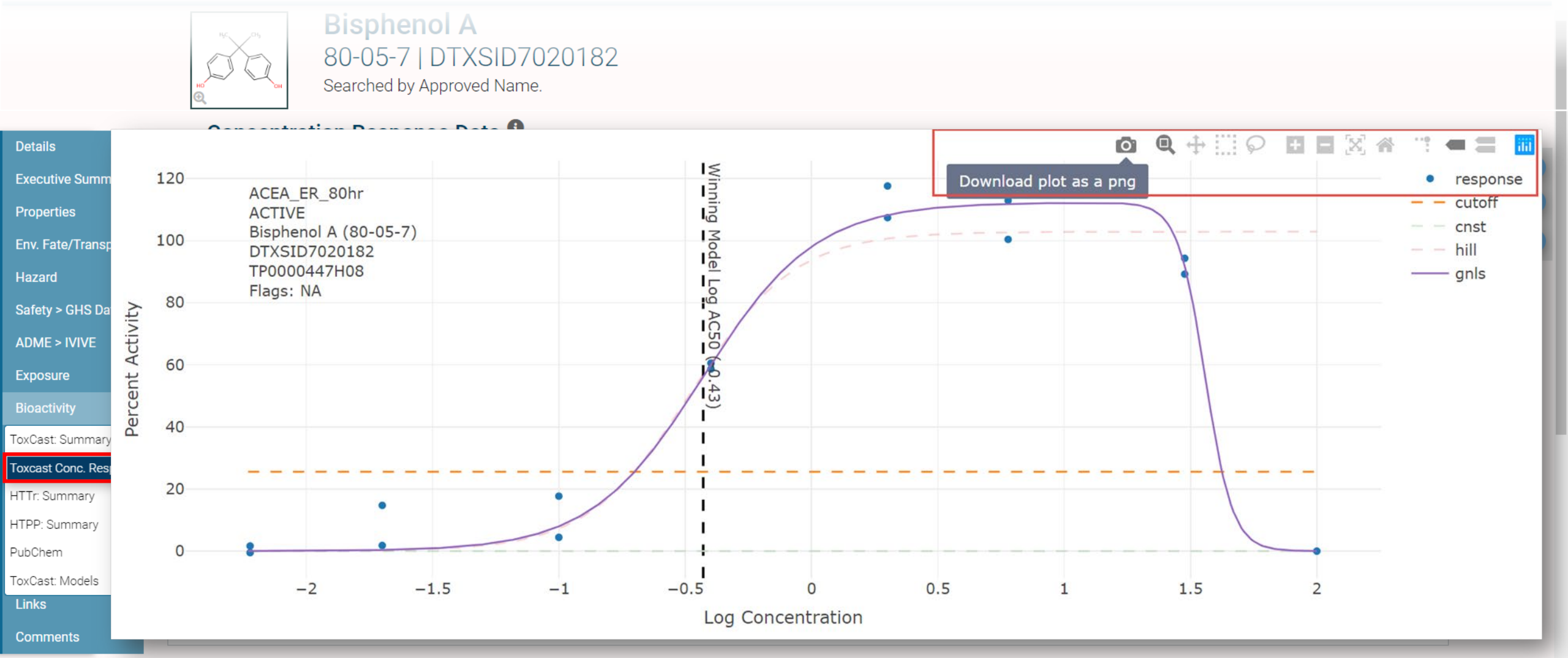
EXPORT

Links out to concentration-response plots

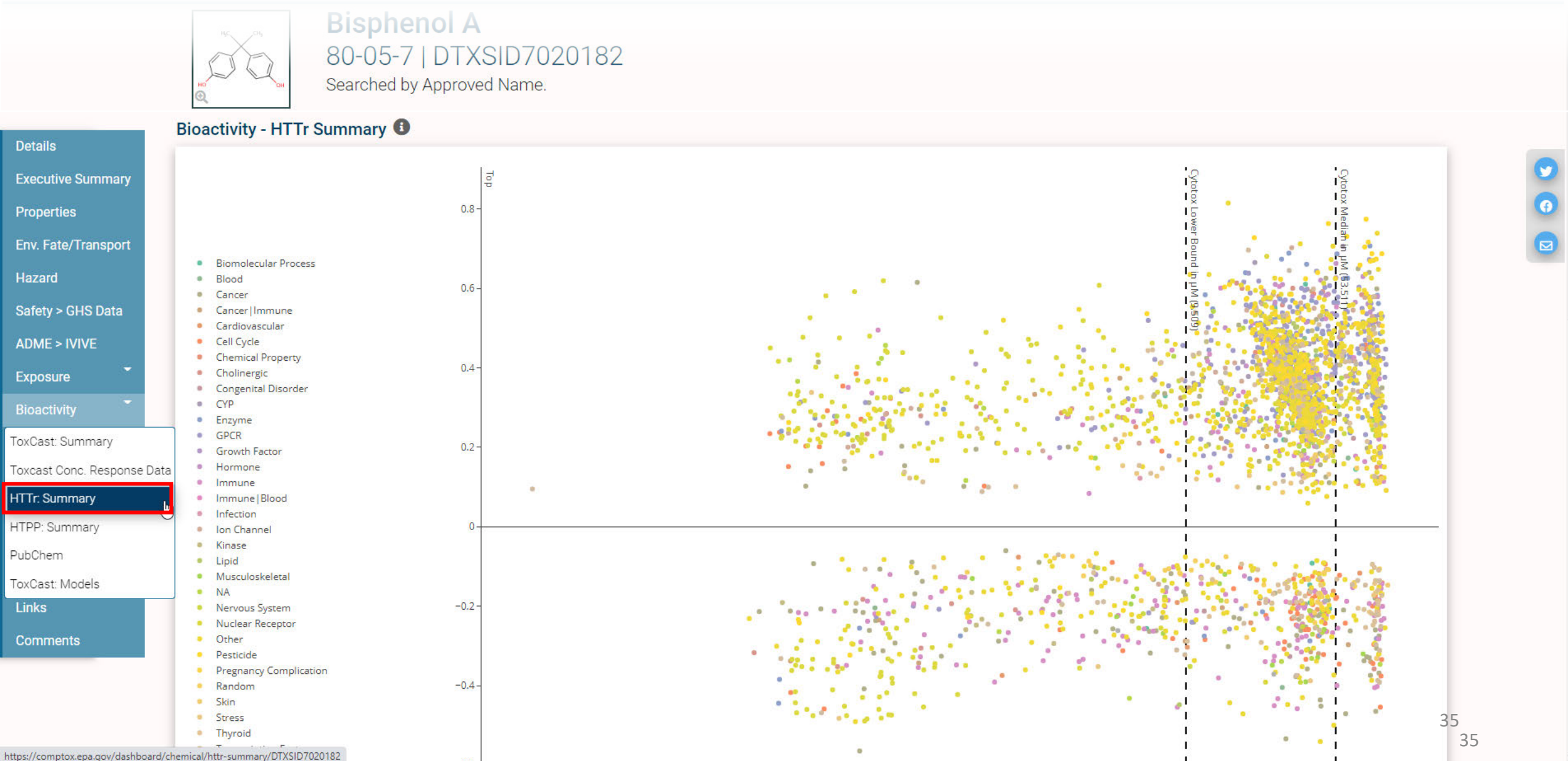
Name	Description	Endpoint Name	Active	Details	Rep. Plot	All Plots	Gene	Intended Target	Cell Line	Cell Format
ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_agonist_80hr	Inactive				AR	steroidal	prostate	cell line
ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_agonist_AUC_viability	Active				-	cytotoxicity	prostate	cell line
ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_antagonist_80hr	Active				AR	steroidal	prostate	cell line
ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_antagonist_AUC_viability	Active				-	cytotoxicity	prostate	cell line
ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_ER_80hr	Active				ESR1	steroidal	breast	cell line
ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_ER_AUC_viability	Inactive				-	cytotoxicity	breast	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_1h_dn	Inactive				-	proliferation	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_1h_up	Inactive				-	arrest	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_24h_dn	Inactive				-	proliferation	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_24h_up	Inactive				-	arrest	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_72h_dn	Inactive				-	proliferation	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_72h_up	Inactive				-	arrest	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellLoss_1h_dn	Inactive				-	cytotoxicity	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellLoss_1h_up	Inactive				-	proliferation	liver	cell line

Rows: 1,398 Total Rows: 1,398

Bioactivity Tab: Conc. Response Data

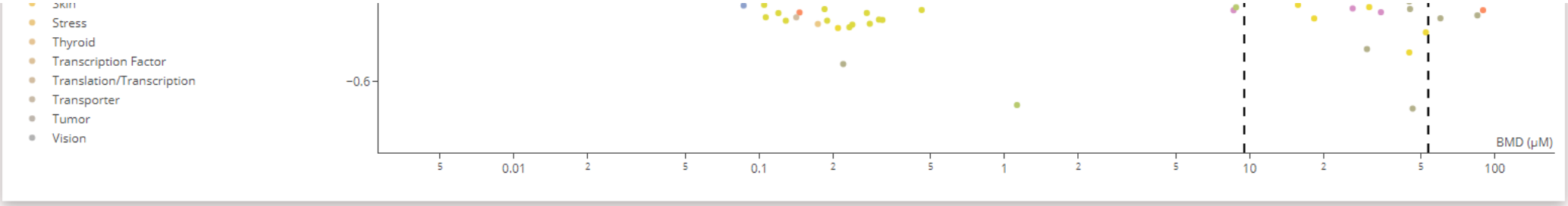


Bioactivity Tab: HTTr: Summary



35

Bioactivity Tab: HTTr: Summary

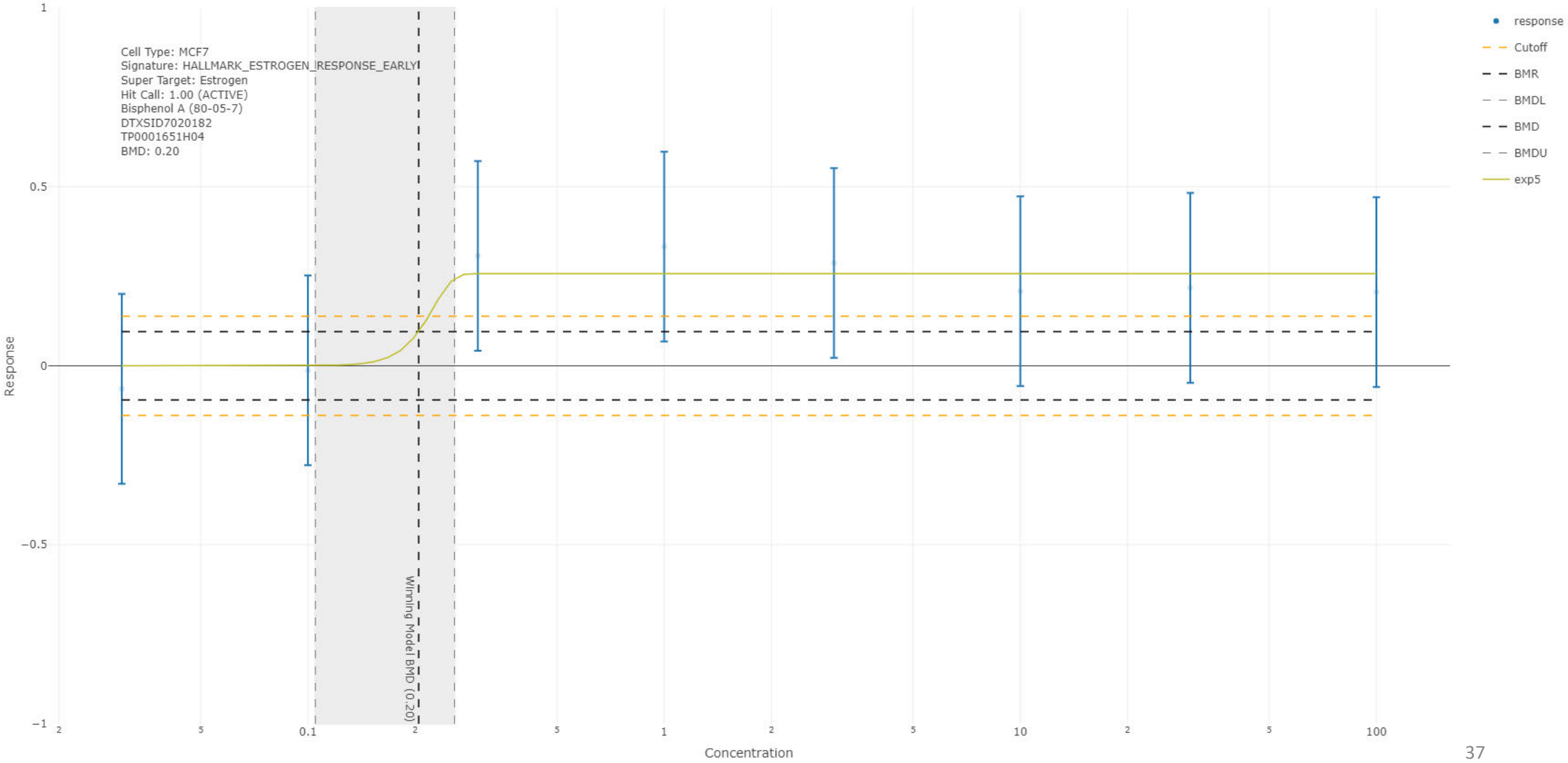


EXPORT

Cell Type	Signature	Target	Hit Call	Top	BMD	Top/Cutoff	QC	QC Flag	Details	Plot	Source	Direction	Sample ID
MCF7	CMAP trifluoperazine 1e-05 100 6424 100	ADR/DRD	0.99	0.39	22.9	2.13	TBD	coming soon			CMAP	dn	TP0001718D10
MCF7	CMAP sirolimus 1e-07 100 934 10 0	mTOR	0.93	0.24	86.3	1.84	TBD	coming soon			CMAP	dn	TP0001718D10
MCF7	CMAP sirolimus 1e-07 100 8359 1 00	mTOR	0.97	0.30	84.6	2.14	TBD	coming soon			CMAP	dn	TP0001718D10
MCF7	CMAP sirolimus 1e-07 100 8179 1 00	mTOR	0.91	0.24	46.3	1.49	TBD	coming soon			CMAP	dn	TP0001718D10
MCF7	CMAP sirolimus 1e-07 100 6478 1 00	mTOR	0.99	0.24	64.1	1.73	TBD	coming soon			CMAP	up	TP0001718D10
MCF7	CMAP sirolimus 1e-07 100 6379 1 00	mTOR	0.90	0.29	51.7	1.33	TBD	coming soon			CMAP	dn	TP0001718D10
MCF7	CMAP sertaconazole 8e-06 100 7933 100	ERG	0.96	0.45	31.2	2.20	TBD	coming soon			CMAP	dn	TP0001718D10
MCF7	CMAP sertaconazole 8e-06 100 3613 100	ERG	0.97	0.29	46.7	1.47	TBD	coming soon			CMAP	dn	TP0001718D10
MCF7	CMAP semustine 1e-04 100 9244 100	Anticancer Drug	0.91	0.20	76.9	1.57	TBD	coming soon			CMAP	up	TP0001718D10

Rows: 3,024 Total Rows: 3,024

Bioactivity Tab: HTTr: Summary



Bioactivity Tab: HTPP: Summary

EPA United States Environmental Protection Agency

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Toxcast Conc. Response Data
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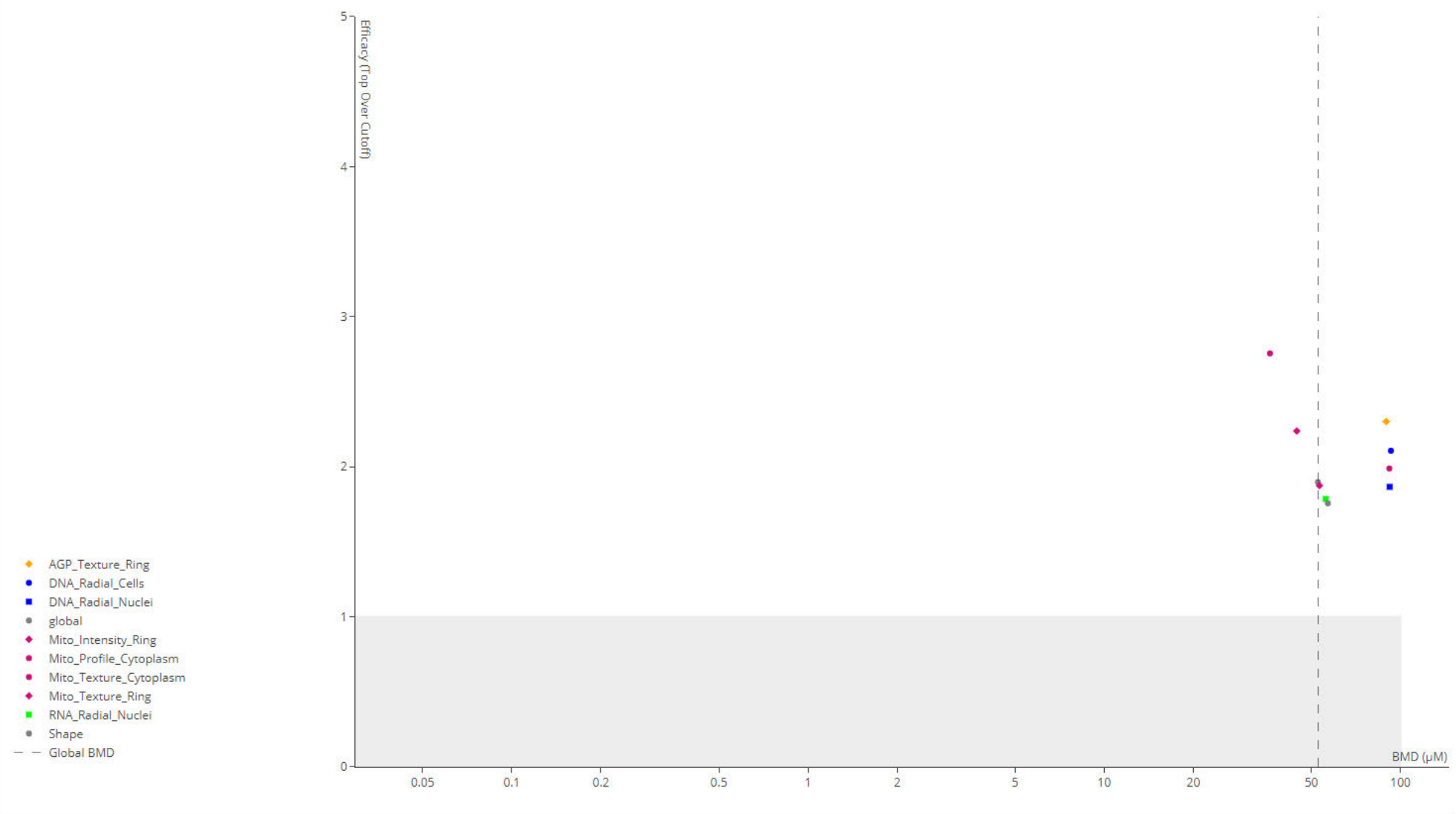
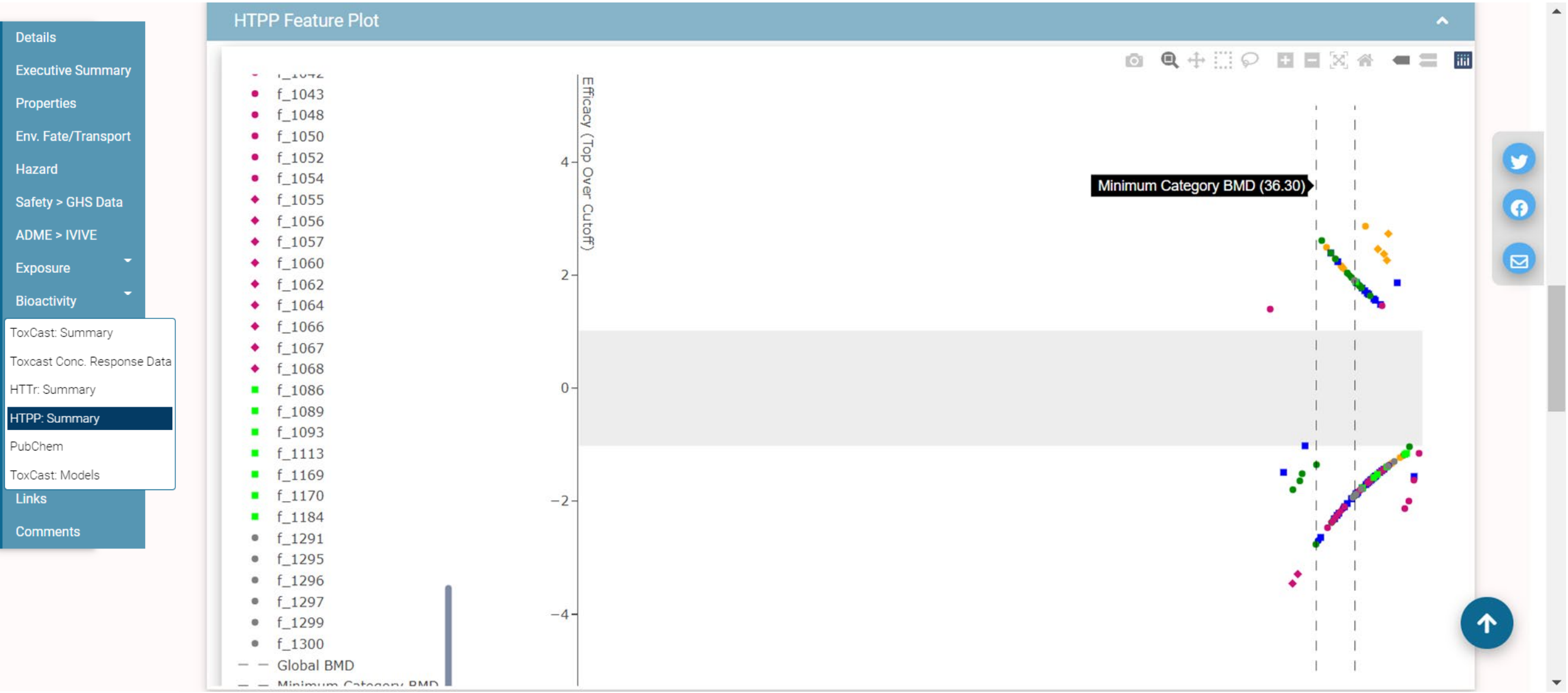
Bioactivity - HTPP Summary

HTPP Category Plot



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

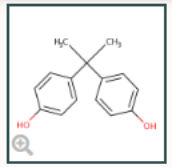
Bioactivity Tab: HTPP: Summary



Bioactivity Tab: HTPP: Summary

EPA United States Environmental Protection Agency

CompTox Chemicals Dashboard | Home | Search | Lists | About | Tools | Submit Comments | Search all data



Bisphenol A

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Bioactivity - HTPP Summary

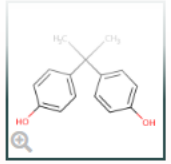
HTPP Category Plot

HTPP Feature Plot

EXPORT

Sample ID	Cell Type	Endpoint	Endpoint Description	BMD	Hit Call	Top/Cutoff	Top	Cutoff	QC	QC Flag	Details	Plot	Channel	Module	Compart
EPAPLT0121D01		f 1069	Position_both_Centroid_Distance	-	0.00	0.12	-0.12	1.00	TBD	coming s...			Position		
EPAPLT0123A01		f 1069	Position_both_Centroid_Distance	-	0.00	0.07	-0.08	1.12	TBD	coming s...			Position		
EPAPLT0121D01		f 1300	Cells Non-Border - Shape_Nuclei Width [um]	56.1	1.00	1.78	-1.83	1.03	TBD	coming s...			Shape		
EPAPLT0123A01		f 1300	Cells Non-Border - Shape_Nuclei Width [um]	46.2	0.99	2.16	-2.22	1.03	TBD	coming s...			Shape		
EPAPLT0121D01		f 1299	Cells Non-Border - Shape_Nuclei Roundness	52.4	0.92	1.91	2.49	1.31	TBD	coming s...			Shape		
EPAPLT0123A01		f 1299	Cells Non-Border - Shape_Nuclei Roundness	-	0.05	0.57	0.61	1.07	TBD	coming s...			Shape		
EPAPLT0121D01		f 1298	Cells Non-Border - Shape_Nuclei Ratio Width to Length	-	0.16	0.74	0.74	1.00	TBD	coming s...			Shape		
EPAPLT0123A01		f 1298	Cells Non-Border - Shape_Nuclei Ratio Width to Length	-	0.00	0.54	-0.54	1.00	TBD	coming s...			Shape		
EPAPLT0121D01		f 1297	Cells Non-Border - Shape_Nuclei Length [um]	53.3	1.00	1.88	-2.14	1.14	TBD	coming s...			Shape		
EPAPLT0123A01		f 1297	Cells Non-Border - Shape_Nuclei Length [um]	83.6	1.00	2.11	-1.99	0.94	TBD	coming s...			Shape		
EPAPLT0121D01		f 1296	Cells Non-Border - Shape_Nuclei Area [um^2]	51.7	1.00	1.94	-2.48	1.28	TBD	coming s...			Shape		
EPAPLT0123A01		f 1296	Cells Non-Border - Shape_Nuclei Area [um^2]	41.8	1.00	2.39	-2.36	0.99	TBD	coming s...			Shape		
EPAPLT0121D01		f 1295	Cells Non-Border - Shape_Cells Width [um]	77.1	0.91	1.30	-1.36	1.05	TBD	coming s...			Shape		
EPAPLT0123A01		f 1295	Cells Non-Border - Shape_Cells Width [um]	59.3	0.93	1.69	-1.77	1.05	TBD	coming s...			Shape		
EPAPLT0121D01		f 1294	Cells Non-Border - Shape_Cells Roundness	-	0.07	0.52	0.55	1.06	TBD	coming s...			Shape		
EPAPLT0123A01		f 1294	Cells Non-Border - Shape_Cells Roundness	-	0.00	0.29	-0.36	1.26	TBD	coming s...			Shape		
EPAPLT0121D01		f 1293	Cells Non-Border - Shape_Cells Ratio Width to Length	-	0.00	0.31	-0.31	0.99	TBD	coming s...			Shape		

Bioactivity Tab: PubChem



Bisphenol A

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- Links
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Bioactivity - PubChem Biological Activities

PRINT PAGE

PUBCHEM > BISPHENOL A > BIOASSAY RESULTS

Links out to external source (PubChem)

BioAssay Results

2,892 items View More Rows & Details

Download

SORT BY Activity Value

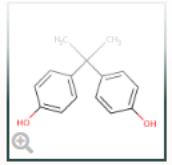
Activity	Activity Value, µM	Activity Type	Target Name	BioAssay Name	BioAssay AID	Substance SID
Inconclusive	0.0014	Potency		qHTS assay to identify small molecule agonists of the endoplasmic reticulum stress response signaling pathway - cell viability counter screen	1159517	144214049
Active	0.00491	IC50	ESRRG - estrogen related receptor gamma (human)	Binding affinity to human ERRgamma	1464223	103308477
Active	0.0055	Kd	Chain A, Estrogen-related receptor gamma (human)	Experimentally measured binding affinity data (Kd) for protein-ligand complexes derived from PDB	977611	87557090
Active	0.0055	Kd	ESRRG - estrogen related receptor gamma (human)	Binding affinity to human ERR gamma	1121409	103308477
Inconclusive	0.0126	Potency	THRB - thyroid hormone receptor beta (human)	qHTS assay for small molecule antagonists of thyroid hormone receptor beta signaling	588547	26752849

1 2 3 ... 579 Next >

PubChem

https://comptox.epa.gov/dashboard/chemical/bio-activity/DTXSID7020182

Bioactivity Tab: ToxCast: Models



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  - PubChem
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- Comments

Bioactivity - ToxCast: Models

EXPORT

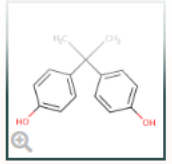
ToxCast Model Predictions

Model	Receptor	Agonist	Antagonist	Binding
COMPARA (Consensus)	Androgen	0.00	1.00	1
ToxCast Pathway Model (AUC)	Androgen	0.00	0.345	-
ToxCast Pathway Model (AUC)	Estrogen	0.450	0.00	-
CERAPP Potency Level (From Literature)	Estrogen	Weak	Strong	Weak
CERAPP Potency Level (Consensus)	Estrogen	1.00	1.00	1

https://comptox.epa.gov/dashboard/chemical/bioactivity-toxcast-models/DTXSID7020182

ADME > IVIVE Tab

EPA United States Environmental Protection Agency



Bisphenol A

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Searched by Approved Name.

ADME – absorption, distribution, metabolism, excretion
IVIVE – *in vitro* to *in vivo* extrapolation

ADME - IVIVE

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- GenRA
- Related Substances
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- Links
- Comments

Search ADME IVIVE

EXPORT

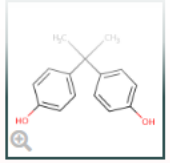
IVIVE

Label	Species	Measured	Predicted	Units	Model	Percentile	Reference	Data Source Species
Intrinsic Hepatic Clearance	Human	19.90	NA	uL/min/million hepatocytes	NA	NA	Wambaugh 2019	Human
Fraction Unbound in Plasma	Human	0.04	NA		NA	NA	Wambaugh 2019	Human
Volume of Distribution	Human	NA	6.34	L/kg	1compartment	NA	NA	Human
PK Half Life	Human	NA	39.61	hours	1compartment	NA	NA	Human
Steady-State Plasma Concentra	Human	NA	3.19	mg/L	3compartmentss	95%	NA	Human

httk R package: CRAN.R-project.org/package=httk

ADME > IVIVE Tab

EPA United States Environmental Protection Agency



Bisphenol A

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ADME – absorption, distribution, metabolism, excretion
IVIVE – *in vitro* to *in vivo* extrapolation

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ADME - IVIVE

Search ADME IVIVE

EXPORT

IVIVE

Label	Species	Measured	Predicted	Units	Model	Percentile	Reference	Data Source Species
Days to Steady State	Human	NA	2.00	Days	PBTK	NA	NA	Human
Days to Steady State	Rat	NA	33.00	Days	PBTK	NA	NA	Human
Fraction Unbound in Plasma	Human	0.04	NA		NA	NA	Wambaugh 2019	Human
Fraction Unbound in Plasma	Rat	0.04	NA		NA	NA	Wambaugh 2019	Human
Intrinsic Hepatic Clearance	Human	19.90	NA	uL/min/million hepatocytes	NA	NA	Wambaugh 2019	Human
Intrinsic Hepatic Clearance	Rat	19.90	NA	uL/min/million hepatocytes	NA	NA	Wambaugh 2019	Human
PK Half Life	Rat	NA	368.30	hours	1compartment	NA	NA	Human
PK Half Life	Human	NA	39.61	hours	1compartment	NA	NA	Human
Steady-State Plasma Concentra	Human	NA	0.39	mg/L	PBTK	50%	NA	Human
Steady-State Plasma Concentra	Human	NA	0.48	mg/L	3compartmentss	50%	NA	Human
Steady-State Plasma Concentra	Rat	NA	1.67	mg/L	PBTK	50%	NA	Human
Steady-State Plasma Concentra	Human	NA	2.35	mg/L	PBTK	95%	NA	Human
Steady-State Plasma Concentra	Rat	NA	2.75	mg/L	3compartmentss	50%	NA	Human
Steady-State Plasma Concentra	Human	NA	3.19	mg/L	3compartmentss	95%	NA	Human
Steady-State Plasma Concentra	Rat	NA	3.21	mg/L	PBTK	95%	NA	Human
Steady-State Plasma Concentra	Rat	NA	5.60	mg/L	3compartmentss	95%	NA	Human
Volume of Distribution	Rat	NA	33.33	L/kg	1compartment	NA	NA	Human
Volume of Distribution	Human	NA	6.34	L/kg	1compartment	NA	NA	Human

httk R package: CRAN.R-project.org/package=httk

Exposure Tabs

Reported and measured data – come from public sources (e.g., MSDS sheets, EPA's Toxics Release Inventory, National Health and Nutrition Examination Survey [NHANES] biomonitoring data)

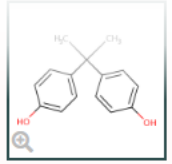
Predicted data – use various inputs, including physchem and environmental/fate transport data

Databases are developed for public consumption, e.g.:

- EPA's Chemical and Products Database (CPDat)
- EPA's Chemical/Product Categories Database (CPCat)

Exposure Tab: Product & Use Categories

EPA United States Environmental Protection Agency



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Searched by Approved Name.

EPA's Chemical and Products Database (CPDat)

EPA's Chemical/Product Categories Database (CPCat)

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Product and Use Categories (PUCs)

Search PUC | EXPORT

Product Use Categories (PUCs)

Product Use Category	Categorization Subtype	Number of Products
Construction and building materials	Article	3
Furniture and Furnishings	Article	1
Not yet Categorized		16

Rows: 3

Search Key Words | EXPORT

General Use Keywords

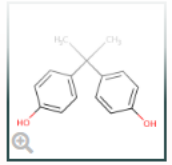
General Use Keywords	Number of Sources
active_ingredient, Pesticides	1
artificial_sweat, detected, emissions, Europe, Other direct contact consumer goods	1
CEDI	1
children, WA Children's Safe Product Act (4/2020)	1
detected, drinking_water, MN Chemical Screening	2
detected, Europe, Other direct contact consumer goods	4
detected, Europe, Toys and children's products	2
detected, ground_water, MN Chemical Screening	1
detected, MN Chemical Screening, surface_water	8
detected, MN Chemical Screening, wastewater	1
detected, wastewater	1
drinking_water, Europe, manufacturing, plastic_additive	1
Europe, nondetect, Other direct contact consumer goods	2
Indirect additives food contact (10/2018)	1
OEHHA Proposition 65 (3/2019)	1

Rows: 15

https://comptox.epa.gov/dashboard/chemical/product-use-categories/DTXSID7020182

Exposure Tab: Chemical Weight Fraction

Reported or predicted by ingredient list



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Chemical Weight Fractions (CWF)

Search Chemical Weight Fractions

EXPORT

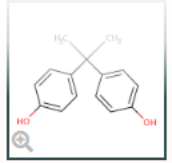
Product Name	Product Use Category	Categorization Subtype	Minimum Weight Fraction	Maximum Weight Fraction	Data Type	Source	Product Count
02y040cat comp b mil-p-23377g ty 1 cl c	Not yet Categorized		0.00	0.500	reported	SIRI	1
032l015 epi-cure 872	Not yet Categorized		0.00	0.100	reported	SIRI	1
0387 hec black	Not yet Categorized		-	-	reported	SIRI	1
039-080055-044_ part b	Not yet Categorized		-	-	reported	SIRI	1
1101/0978-0979_ belzona 1321 (belzona (supp	Not yet Categorized		0.100	0.300	reported	SIRI	1
1:1 adduct for epoxy fill primer_ 120900	Not yet Categorized		0.00	5.00e-2	reported	SIRI	1
1961a concise orthodontic bonding system paste b	Not yet Categorized		0.00	1.00e-2	reported	SIRI	1
1961a concise orthodontic bonding syst paste_ part b (suppl)	Not yet Categorized		0.00	1.00e-2	reported	SIRI	1
3135 a (epoxy resin)_ part a	Not yet Categorized		-	-	reported	SIRI	1
3197 steel works	Not yet Categorized		1.00e-2	7.00e-2	reported	SIRI	1
3303/1358_ 4911 (belzona magma tx (supdat)	Not yet Categorized		1.00e-2	5.00e-2	reported	SIRI	2
3303/1358_ belzona 4911 solidifier	Not yet Categorized		1.00e-2	5.00e-2	reported	SIRI	1

Rows: 250

https://comptox.epa.gov/dashboard/chemical/chemical-weight-fraction/DTXSID7020182

Exposure Tab: Chemical Functional Use

Reported and predicted values



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Exposure - Collected Data on Functional Use

Search Reported | EXPORT

Collected Data on Functional Use

Harmonized functional use	Reported functional use
Antioxidant	antioxidants>phenolics
Binder	binder
Catalyst	catalyst
Hardener	curing agent
Flame retardant	fire retardant
Hardener	hardener
Monomers	monomer, bisphenol a-epichlorohydrin acrylate
Monomers	monomer, epichlorohydrin bisphenol a resin
Monomers	monomer, epichlorohydrin-bisphenol a resin
Monomers	monomer, polycarbonate

Rows: 10

Search Predicted | EXPORT

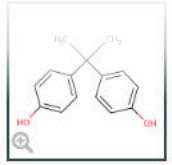
Predicted Probability of Associated Functional Use

Harmonized functional use	Probability
antioxidant	0.894
uv_absorber	0.805
crosslinker	0.774
heat_stabilizer	0.512
antimicrobial	0.372
flame_retardant	0.221
fragrance	0.207
catalyst	0.203
colorant	0.156

Rows: 9

https://comptox.epa.gov/dashboard/chemical/chemical-functional-use/DTXSID7020182

Exposure Tab: Toxics Release Inventory



Bisphenol A
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Searched by Approved Name.

www.epa.gov/trinationalanalysis

awsedap.epa.gov/public/extensions/TRINA_dashboard_2020/TRINA_dashboard_2020.html

Exposure - Toxics Release Inventory

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2019 TRI Factsheet: Chemical - 4,4'-Isopropylidenediphenol, 0000080057

Data Source: 2020 Updated Dataset (released May 2022)

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

Map of TRI Facilities Reporting 4,4'-Isopropylidenediphenol

Quick Facts for 2019

	Chemical	United States
Number of TRI Facilities:	126	21,789
Total Production-Related Waste Managed:	11.6 million lbs	30.6 billion lbs
Total On-site and Off-site Disposal or Other Releases:	2.8 million lbs	3.4 billion lbs
Total On-site:	832.9 thousand lbs	2.9 billion lbs
• Air:	32.1 thousand lbs	602.7 million lbs
• Water:	1.3 thousand lbs	200.7 million lbs
• Land:	799.5 thousand lbs	2.1 billion lbs
Total Off-site:	2.0 million lbs	459.6 million lbs

4,4'-Isopropylidenediphenol ranks **64** out of **490** chemicals reported to TRI in 2019 (Rank 1 = highest releases)

Under the Pollution Prevention Act of 1990, TRI collects information to track industry progress in reducing waste generation and moving towards safer waste management alternatives. EPA encourages facilities to first eliminate waste at its source (source reduction). For waste that is generated, the preferred management method is recycling, followed by energy recovery, treatment, and as a last resort, disposing of or otherwise releasing the waste. Learn more about Pollution Prevention and TRI.

The Waste Management Hierarchy

Source Reduction

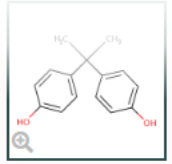
Production-related waste managed
4,4'-Isopropylidenediphenol, 2003 – 2020

20M

https://comptox.epa.gov/dashboard/chemical/toxics-release-inventory/DTXSID7020182

Exposure Tab: Biomonitoring Data

Measured values



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National Health and Nutrition Examination Survey (NHANES) Inferences (mg/kg-bw/day)

Search Monitoring Data

EXPORT

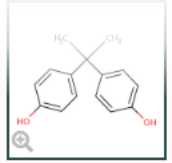
Monitoring Data

Demographic	Lower Bound (Median)	Upper Bound (Median)	Median
Age 6-11	3.80e-5	4.92e-5	4.33e-5
Age 12-19	2.55e-5	3.38e-5	2.93e-5
Age 20-65	2.79e-5	3.27e-5	3.02e-5
Age 65+	1.91e-5	2.31e-5	2.10e-5
BMI < 30	3.02e-5	3.30e-5	3.16e-5
BMI > 30	2.38e-5	2.74e-5	2.55e-5
Females	2.58e-5	3.03e-5	2.80e-5
Males	2.94e-5	3.37e-5	3.15e-5
Repro. Age Females	2.83e-5	3.31e-5	3.06e-5
Total	2.86e-5	3.08e-5	2.97e-5

https://comptox.epa.gov/dashboard/chemical/monitoring-data/DTXSID7020182

Exposure Tab: Exposure Predictions

Predicted values



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Exposure - Exposure Predictions (mg/kg-bw/day)

Search Demographics Predictions Data

EXPORT

Demographics Predictions Data

Demographic	Predictor	Median	Upper 95%ile	Units
Age 6-11	SEEM2 Heuristic	6.30e-5	1.05e-2	mg/kg/day
Age 12-19	SEEM2 Heuristic	5.87e-5	1.72e-2	mg/kg/day
Age 20-65	SEEM2 Heuristic	5.68e-5	1.15e-2	mg/kg/day
Age 66+	SEEM2 Heuristic	6.61e-5	1.95e-2	mg/kg/day
BMI <= 30	SEEM2 Heuristic	6.25e-5	1.36e-2	mg/kg/day
BMI > 30	SEEM2 Heuristic	7.07e-5	1.86e-2	mg/kg/day
Females	SEEM2 Heuristic	1.24e-5	2.90e-3	mg/kg/day
Males	SEEM2 Heuristic	3.87e-5	6.31e-3	mg/kg/day
Repro. Age Females	SEEM2 Heuristic	1.36e-5	4.18e-3	mg/kg/day
Total	SEEM3 Consensus	5.50e-5	2.04e-2	mg/kg/day

EXPORT

General Predictions Data

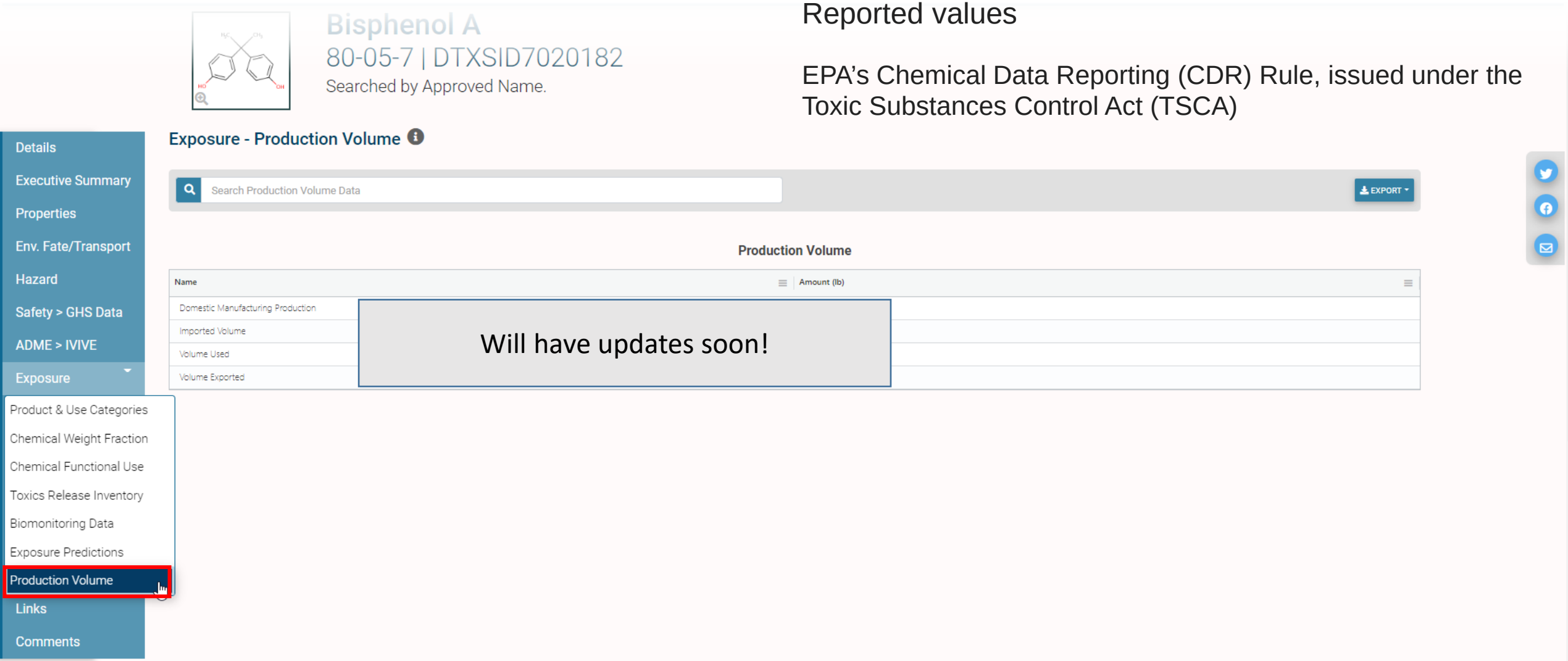
Predictor	Value	Units
Production Volume	2,780,000	kg/day
Stockholm Convention	0	Presence/Absence
Probability Far-Field Pesticide	0	Likelihood from 0 (none) to 1 (certain)
Probability Industrial	0	Likelihood from 0 (none) to 1 (certain)
Probability Residential	1	Likelihood from 0 (none) to 1 (certain)

https://comptox.epa.gov/dashboard/chemical/exposure-predictions/DTXSID7020182

Exposure Tab: Production Volume

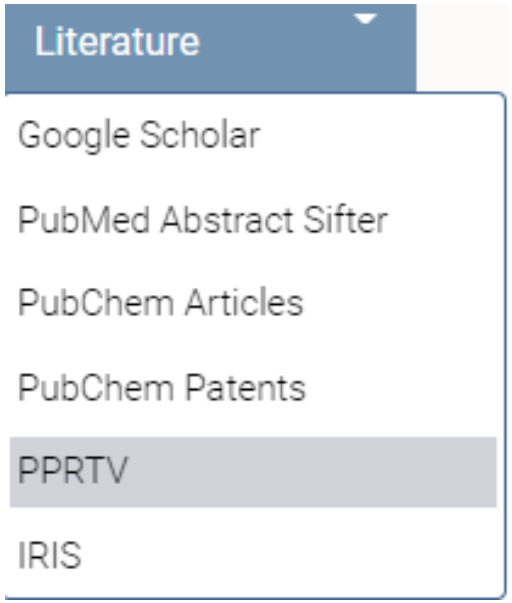
Reported values

EPA's Chemical Data Reporting (CDR) Rule, issued under the Toxic Substances Control Act (TSCA)



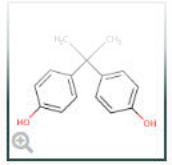
Literature Tabs

- Perform searches of publications containing the chemical, as well as user-defined terms
  - Google Scholar
  - PubMed Abstract Sifter
- Direct visualization of curated chemical database information
  - PubChem Articles
  - PubChem Patents
  - PPRTV (EPA's Provisional Peer-Reviewed Toxicity Value)
  - IRIS (EPA's Integrated Risk Information System)



External Links

United States Environmental Protection Agency



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General

- ACS Reagent Chemicals
- CAMEO Chemicals
- ChEBI
- ChemAgora
- ChEMBL
- Chemspider
- Consumer Product Information Database
- CPCat
- DrugBank
- ECHA Brief Profile
- ECHA Infocard
- EPA Substance Registry Service
- MSDS Lookup
- NIOSH Chemical Safety Cards
- NIST Chemistry Webbook
- PubChem
- PubChem 3D conformer download
- PubChem 3D Structure Display
- PubChem: Chemical Vendors
- PubChem Safety Sheet
- State-Specific Water Quality Standards
- ToxPlanet
- WEBWISER
- Wikidata
- Wikipedia
- Wolfram Alpha

Toxicology

- ACToR
- ACToR PDF Report
- BindingDB
- CalEPA OEHHA
- Chemical Checker
- ChemView
- CTD
- DrugPortal
- eChemPortal
- ECOTOX
- National Air Toxics Assessment
- NIOSH IDLH Values

Publications

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

Analytical

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

Prediction

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

CCD Help Page

www.epa.gov/chemical-research/comptox-chemicals-dashboard-help

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CompTox Chemicals Dashboard | Home | Search | Lists | About | Tools | Submit Comments

- About
- News
- Help
- Downloads
- Comments
- Release Notes

CompTox Chemicals Dashboard

Search 1,200,059 Chemicals

Chemicals | Products/Use Catego

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

Identifier substring search

Latest News

Read More News

CompTox Chemicals Dashboard Release 2.0.2

Updated at July 19, 2022

We apologize for the inconvenience. We had some technical challenges after a fix to correct an error due to internal maintenance, which led to several issues. An updated fix has been implemented. Please see the release notes. Thank you.

https://s3.amazonaws.com/dmap-ccte-ccd/current/manual/index.html

Submit Comments

EPA United States Environmental Protection Agency

CompTox Chemicals Dashboard | Home | Search | Lists | About | Tools | Submit Comments

New Comment

Your email

Message

SEND

Chemicals | Products/Use Categories | Assa

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

Identifier substring search

Latest News

Read More News

The new Dashboard is a complete rebuild and is replacing the CompTox Chemicals Dashboard released on July 12th 2020.

Updated at December 8, 2021

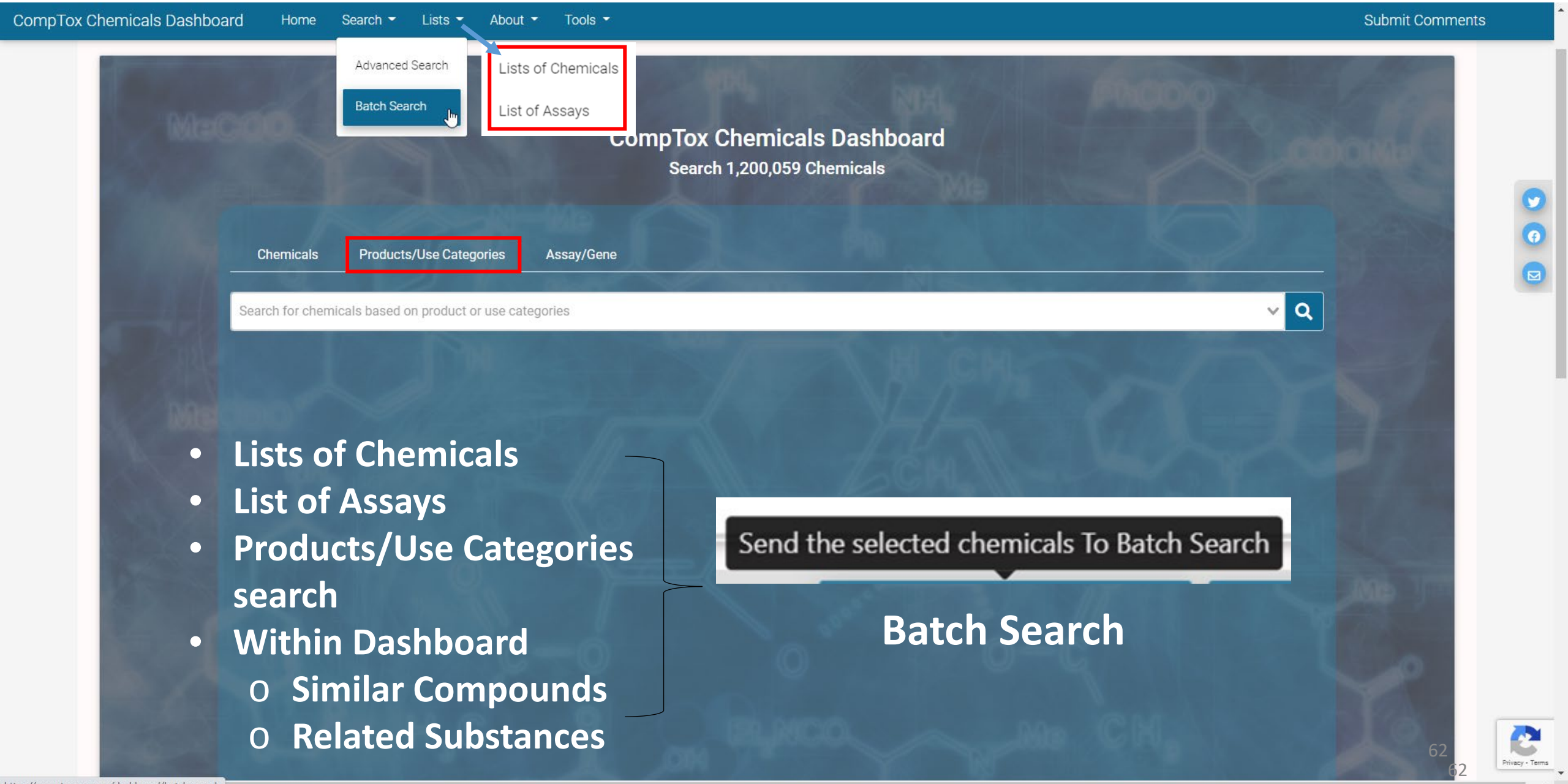
Check out the new CCD Dashboard About Page for details about the CCD Dashboard. The CCD Users Manual can help get you started.
Please log issues or questions using the Submit Comments function/button in the Menu bar.

Known Issues

1. Browser Cache: In order to properly load the new Comptox Chemical Dashboard and data, please clear the browser cache. We are observing issues caused by browser cache. Refer to the specific instructions on how to clear the cache for the various browsers.
2. Chemical Lists:
    1. Issue: Some hyperlinks for the list acronyms (e.g. toxcast_phase1, etc.) in the chemical list description are not functional i.e. all chemicals in the list are not displayed

Please report bugs using “Submit Comments.”

Batch Search



- Lists of Chemicals
- List of Assays
- Products/Use Categories search
- Within Dashboard
  - Similar Compounds
  - Related Substances

Batch Search

Batch Search

EPA United States Environmental Protection Agency

CompTox Chemicals Dashboard | Home | Search | Lists | About | Tools | Submit Comments

Lists of Chemicals
List of Assays

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

Identifier substring search

https://comptox.epa.gov/dashboard/chemical-lists

Batch Search

EPA United States Environmental Protection Agency

CompTox Chemicals Dashboard | Home | Search | Lists | About | Tools | Submit Comments | Search all data

Chemical Lists

Search Chemical Lists

EXPORT | COPY URL

Showing 410 Records

List Acronym	List Name	# Chemicals	Updated	List Description
40CFR1164	40 CFR 116.4 Designation of Hazardous Sub...	333	2020-06-25	Hazardous Substance List associated with the Federal Water Pollution Control Act, as amended by the Federal Water Pollution Control Act Amendments of 1972 (Pub. L. 92-500), and as further amended by the Clean Water Act of 1977 (Pub. L. 95-217), 33 U.S.C. 1251 et seq.; and as further amended by the Clean Water Act Amendments of 1978 (Pub. L. 95-676)The current list can be found at 40 CFR 116.4 list. Other lists of interest are: List of constituents of motor fuels relevant to leaking underground storage tank sites List of constituents of motor fuels relevant to leaking underground storage tank sites Chemicals present in Underground Storage Tanks Chemicals present in Underground Storage Tanks
40CFR355	40CFR355 Extremely Hazardous Substance ...	354	2018-01-05	Extremely Hazardous Substance List and Threshold Planning Quantities; Emergency Planning and Release Notification Requirements; Final Rule. (52 FR 13378) This FR notice contains the EHS list of chemicals as published in 1987. This list has been revised over time and should not be used for current compliance purposes. The current EHS list can be found at 40 CFR 355.
				The ACS Committee on Analytical Reagents sets purity specifications for almost 500 reagent chemicals and over 500 standard-grade reference materials. These specifications have become the de facto

Rows: 410

Batch Search

EPA United States Environmental Protection Agency

CompTox Chemicals Dashboard | Home | Search | Lists | About | Tools | Submit Comments | Search all data

Chemical Lists

Fat Minnow

EXPORT | COPY URL

Showing 1 of 410 Records

List Acronym	List Name	# Chemicals	Updated	List Description
EPAFHM	EPA|ECOTOX: Fathead Minnow Acute Toxicity	617	2008-02-15	The EPA Fathead Minnow Acute Toxicity database was generated by the U.S. EPA Mid-Continental Ecology Division (MED) for the purpose of developing an expert system to predict acute toxicity from chemical structure based on mode of action considerations. Hence, an important and unusual characteristic of this toxicity database is that the 617 tested industrial organic chemicals were expressly chosen to serve as a useful training set for development of predictive quantitative structure-activity relationships (QSARs). A second valuable aspect of this database, from a QSAR modeling perspective, is the inclusion of general mode-of-action (MOA) classifications of acute toxicity response for individual chemicals derived from study results. These MOA assignments are biologically based classifications, allowing definition of chemical similarity based upon biological activity instead of organic chemistry functional class as most commonly employed in QSAR study. MOA classifications should strengthen the scientific basis for construction of individual QSARs. However, it is cautioned that the broad MOA categorizations should not be construed to represent a single molecular mechanism; for example, CNS seizure agents and respiratory inhibitors are known to act through a variety of receptors. The DSSTox EPAFHM database includes information pertaining to organic chemical class assignments (ChemClass_FHM), acute toxicity in fathead minnow (LC50_mg), dose-response assessments (LC50_Ratio, ExcessToxicityIndex), behavioral assessments (FishBehaviorTest), joint toxicity MOA evaluations of mixtures (MOA_MixtureTest), and additional MOA evaluation of fish acute toxicity syndrome (FishAcuteToxSyndrome) in rainbow trout. All of these indicators, to the extent available, were considered in the determination of MOA and, additionally, were used to determine a level of confidence in the MOA assignment for each chemical (MOA_Confidence).

Rows: 1 of 410

Privacy - Terms

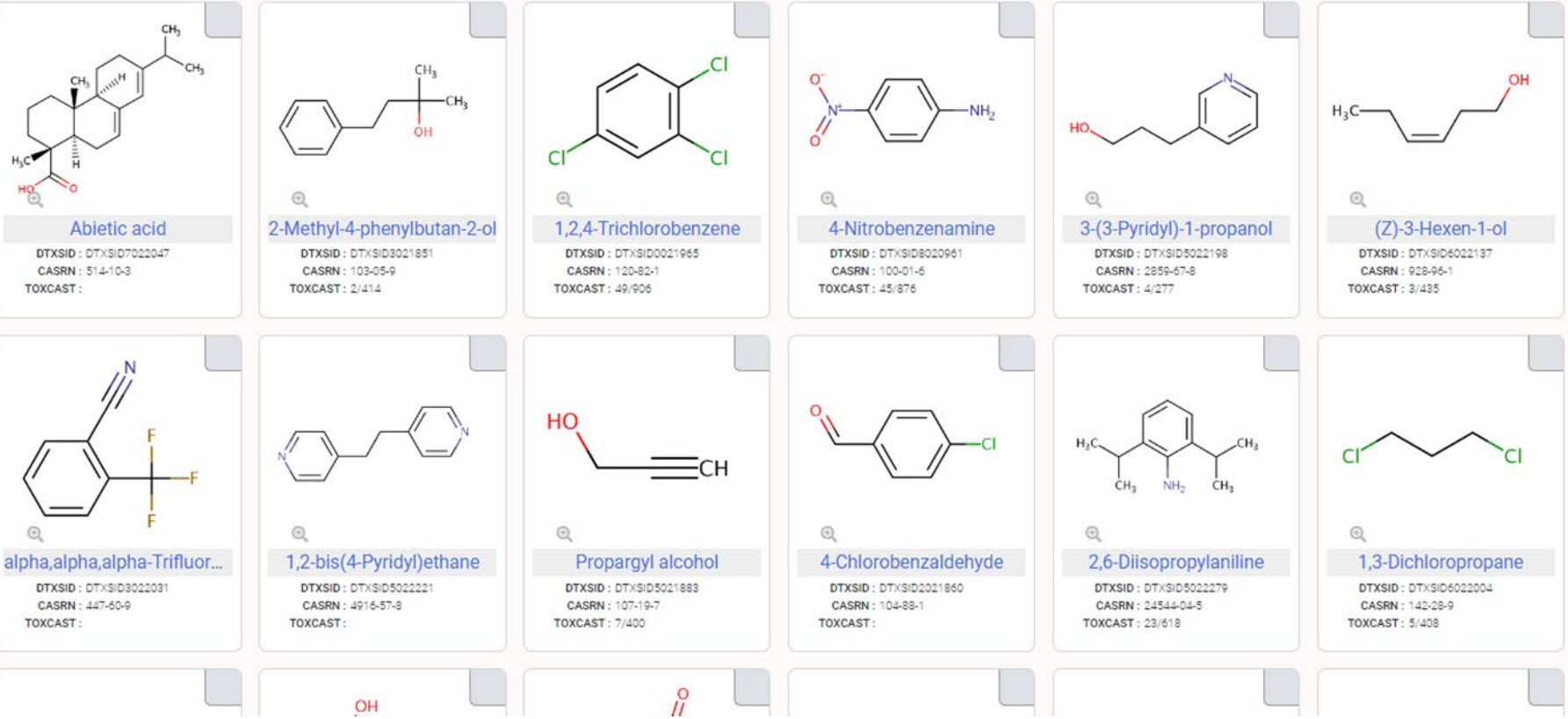
Batch Search

characteristic of this toxicity database is that the 617 tested industrial organic chemicals were expressly chosen to serve as a useful training set for development of predictive quantitative structure-activity relationships (QSARs). A second valuable aspect of this database, from a QSAR modeling perspective, is the inclusion of general mode-of-action (MOA) classifications of acute toxicity response for individual chemicals derived from study results. These MOA assignments are biologically based classifications, allowing definition of chemical similarity based upon biological activity instead of organic chemistry functional class as most commonly employed in QSAR study. MOA classifications should strengthen the scientific basis for construction of individual QSARs. However, it is cautioned that the broad MOA categorizations should not be construed to represent a single molecular mechanism; for example, CNS seizure agents and respiratory inhibitors are known to act through a variety of receptors. The DSSTox EPAFHM database includes information pertaining to organic chemical class assignments (ChemClass_FHM), acute toxicity in fathead minnow (LC50_mg), dose-response assessments (LC50_Ratio, ExcessToxicityIndex), behavioral assessments (FishBehaviorTest), joint toxicity MOA evaluations of mixtures (MOA_MixtureTest), and additional MOA evaluation of fish acute toxicity syndrome (FishAcuteToxSyndrome) in rainbow trout. All of these indicators, to the extent available, were considered in the determination of MOA and, additionally, were used to determine a level of confidence in the MOA assignment for each chemical (MOA_Confidence).

Number of Chemicals: 617

Search Results | SEND 617 TO BATCH SEARCH | TILE INFO | FILTER | EXPORT | PREFERRED VIEW

Showing 617 of 617 chemicals



Batch Search

EPA United States Environmental Protection Agency

CompTox Chemicals Dashboard | Home | Search | Lists | About | Tools | Submit Comments | Search all data

Batch Search

1 Select Input Type(s)

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

2 Enter Identifiers to Search

(Please enter one identifier per line and limit the number of identifiers to 10,000 or less)

```
DTXSID7022047
DTXSID3021851
DTXSID0021965
DTXSID8020961
DTXSID5022198
DTXSID6022137
DTXSID3022031
DTXSID5022221
```

3 DISPLAY ALL CHEMICALS or CHOOSE EXPORT OPTIONS

Customize Export Results

4 CHOOSE EXPORT FORMAT

- Excel
- CSV
- SDF v2000 MOL Format (.sdf)
- SDF v3000 MOL Format (.sdf)

Please select output format.

Batch Search

EPA United States Environmental Protection Agency

Customize Export Results

4 CHOOSE EXPORT FORMAT

Your file will be exported in Microsoft Excel Format (.xlsx)

Select All columns available

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
- Safety Data
- NHANES/Predicted Exposure
- Data Sources
- Include ToxVal Data Availability
- Assay Hit Count
- Number of PubMed Articles
- PubChem Data Sources
- CPDat Product Occurrence Count
- IRIS
- PPRTV
- Wikipedia Article
- QC Notes
- Include links to ACToR reports

Enhanced Data Sheets

- MetFrag Input File (Beta)
- ToxPrint single fingerprints
- Abstract Sifter Input File
- Synonyms and Identifiers
- Related Substance relationships
- ToxPrint fingerprints (ChemoTyper)
- Associated ToxCast Assays
- ToxValDB Details
- Physicochemical Property Values

Presence in Lists

Title	Description
40CFR1164	40 CFR 116.4 Designation of Hazardous Substances (Above Ground Storage Tanks)
40CFR355	40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities
ACSREAG	LIST: ACS Reagent Chemicals
AEGLVALUES	AEGLS: Acute Exposure Guideline Levels
AGCHEMWEAPONS	WEAPONS: Australia Group
ALGALTOX	LIST: Algal Toxins
ALLSURFACTANTS	CATEGORY: Surfactants
AMINOACIDS	CATEGORY: Amino acids
AMPHIBOLES	Amphibole minerals
ANITMICROB2	Antimicrobial Ingredients in Building Materials
ANTIBIOTICS	CATEGORY|PHARMACEUTICALS: Antibiotics
ANTIMICROBIALS	CATEGORY|WIKILIST|ANTIMICROBIALS: Antimicrobials from Wikipedia
AOPSTRESSORS	List of Adverse Outcome Pathway Stressors

Rows: 410

Download Export file for the chemicals selected

5 DOWNLOAD EXPORT FILE

United States Environmental Protection Agency

Summary

Summary

- Developed public access of environmental chemical data to support EPA and partner decision making.
- Provides chemistry, toxicity and exposure information for more than 1.2 million chemicals on the Dashboard.
- The idea is that easy access to data improves efficiency and accelerates chemical risk assessment.

United States Environmental Protection Agency

Questions

Future NAMs Trainings: Potential Topics

Topic Area	Specific Products, Including Web Applications, Databases, Tools and Workflows
CompTox Chemicals Dashboard	CompTox Chemicals Dashboard: overview, all sub-modules and their functionality tailored to be a chemical specific case study approach that is trainee/user-defined
Ecotoxicology	ECOTOX Knowledgebase, SeqAPASS
Exposure	CPDat (CPCat, CPCPdb, Ingredient Lists, Functional Use Data, Measured Data), Expocast/SEEM3; SHEDS HT
Databases relevant to toxicity and bioactivity	ToxCast, ToxRefDB, ToxVal, TEST; invitroDB
Toxicokinetics and dosimetry	High-Throughput Toxicokinetics R Package (httk)
Chemical safety proof-of-concept (POC) workflows	Toxic Substances Control Act (TSCA) POC, Bioactivity:Exposure Ratio
Chemistry	GenRA; phys-chem properties (OPERA models); ENTACT; Non-Targeted Analysis (NTA)

For more information: www.epa.gov/chemical-research/new-approach-methods-nams-training

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Research Planning and Implementation Staff

US EPA ORD Center for Computational Toxicology and Exposure

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

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Thank You!