



CompTox Chemicals Dashboard

Nisha S. Sipes, PhD

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

Presented at the Tribal Environmental Summit

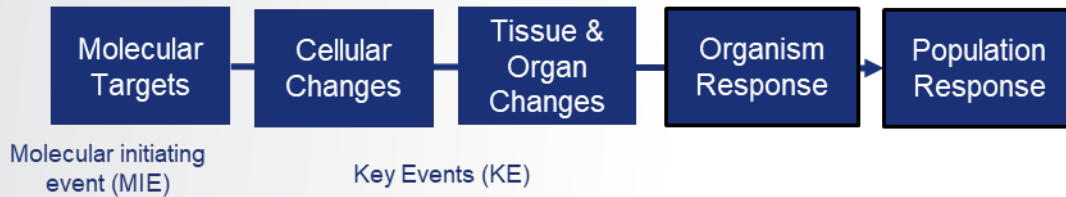
May 5, 2022

Sipes.Nisha@epa.gov

- Intro to Computational Toxicology
- Vision of the Dashboard
- CompTox Chemicals Dashboard Navigation
 - Simple search
 - Batch search
- Case Example for Clean Water Act Programs

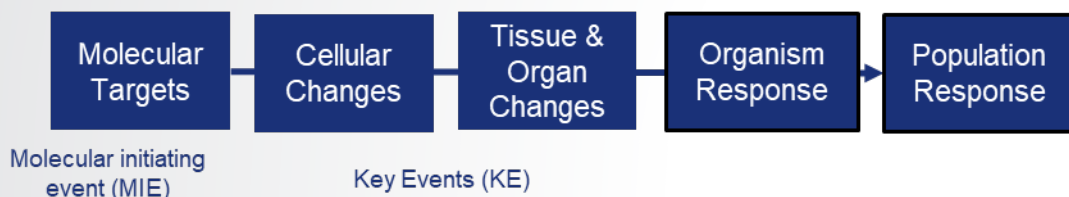
- Developing, gathering, integrating, and evaluating data and information using mathematical and computer-based approaches to better understand chemical hazards and risks to human health and the environment
- Typically refers to non-*in vivo* toxicological tools and approaches
 - New Approach Methodologies (NAMs)—*in silico*, *in vitro*, hazard + exposure
- Some tools and approaches are already used in hazard and/or risk assessments
 - E.g., Quantitative Structure-Activity Relationships (QSARs)

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



- **Adverse outcome pathways (AOPs)**

Pathway identification and knowledge integration



- ***In vitro* assays**

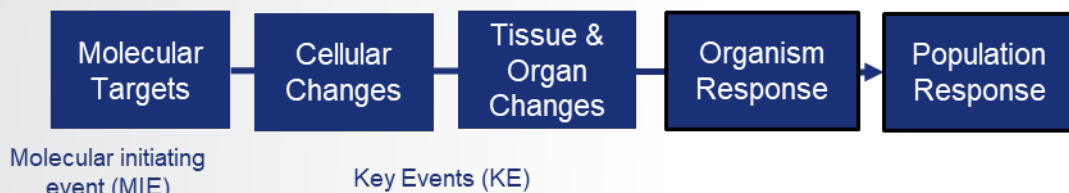
- Broad / screening (transcriptomics, cell painting)
- Targeted (receptors, enzymes)
- *In vitro* PODs, modes/mechanisms of action

- ***In vitro* toxicokinetics**

Allow conversion of an *in vitro* POD to *in vivo* (IVIVE)



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



- ***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)

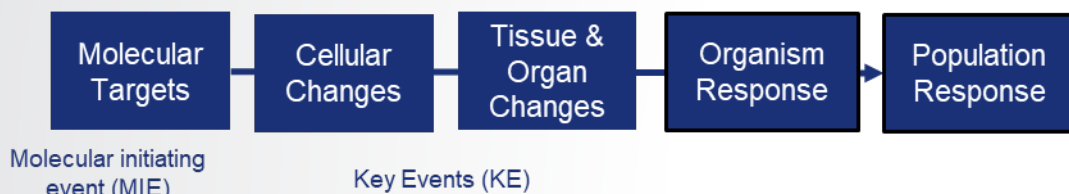


Image: <https://ncats.nih.gov/news/releases/2018/tox21-strategic-plan>



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

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



- ***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>



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



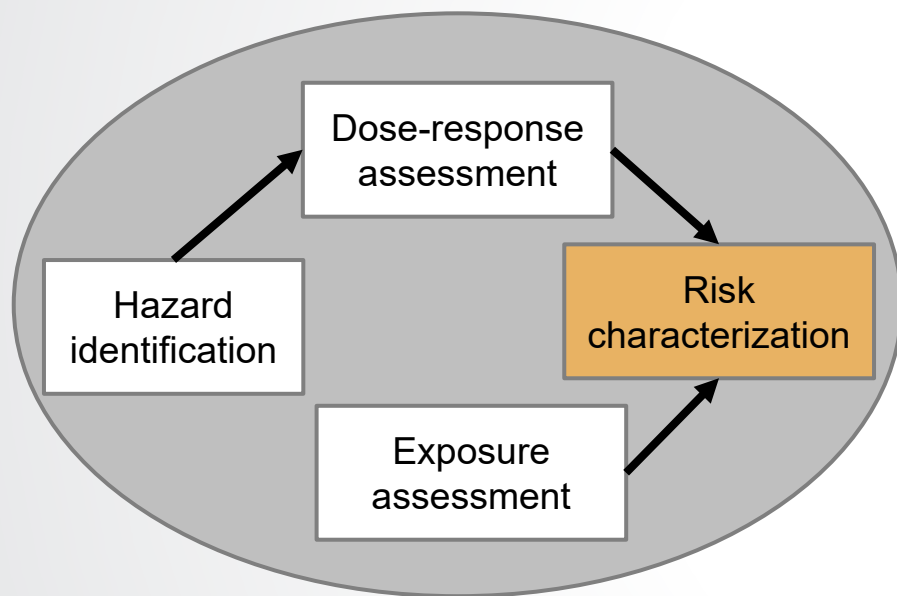
Image: <https://comptox.epa.gov/dashboard>

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



Vision of the CompTox Chemicals Dashboard

- Develop public access 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



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

+ online web applications: chemical similarity search, read-across, literature search



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

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

Welcome to the new EPA CompTox Chemicals Dashboard

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

CompTox Chemicals Dashboard

★ Search 906,511 Chemicals

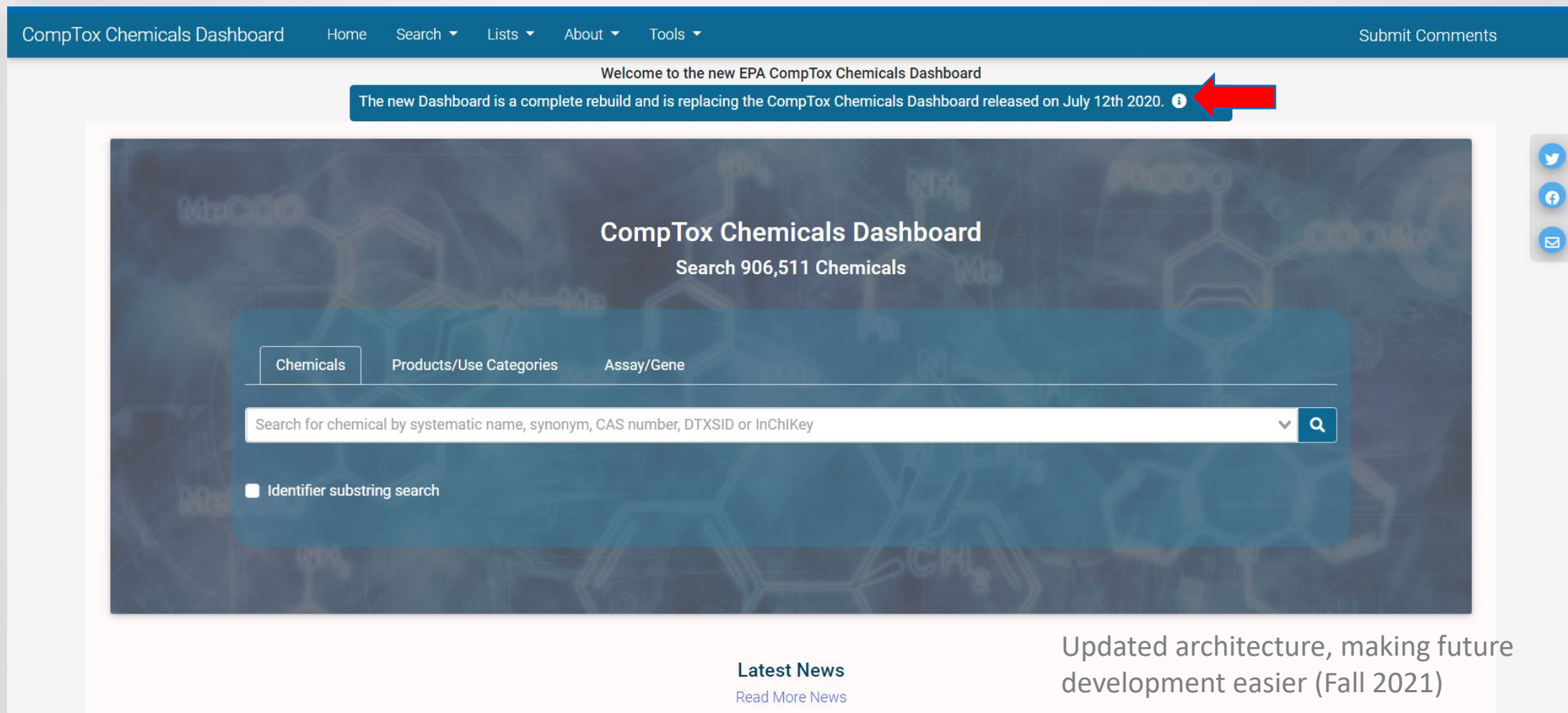
Chemicals Products/Use Categories Assay/Gene

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

☐ Identifier substring search

Latest News
[Read More News](#)

Updated architecture, making future development easier (Fall 2021)



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

Welcome to the new EPA CompTox Chemicals Dashboard

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

CompTox Chemicals Dashboard

Search 906,511 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](#)

Updated architecture, making future development easier (Fall 2021)



Provides the latest important information

Important Dashboard Information

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.

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_phasel, 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
 - Enter the list acronym in the filter box below the "List Acronym" header
 - Select the list to see all of the chemicals in that list
3. Chemical Result Sets:
 1. Issue: Anywhere within the Comptox Chemicals Dashboard that displays a list of chemicals, either from a user entered search or preconfigured lists linked from a searched chemical details. The sort function on the upper toolbar does not always work.
 2. Workaround: The initial view of all these result sets is the Ag-grid view. Use the column header sort function to get your desired sort:
 - Click on the header of the column you desire to sort on.
 - Once you click on the header it will show an arrow icon pointing up for an ascending order sort or down for descending order sort.
 - Clicking on the column header multiple times will cycle through ascending, descending, and then removing the sort order.

Latest News

[Read More News](#)

Updated architecture, making future development easier (Fall 2021)



Basic Search

[CompTox Chemicals Dashboard](#) [Home](#) [Search ▾](#) [Lists ▾](#) [About ▾](#) [Tools ▾](#) [Submit Comments](#)

Welcome to the new EPA CompTox Chemicals Dashboard

The new Dashboard is a complete rebuild and is replacing the CompTox Chemicals Dashboard released on July 12th 2020. [i](#)

CompTox Chemicals Dashboard

Search 906,511 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 – 3 ways

- chemical
- product/use category
- assay/gene

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

Welcome to the new EPA CompTox Chemicals Dashboard

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

CompTox Chemicals Dashboard

Search 906,511 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 – by chemical: “bisphenol a”

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

Welcome to the new EPA CompTox Chemicals Dashboard




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

CompTox Chemicals Dashboard

Search 906,511 Chemicals

Chemicals Products/Use Categories Assay/Gene

bisphenol a

-  Bisphenol A
DTXSID7020182
-  Bisphenol A-13C12 beta-D-Glucuronide
DTXSID601017638
-  Bisphenol A bis(2-hydroxyethyl ether) diacrylate
DTXSID6060000

16

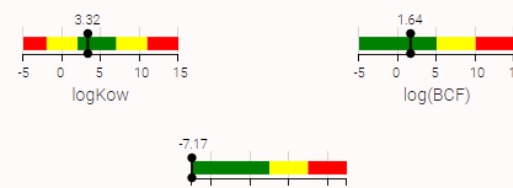


- Quantitative toxicity values
- ADME
- Exposure
- Adverse Outcome Pathway (AOP) links
- Physchem & fate & transport
- Plots: hazard Point-of-Departure (POD) oral/inhalation and in vitro bioactivity summary

Regional Screening ¹

Class	Risk Level
RfDo (mg/kg-day)	
risk-based SSL (mg/kg soil)	Tr
screening level (tap water) (ug/L)	Tr
screening level (residential soil) (mg/kg soil)	Tr
screening level (industrial soil) (mg/kg soil)	Tr
risk-based SSL (mg/kg soil)	THQ = 1 3.0e+3
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 ⓘ





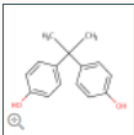
Executive Summary tab

- EPA's Integrated Risk Information System (IRIS)
- A Provisional Peer-Reviewed Toxicity Value (PPRTV) –for Superfund Program
- Regional Screening Level (RSL)
- Reference Dose (RfD)
- Reference Concentration (RfC)
- Point of Departure Value (POD)

CompTox Chemicals Dashboard Home Search Lists About Tools Submit Comments

Welcome to the new EPA CompTox Chemicals Dashboard

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

 **Bisphenol A**
80-05-7 | DTXSID7020182
Searched by Approved Name.

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
- **Subchronic Toxicology**
 - ✓ Subchronic toxicity PODs available
- **Developmental Toxicology**
 - ✓ Developmental toxicity PODs available

Regional Screening

Class	Risk Level
RfDo (mg/kg-day)	
risk-based SSL (mg/kg soil)	TH
screening level (tap water) (ug/L)	TH
screening level (residential soil) (mg/kg soil)	TH
screening level (industrial soil) (mg/kg soil)	TH
risk-based SSL (mg/kg soil)	TH
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

logKow: 3.32

log(BCF): 1.64

logKow: -7.17

Overview of data

- Quantitative toxicity values
- ADME
- Exposure
- Adverse Outcome Pathway (AOP) links
- Physchem & fate & transport
- Plots: hazard Point-of-Departure (POD) oral/inhalation and in vitro bioactivity summary

Scroll to see more 18



Executive Summary tab

Synonyms

Literature

Links

Comments

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

Acute toxicity PODs available

Subacute Toxicology

Subacute toxicity PODs available

Endocrine System

Endocrine Disruption Potential: Significant Estrogen and Androgen Receptor activity seen. Chemical was positive in 17 ER assay (out of 21) and was positive in 9 AR assay (tested in 17)

ADME

HTTK Oss data are available

Fate Transport

No bioaccumulation concern

No volatility concern

Biodegradation predictions are available

BOF predictions are available

Vapor Pressure predictions are available

Exposure

Exposure estimates are available based on NHANES and SEEM

AOP Information

AOP Links:

6, 8, 11, 14, 18, 19, 21, 23, 27, 29, 30, 33, 34, 36, 37, 41, 46, 51, 52, 53, 57, 58, 60, 61, 62, 64, 66, 67, 71, 72, 91, 93, 94, 96, 107, 111, 112, 117, 131, 150, 163, 165, 166, 167, 187, 197, 200, 214, 307, 310, 318

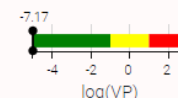
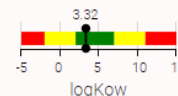
Other Notes

No water quality values available

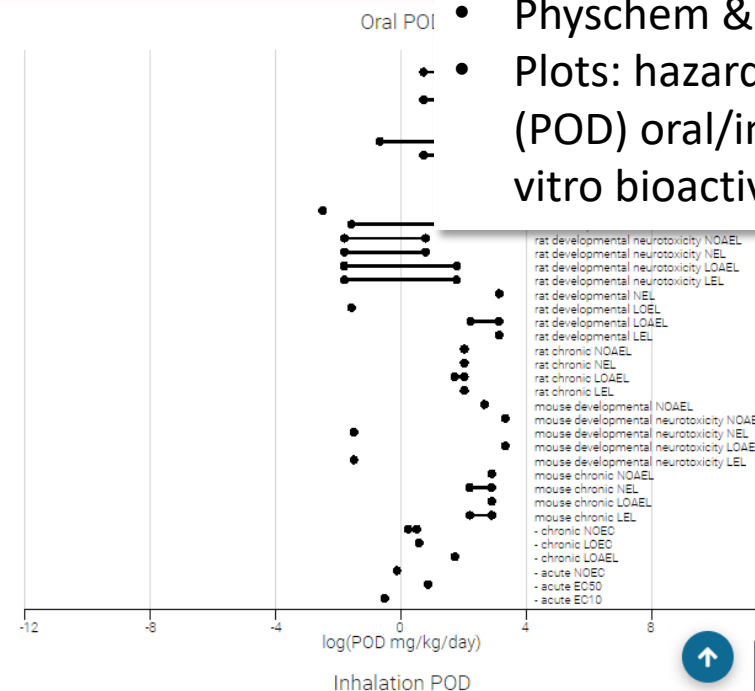
No air quality values available

No occupational exposure values available

PhysChem Parameters



Point-of-Departure Plots



Overview of data

- Quantitative toxicity values
- ADME
- Exposure
- Adverse Outcome Pathway (AOP) links
- Physchem & fate & transport
- Plots: hazard Point-of-Departure (POD) oral/inhalation and in vitro bioactivity summary

Scroll to see more 19



Executive Summary tab

- Synonyms
- Literature
- Links
- Comments

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

Acute toxicity PODs available

Subacute Toxicology

Subacute toxicity PODs available

Endocrine System

Endocrine Disruption Potential: Significant Estrogen and Androgen Receptor activity seen. Chemical was positive in 17 ER assay (out of 21) and was positive in 9 AR assay (tested in 17)

ADME

HTTK Oss data are available

Fate Transport

No bioaccumulation concern

Exposure limits

- Water quality, air quality, and occupational exposure values (e.g., EPA's Office of Water, Occupational Safety and Hazard (OSHA))

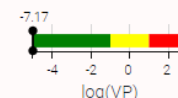
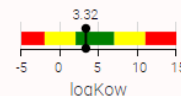
AOP Links:

6, 8, 11, 14, 18, 19, 21, 23, 27, 29, 30, 33, 34, 36, 37, 41, 46, 51, 52, 53, 57, 58, 60, 61, 62, 64, 66, 67, 71, 72, 91, 93, 94, 96, 107, 111, 112, 117, 131, 150, 163, 165, 166, 167, 187, 197, 200, 214, 307, 310, 318

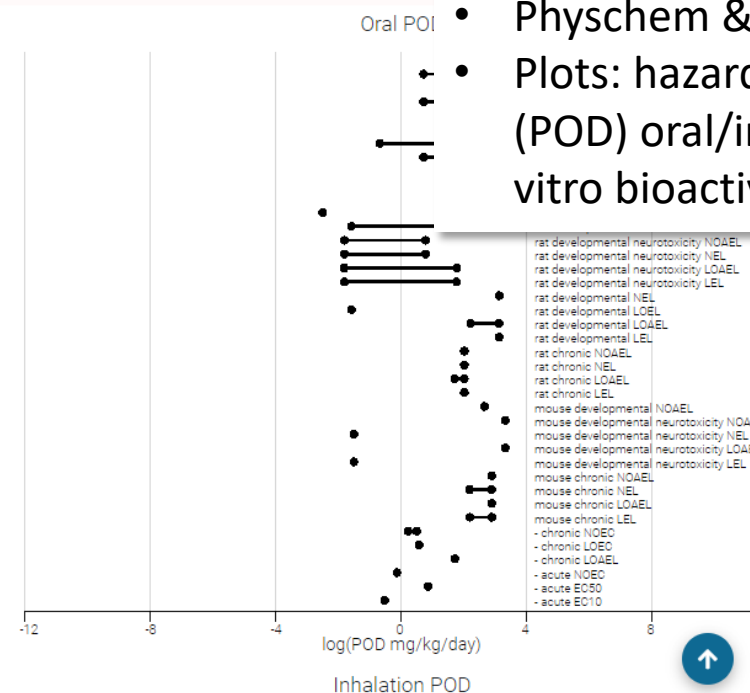
Other Notes

- No water quality values available
- No air quality values available
- No occupational exposure values available

PhysChem Parameters



Point-of-Departure Plots



Overview of data

- Quantitative toxicity values
- ADME
- Exposure
- Adverse Outcome Pathway (AOP) links
- Physchem & fate & transport
- Plots: hazard Point-of-Departure (POD) oral/inhalation and in vitro bioactivity summary

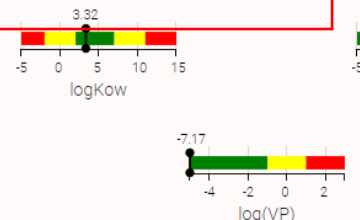
Functional Informational Features

- Synonyms
- Literature
- Links
- Comments

PhysChem Parameters

These PhysChem Parameters are those of primary concern for the distribution and bioavailability of chemicals in the environment: logP, Bioconcentration Factor and Vapor Pressure. The color coding illustrates the acceptable ranges.

PhysChem Parameters



Subchronic Toxicology

Subchronic toxicity PODs available

Developmental Toxicology

Developmental toxicity PODs available

Acute Toxicology

Acute toxicity PODs available

Subacute Toxicology

Subacute toxicity PODs available

Endocrine System

Endocrine Disruption Potential: Significant Estrogen and Androgen Receptor activity seen. Chemical was positive in 17 ER assay (out of 21) and was positive in 9 AR assay (tested in 17)

ADME

HTTK Oss data are available

Fate Transport

No bioaccumulation concern

No volatility concern

Biodegradation predictions are available

BOF predictions are available

Vapor Pressure predictions are available

Exposure

Exposure estimates are available based on NHANES and SE

AOP Information

AOP Links:

6, 8, 11, 14, 18, 19, 21, 23, 27, 29, 30, 33, 34, 36, 37, 41, 46, 51, 52, 53, 57, 58, 60, 61, 62, 64, 66, 67, 71, 72, 91, 93, 94, 96, 107, 111, 112, 117, 131, 150, 163, 165, 166, 167, 187, 197, 200, 214, 307, 310, 318

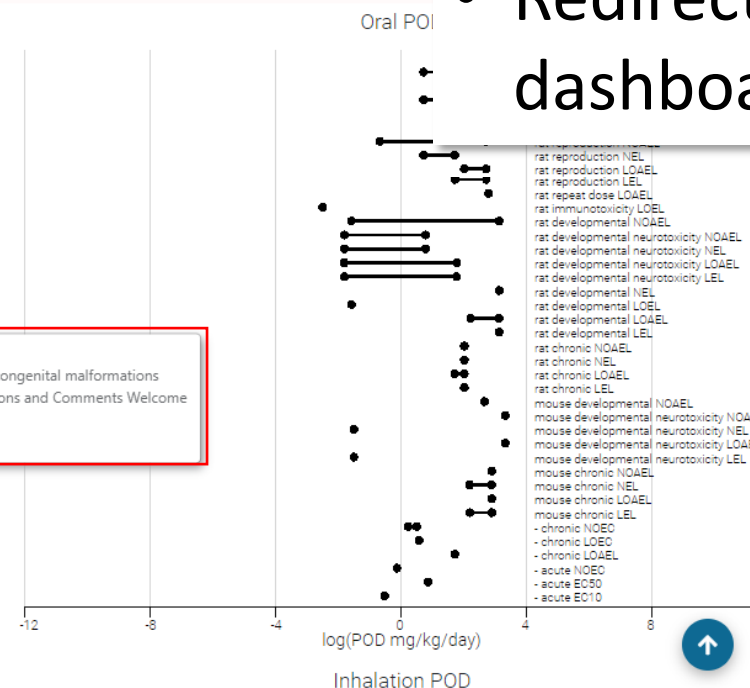
Other Notes

No water quality values available

No air quality values available

No occupational exposure values available

Point-of-Departure Plots



ID: 94

AOP TITLE Sodium channel inhibition leading to congenital malformations
AUTHOR STATUS Under Development: Contributions and Comments Welcome
OECD STATUS
SAAOP STATUS Under Development

- Hover over information
- Links to external resources
- Redirect links within dashboard

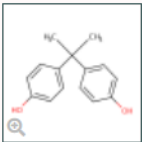


Properties tab: Experimental and Predicted Values

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

Welcome to the new EPA CompTox Chemicals Dashboard

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

 **Bisphenol A**
80-05-7 | DTXSID7020182
Searched by DTXSID

Properties: Summary

Summary

EXPORT

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-m ³ /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	dyn/cm
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

New Data Table Functional Features

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

Details

Executive Summary

Properties

Env. Fate/Transport

Hazard

Safety > GHS Data

ADME > IVIVE

Exposure

Bioactivity

Similar Compounds

GenRA

Related Substances

Synonyms

Properties: Summary

Summary

EXPORT

CSV (.csv)

Excel (.xlsx)

Experimental average

Experimental median

Predicted median

Experimental range

Predicted range

Unit

Search...

Property

Experimental average

Predicted average

Experimental median

Predicted median

Experimental range

Predicted range

Unit

Boiling Point

Flash Point

Melting Point

Molar Refractivity

Molar Volume

Viscosity

Surface Tension

Density

Vapor Pressure

Water Solubility

2100 (1)

-

155 (7)

-

-

-

-

-

1.07e-6 (3)

8.55e-4 (3)

362

190

132

68.2

200

9.66

46.0

1.17

5.34e-7

1.69 (4)

200

-

153 to 156

-

-

-

-

-

-

5.26e-4

27.0

1.25e-7

343 to 401

125 to 153

68.2

200

9.66

1.14 to 1.20

6.78e-8 to 2.59e-6

5.25e-4 to 1.51e-3

Å^3

atm-m3/mole

°C

°C

cm^3

cm^3

cP

g/cm^3

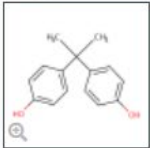
mmHg

mol/L

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

Welcome to the new EPA CompTox Chemicals Dashboard

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



Bisphenol A
80-05-7 | DTXSID7020182
Searched by DTXSID

Env. Fate/Transport: Summary

Summary

EXPORT

Property ↓↑	Experimental average ↓↑	Predicted average ↓↑	Experimental median ↓↑	Predicted median ↓↑	Experimental range ↓↑	Predicted range ↓↑
Atmos. Hydroxylation Rate		1.64e-11 (1)		1.64e-11	-	1.64e-11
Biodeg. Half-Life		15.1 (1)		15.1	-	15.1
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

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

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

Ability to look at parameter-specific tables

Physical-Chemical & Environmental Fate/Transport Properties

- Input into broader models – e.g., hazard, toxicokinetics, exposures
- Use as flags related to persistence and bioaccumulation
- Experimental design – e.g., knowing what chemicals are too volatile when designing bioactivity screens

- **Similar Compounds**, based on similarity of molecular fingerprints
- **Related Substances**, based on
 - Salt Form
 - Monomer
 - Polymer
 - Predecessor: Component
 - Component
 - Markush Parent
 - Markush Child
 - Transformation Parent
 - Transformation Product



Related Substances

- Interactive workflow to:
 - search for target or draw it;
 - define fingerprints for similarity and number of analogs;
 - Examine what data exist for source analogs;
 - Inspect the consistency, concordance, and range of effects for analogs
 - Understand confidence in the prediction(s)

Neighbors by:

Chem: Morgan Fgrprts

Chem: Morgan Fgrprts

Chem: Torsion Fgrprts

Chem: ToxPrints

Biology: ToxCast data

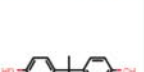
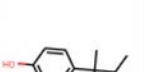
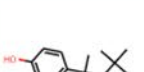

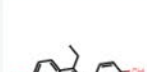
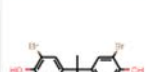
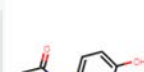
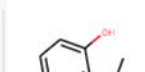
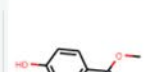
Toxicity: ToxRef data

Custom hybrid

Filter by:

In vivo data

Run Read-Across GenRA Min+ 1 Min- 1 Similarity Weights Hide Pagination Download: File Type

Assay endpoint	1.00	0.48	0.45	0.41	0.29	0.29	0.28	0.28	0.28
Bisphenol A									
CHR:adrenal gland	Blue	Grey	Grey	Blue	Grey	Grey	Blue	Blue	Grey
CHR:alanine aminotransferase	Grey	Grey	Grey	Red	Grey	Grey	Grey	Grey	Grey
CHR:albumin	Grey	Grey	Grey	Red	Grey	Grey	Grey	Grey	Grey
CHR:alkaline phosphatase	Grey	Grey	Grey	Red	Grey	Grey	Grey	Grey	Grey
CHR:blood	Grey	Grey	Grey	Red	Grey	Grey	Grey	Grey	Grey
CHR:body weight	Red	Grey	Grey	Red	Grey	Grey	Red	Red	27

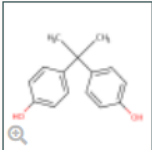
Traditional animal studies toward human toxicity & ecotoxicology

ToxVal Database – 30 worldwide sources

- e.g., IRIS, ECHA, EFSA ...
- + ECOTOXicology Knowledgebase (ECOTOX) – aquatic life, terrestrial plants and wildlife

CompTox Chemicals Dashboard
Home
Search
Lists
About
Tools
Submit

Welcome to the new EPA CompTox Chemicals Dashboard
The new Dashboard is a complete rebuild and is replacing the CompTox Chemicals Dashboard release



Bisphenol A

80-05-7 | DTXSID7020182

Searched by DTXSID

Hazard: Point of Departure

Point of Departure
Search Hazard

☒ human
☐ eco

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	-	-
	3	ECHA POC	NOAEL	-	repeat dose	=	750	ppm	repeat dose	oral	reduced body weight (males) and females, delayed vaginal patency, preputial separation (males), reduced litter size	rat	2002
	3	ECHA POC	LOAEL	-	subchronic	=	250	ppm	subchronic	oral	cecal enlargement	mouse rat	1982
	3	ECHA POC	NOAEL	-	reproduction	=	750	ppm	reproducti...	oral	body weight and weight gain	rat	2002
	3	ECHA POC	NOAEL	-	developmental	=	300	ppm	developm...	oral	-	mouse	2007
	3	ECOTOX	LOEL	-	acute development	-	125	mg/kg bd...	Developm...	Intraperito...	Abnormal	norway rat	1981
	3	ECHA POC	NOAEL	-	reproduction	=	750	mg/m3	reproducti...	oral	body weight and weight gain	rat	2002
	3	ECHA POC	NOAEL	-	reproduction	=	750	ppm	reproducti...	oral	body weight and weight gain	rat	2000

Rows: 223
Total Rows: 223

Exposure limits

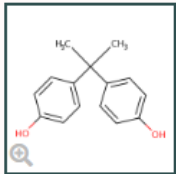
Water quality, air quality, and occupational exposure values

e.g., EPA's Office of Water, Occupational Safety and Hazard (OSHA), Food and Drug Administration, State-specific values

CompTox Chemicals Dashboard
Home
Search
Lists
About
Tools

Welcome to the new EPA CompTox Chemicals Dashboard

The new Dashboard is a complete rebuild and is replacing the CompTox Chemicals Dashboard



Bisphenol A

80-05-7 | DTXSID7020182

Searched by DTXSID7020182.

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

Exposure Limit

Search Hazard

☒ human
☐ eco

EXPORT

More	Priority ↑	Source	Type	Subtype	Risk Assessment	Qualifier	Value	Units	Study Type	Exposure Route	Critical effect	Species	Year
	2	FDA CEDI	cumulative estimated daily intake	-	chronic	=	1.85e-4	mg/...	-	oral	-	-	-
	2	FDA CEDI	cumulative daily concentration	-	chronic	=	3.70	ppb	-	oral	-	-	-
	5	EFSA	TDI	-	chronic	=	4.00	ug/k...	-	oral	-	-	2008
	5	EFSA	TDI	-	chronic	=	5.00e-2	mg/...	-	oral	-	-	2008
	7	DOE Protective ...	PAC-3	PAC 3	acute	=	650	mg/...	acute	inhal...	-	-	-
	7	DOE Protective ...	PAC-1	PAC 1	acute	=	15.0	mg/...	acute	inhal...	-	-	-
	7	DOE Protective ...	PAC-2	PAC 2	acute	=	110	mg/...	acute	inhal...	-	-	-

29



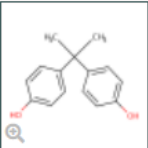
Safety > GHS Data

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.

CompTox Chemicals Dashboard Home Search Lists About Tools Submit Comments

Welcome to the new EPA CompTox Chemicals Dashboard

The new Dashboard is a complete rebuild and is replacing the CompTox Chemicals Dashboard released on July 12th 2021

 **Bisphenol A**
80-05-7 | DTXSID7020182
Searched by DTXSID

Safety - GHS Data

PRINT PAGE




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.)

e.g., sources:

- EU Regulation
- European Chemicals Agency (ECHA)
- Safe Work Australia
- Hazardous Substances Data Bank (HSDB)
- Japan National Institute of Technology and Evaluation (NITE)

Links out to external source (PubChem)

US EPA's Toxicity Forecasting (ToxCast) Program

<https://www.epa.gov/chemical-research/toxicity-forecasting>

Bioactivity

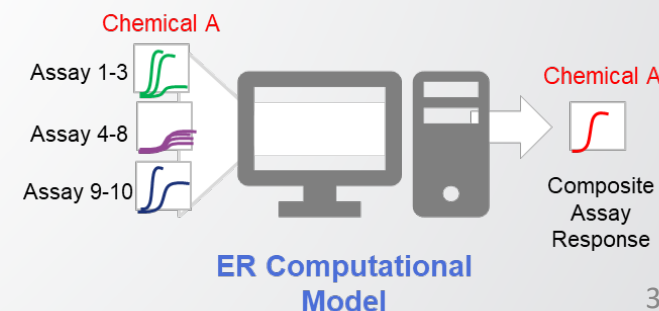
ToxCast: Summary

Conc. Response Data

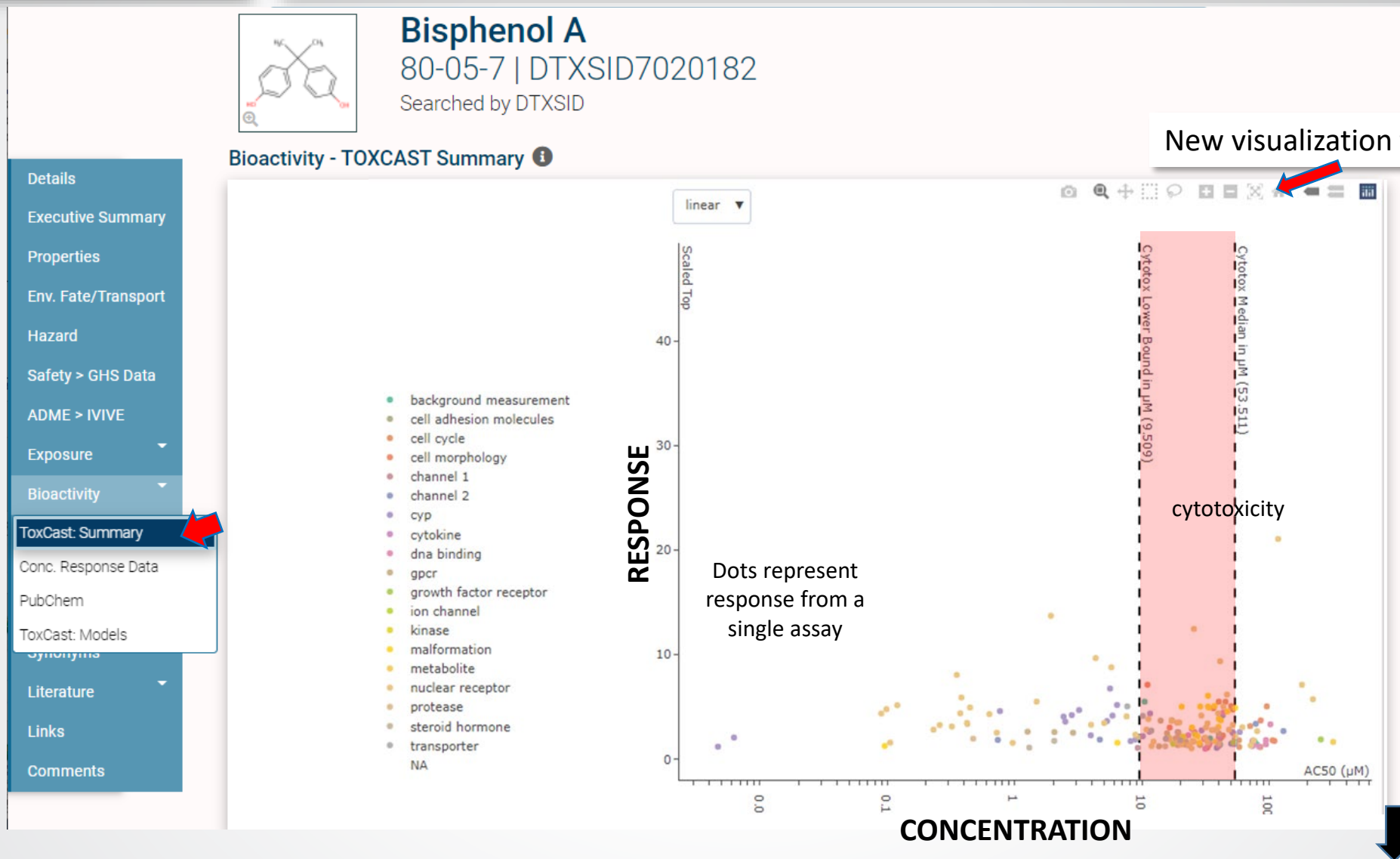
PubChem

ToxCast: Models

- High throughput chemical screens to generate biological data on hundreds to thousands of chemicals
 - E.g., chemical-biological receptor interaction, metabolomics changes, functional cellular changes (neural network function), zebrafish development
 - Tox21 – intergovernmental US collaboration
- Development of predictive models utilizing individual assay data (e.g., estrogen receptor (ER) model)



Bioactivity tab: ToxCast Summary



New visualization features



Bioactivity tab: ToxCast Summary

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

☒ Filter out 'background' from Intended Target Family

Activity concentration where there is a 50% change in response

<input type="checkbox"/>	Name	Details	SeqAPASS	Gene Symbol	AOP	Event	Hit Call	Top	AC50	logAC50	Max Med	Cutoff	Modl Acc	Intended Target Family
<input type="checkbox"/>							(1)							background
<input type="checkbox"/>	ACEA_AR_agonist...				-	-	Active	148	40.0	1.60	123.326 - percent_a...	26.9	1.14	cell cycle
<input type="checkbox"/>	ACEA_AR_antagon...			AR	-	-	Active	3.43	41.0	1.61	2.860 - log2_fold_in...	0.3...	1.07	nuclear receptor
<input type="checkbox"/>	ACEA_AR_antagon...				-	-	Active	141	36.3	1.56	116.273 - percent_ac...	29.0	1.10	cell cycle
<input type="checkbox"/>	ACEA_ER_80hr		NP_000116.2	ESR1	-	-	Active	112	0.373	-0.428	112.502 - percent_ac...	25.6	-0....	nuclear receptor
<input type="checkbox"/>	APR_HepG2_CellL...				-	-	Active	1.20	106	2.02	1.197 - log2_fold_ind...	0.6...	2.03	cell cycle
<input type="checkbox"/>	APR_HepG2_CellL...				-	-	Active	4.49	95.2	1.98	4.435 - log2_fold_in...	0.8...	1.75	cell cycle
<input type="checkbox"/>	APR_HepG2_Mito...				-	-	Active	0.8...	109	2.04	0.867 - log2_fold_in...	0.4...	2.05	cell morphology
<input type="checkbox"/>	APR_HepG2_Mito...				-	-	Active	5.92	11.0	1.04	6.453 - log2_fold_in...	0.831	0.811	cell morphology
<input type="checkbox"/>	APR_HepG2_Mito...				-	-	Active	2.71	85.3	1.93	2.255 - log2_fold_in...	0.7...	1.70	cell morphology
<input type="checkbox"/>	APR_HepG2_Mitoti...			H3F3A	-	-	Active	1.66	84.7	1.93	1.443 - log2_fold_in...	1.42	2.29	cell cycle
<input type="checkbox"/>	APR_HepG2_P-H2...		NP_002096.1	H2AFX	-	-	Active	1.20	110	2.04	1.192 - log2_fold_ind...	0.821	2.08	dna binding
<input type="checkbox"/>	APR_HepG2_P-H2...		NP_002096.1	H2AFX	-	-	Active	1.80	106	2.02	1.596 - log2_fold_in...	1.10	2.08	dna binding
<input type="checkbox"/>	ATG_Ahr_CIS_up		NP_001612.1	AHR	57 131 21 41 150 310	165	Active	1.31	23.4	1.37	1.281 - log2_fold_ind...	0.9...	1.56	dna binding
<input type="checkbox"/>	ATG_AP_1_CIS_up		NP_005243.1 NP_002219.1	FOS TFAP2A	-	-	Active	0.8...	33.7	1.53	0.746 - log2_fold_in...	0.5...	1.67	dna binding
<input type="checkbox"/>	ATG_AP_2_CIS_dn		NP_003211.1 NP_003212.2 NP_758438.2	TFAP2B	-	-	Active	0.4...	93.8	1.97	0.456 - log2_fold_in...	0.318	2.02	dna binding

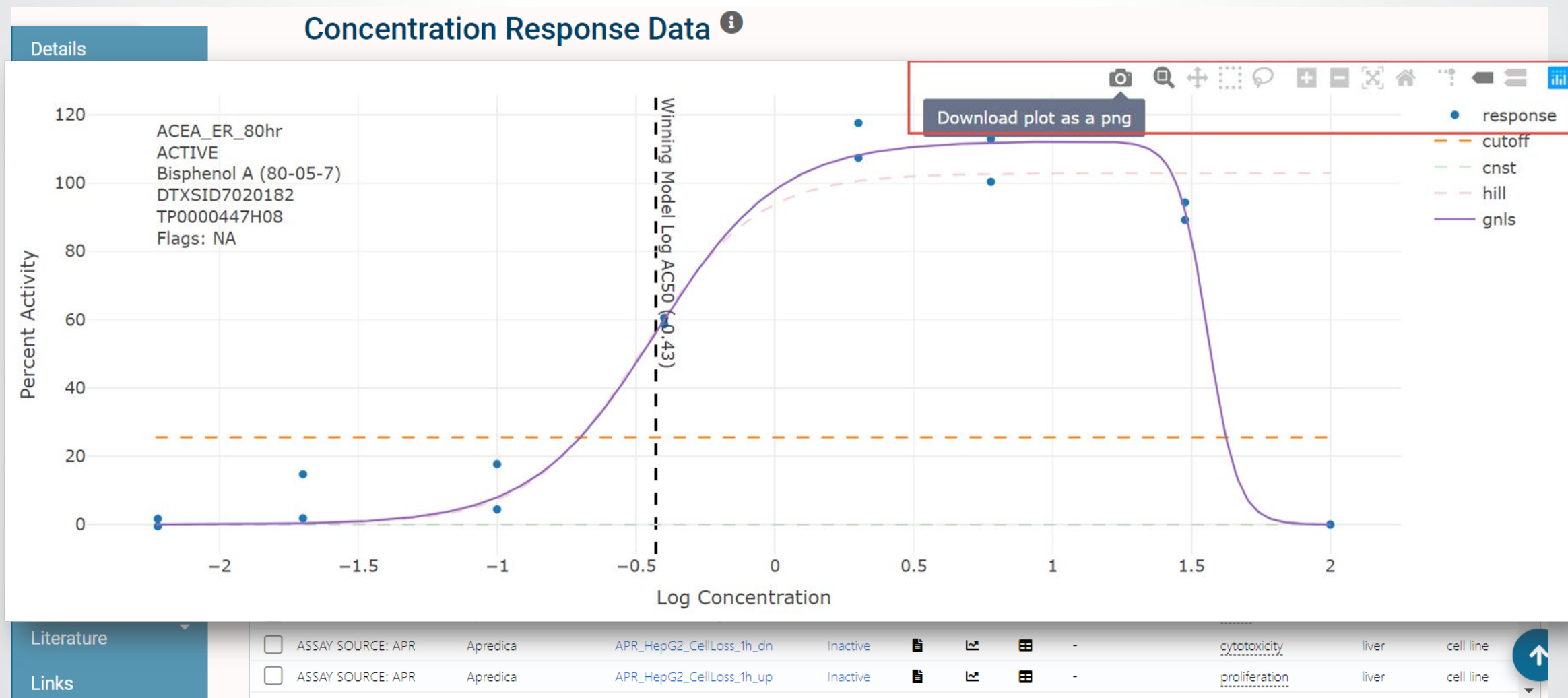


Analytical Data on Tox21 Browser [↗](#)

EXPORT ▼

Links out to concentration-response plots

<input type="checkbox"/>	Name ↑	Description	Endpoint Name	Active	Details	SEP	Cell	Gene	Intended Target	Cell Line	Cell
<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_via...	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_1...	Inactive				-	proliferation	liver	cell line
<input type="checkbox"/>	ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_1...	Inactive				-	arrest	liver	cell line
<input type="checkbox"/>	ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_2...	Inactive				-	proliferation	liver	cell line
<input type="checkbox"/>	ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_2...	Inactive				-	arrest	liver	cell line
<input type="checkbox"/>	ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_7...	Inactive				-	proliferation	liver	cell line
<input type="checkbox"/>	ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_7...	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



Details

Executive Summary

Properties

Env. Fate/Transport

Hazard

Safety > GHS Data

ADME > IVIVE

Exposure

Bioactivity

ToxCast: Summary

Conc. Response Data

PubChem

ToxCast: Models

Synonyms

Literature

Links

Comments

Bioactivity - PubChem Biological Activities

PRINT PAGE

PUBCHEM > BISPHENOL A > BIOASSAY RESULTS

Links out to external source (PubChem)

BioAssay Results

2,858 items View More Rows & Details

Download

SORT BY

Activity Value

Activity ?	Activity Value, μ M	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

...

572

Next >



Bioactivity tab: ToxCast: Models

Bioactivity - ToxCast: Models

EXPORT

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)

Details

Executive Summary

Properties

Env. Fate/Transport

Hazard

Safety > GHS Data

ADME > IVIVE

Exposure

Bioactivity

ToxCast: Summary

Conc. Response Data

PubChem

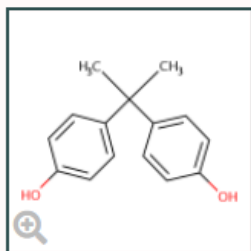
ToxCast: Models

Synonyms



What can be done with the bioactivity data?

- Valuable for chemical safety and risk assessment
 - Routinely used by industries and regulatory authorities (e.g., genotoxicity)
- Informing Adverse Outcome Pathways
- Estrogen Pathway model is an alternate Tier 1 screen for the US EPA's Endocrine Disruptor Screening Program (EDSP)
- Toward prioritization: In vitro to in vivo extrapolation (IVIVE)
 - Calculate an external exposure dose based on the *in vitro* bioactivity data and compare with predicted exposures



Bisphenol A

80-05-7 | DTXSID7020182

Searched by Approved Name.

ADME - IVIVE



EXPORT

IVIVE

Label	Measured	Predicted	Computed	Unit
<u>In Vitro Intrinsic Hepatic Clearance</u>	19.90	-	-	uL/min/million hepatocytes
<u>Fraction Unbound in Human Plasma</u>	0.04	-	-	
<u>Volume of Distribution</u>	-	-	5.01	L/kg
<u>Days to Steady State</u>	-	-	1.00	Days
<u>PK Half Life</u>	-	-	31.70	hours
<u>Human Steady-State Plasma Concentration</u>	-	-	3.30	mg/L

Details

Executive Summary

Properties

Env. Fate/Transport

Hazard

Safety > GHS Data

ADME > IVIVE

Exposure

Bioactivity

Similar Compounds





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 env./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

- Product & Use Categories
- Chemical Weight Fraction
- Chemical Functional Use
- Toxics Release Inventory
- Monitoring Data
- Exposure Predictions
- Production Volume



Exposure tab: Product & Use Categories

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

- Details
- Executive Summary
- Properties
- Env. Fate/Transport
- Hazard
- Safety > GHS Data
- ADME > IVIVE
- Exposure
 - Product & Use Categories**
 - Chemical Weight Fraction
 - Chemical Functional Use
 - Toxics Release Inventory
 - Monitoring Data
 - Exposure Predictions
 - Production Volume
- Links
- Comments

Product and Use Categories (PUCs)

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

EXPORT

General Use Keywords ⓘ

General Use Keywords	Number of Sources
active_ingredient, Pesticides	1
artificial_sweat, detected, emissions, Europe, Other direct c...	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



Exposure tab: Chemical Weight Fraction

Reported or predicted by ingredient list

Details

Executive Summary

Properties

Env. Fate/Transport

Hazard

Safety > GHS Data

ADME > IVIVE

Exposure

Product & Use Categories

Chemical Weight Fraction

Chemical Functional Use

Toxics Release Inventory

Monitoring Data


Exposure Predictions

Production Volume

Chemical Weight Fractions (CWF)



 EXPORT 

Product Name	Product Use Category	Minimum Weight Fraction	Maximum Weight Fraction	Data Type	Product Count
<input type="text"/>		<input type="text"/>	<input type="text"/>	<input type="text"/>	<input type="text"/>
02y040cat comp b mil-p-23377g...	Not yet Categorized	0.00	0.500	reported	1
032l015 epi-cure 872	Not yet Categorized	0.00	0.100	reported	1
0387 hec black	Not yet Categorized	-	-	reported	1
039-080055-044_part b	Not yet Categorized	-	-	reported	1
1101/0978-0979_belzona 1321 (b...	Not yet Categorized	0.100	0.300	reported	1
1:1 adduct for epoxy fill primer_1...	Not yet Categorized	0.00	5.00e-2	reported	1
1961a concise orthodontic bondi...	Not yet Categorized	0.00	1.00e-2	reported	1
1961a concise orthodontic bondi...	Not yet Categorized	0.00	1.00e-2	reported	1
3135 a (epoxy resin)_part a	Not yet Categorized	-	-	reported	1
3197 steel works	Not yet Categorized	1.00e-2	7.00e-2	reported	1
3303/1358_4911 (belzona magm...	Not yet Categorized	1.00e-2	5.00e-2	reported	2
3303/1358_belzona 4911 solidifier	Not yet Categorized	1.00e-2	5.00e-2	reported	1

Rows: 250





Exposure tab: Functional Use

Reported and predicted values

Details

Executive Summary

Properties

Env. Fate/Transport

Hazard

Safety > GHS Data

ADME > IVIVE

Exposure

Product & Use Categories

Chemical Weight Fraction

Chemical Functional Use

Toxics Release Inventory

Monitoring Data

Exposure Predictions

Production Volume

Exposure - Collected Data on Functional Use



EXPORT

Collected Data on Functional Use

Harmonized functional use	Reported functional use
<input type="text"/>	<input type="text"/>
crosslinker	antioxidant
crosslinker	coupling agent
crosslinker	crosslinker
crosslinker	curing agent
crosslinker	phenol
Rows: 5	



EXPORT

Predicted Probability of Associated Functional Use

Harmonized functional use	Probability
<input type="text"/>	<input type="text"/>
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	



Exposure tab: Toxics Release Inventory

Reported values

<https://www.epa.gov/trinationalanalysis>

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

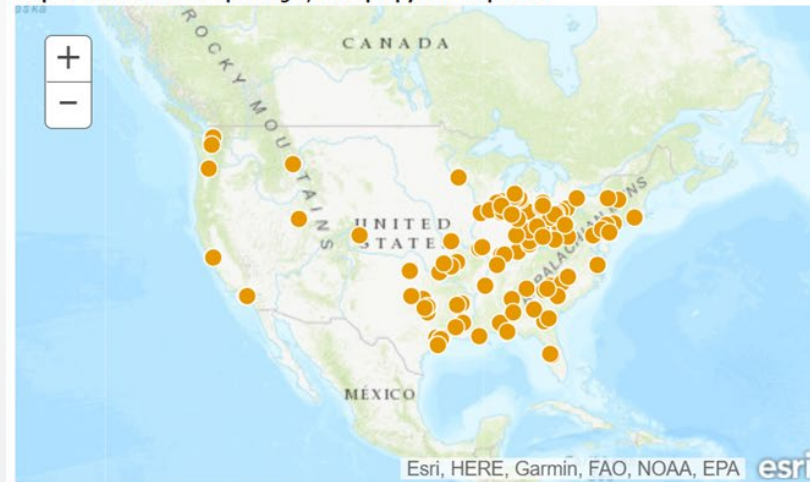
Not currently working, but should look like this:

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

Data Source: 2020 National Analysis Dataset (October 2021, released October 2021)

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:	125	21,705
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:	832.8 thousand lbs	2.9 billion lbs
• Air:	32.1 thousand lbs	602.1 million lbs
• Water:	1.3 thousand lbs	200.7 million lbs
• Land:	799.4 thousand lbs	2.1 billion lbs
Total Off-site:	2.0 million lbs	459.4 million lbs

Exposure

Product & Use Categories

Chemical Weight Fraction

Chemical Functional Use

Toxics Release Inventory

Monitoring Data

Exposure Predictions

Production Volume



Exposure tab: Monitoring data

Measured values

Details

Executive Summary

Properties

Env. Fate/Transport

Hazard

Safety > GHS Data

ADME > IVIVE

Exposure

Product & Use Categories

Chemical Weight Fraction

Chemical Functional Use

Toxics Release Inventory

Monitoring Data

Exposure Predictions

Production Volume

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



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



Exposure tab: Exposure Predictions

Predicted values

Details

Executive Summary

Properties

Env. Fate/Transport

Hazard

Safety > GHS Data

ADME > IVIVE

Exposure

Product & Use Categories

Chemical Weight Fraction

Chemical Functional Use

Toxics Release Inventory

Monitoring Data

Exposure Predictions

Production Volume

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



 EXPORT

Exposure Predictions

Demographic	Median	95th Percentile
Age 6-11	6.30e-5	5.82e-3
Age 12-19	2.68e-5	2.00e-3
Age 20-65	2.05e-5	1.61e-3
Age 65+	1.61e-5	2.18e-3
BMI < 30	2.67e-5	2.26e-3
BMI > 30	1.69e-5	1.45e-3
Females	1.11e-5	9.09e-4
Males	3.89e-5	3.34e-3
Repro. Age Females	1.11e-5	1.57e-3
Total	5.50e-5	2.04e-2



Exposure tab: Production Volume

Reported values

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

Details

Executive Summary

Properties

Env. Fate/Transport

Hazard

Safety > GHS Data

ADME > IVIVE

Exposure

Product & Use Categories

Chemical Weight Fraction

Chemical Functional Use

Toxics Release Inventory

Monitoring Data

Exposure Predictions

Production Volume

Exposure - Production Volume



Production Volume

Name	Amount (lb)
Domestic Manufacturing Production	187836000*
Imported Volume	16973090*
Volume Used	0*
Volume Exported	43815500*

- 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)



Literature tab: Google Scholar

Literature

Google Scholar

PubMed Abstract Sifter

PubChem Articles

PubChem Patents

PPRTV

IRIS

Choose Query Term

Choose Query Term

Choose Query Term

Hazard

Fate and Transport

Metabolism

Exposure

Male Reproduction

Androgen Disruption

Female Reproduction

Genotoxicity

Embryonic development

May choose terms from dropdown menu
or type your own

SUBMIT QUERY TO GOOGLE SCHOLAR

Query to send to Google Scholar

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

Google Scholar

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



Articles

About 17,400 results (0.03 sec)

My profile

Any time

Since 2022

Since 2021

Since 2018

Custom range...

Sort by relevance

Sort by date

Any type

Review articles

☐ include patents

☒ include citations

☒ Create alert

A review of the carcinogenic potential of **bisphenol A**

[HTML] nih.gov

DD Seachrist, KW Bonk, SM Ho, GS Prins... - Reproductive ..., 2016 - Elsevier

The estrogenic properties of **bisphenol A** (BPA), a ubiquitous synthetic monomer that can leach into the food and water supply, have prompted considerable research into exposure...

☆ Save ↗ Cite Cited by 323 Related articles All 8 versions

In vitro molecular mechanisms of **bisphenol A** action

[PDF] tulane.edu

YB Wetherill, BT Akingbemi, J Kanno... - Reproductive ..., 2007 - Elsevier

Bisphenol A (BPA, 2,2-bis (4-hydroxyphenyl) propane; CAS# 80-05-7) is a chemical used primarily in the manufacture of polycarbonate plastic, epoxy resins and as a non-polymer ...

☆ Save ↗ Cite Cited by 978 Related articles All 14 versions

An evaluation of evidence for the carcinogenic activity of **bisphenol A**

[HTML] nih.gov

RA Keri, SM Ho, PA Hunt, KE Knudsen, AM Soto... - Reproductive ..., 2007 - Elsevier

..., particularly with knowledge and research on **bisphenol A** (BPA). Five subpanels were charged ... These were presented and discussed at an open forum entitled "**Bisphenol A**: An Expert ...

☆ Save ↗ Cite Cited by 332 Related articles All 15 versions



Literature tab: PubMed Abstract Sifter

Literature

Google Scholar

PubMed Abstract Sifter

PubChem Articles

PubChem Patents

PPRTV

IRIS

Literature - PubMed Abstract Sifter

Abstract Sifter Instructions

May choose terms from dropdown menu or type your own

1 Select PubMed starting point query

query

Choose Query Term

Choose 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

2 Optionally, enter any PubMed query or edit the query from step 1

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

3 Click Retrieve Articles to begin download.

RETRIEVE ARTICLES

0 of 16058 articles loaded

4 Optionally, export articles

SEND TO

<input type="checkbox"/>	PubMed ID	Year $\uparrow\downarrow$	Title $\uparrow\downarrow$	Authors $\uparrow\downarrow$	Journal $\uparrow\downarrow$	Rev $\uparrow\downarrow$	DOI $\uparrow\downarrow$	Vol $\uparrow\downarrow$	Issue $\uparrow\downarrow$	Page $\uparrow\downarrow$
<input type="checkbox"/>	35376969	2022	Pharmacokinetics and toxicit...	Lee; An; Kim; Noh; Lee; Lee; ...	Archives of toxicology		10.1007...	-	-	-
<input type="checkbox"/>	35278557	2022	Bisphenol chemicals disturb i...	Zhu; Wei; Li; Li; Dong; Chen; ...	The Science of the total envir...		10.1016...	828	-	154
<input type="checkbox"/>	35168014	2022	Bisphenol A and declining se...	Kortenkamp; Martin; Ermler; ...	International journal of hygie...		10.1016...	241	-	113.
<input type="checkbox"/>	34884472	2021	Alteration of Extracellular Ma...	Sanannam; Looprasertkul; Ka...	International journal of molec...		10.3390...	22	23	-
<input type="checkbox"/>	34773844	2021	Acute and subacute repeate...	Kim; Maruthupandy; An; Lee;...	Ecotoxicology and environm...		10.1016...	228	-	112.
<input type="checkbox"/>	34712366	2021	Opinion on the impact of no...	More; Benford; Hougaard Be...	EFSA journal. European Food...		10.2903...	19	10	e06
<input type="checkbox"/>	34408969	2021	A critical assessment of the e...	Natsch; Hostettler; Haupt; La...	Toxicology reports		10.1016...	8	-	100
<input type="checkbox"/>	34383603	2021	Multi- and Transgenerational...	López-Rodríguez; Aylwin; De...	Environmental health perspe...		10.1289...	129	8	870
<input type="checkbox"/>	34363818	2021	Bisphenol A and genistein ha...	Gao; Gao; Fan; Liu; Li; Miao; ...	Chemico-biological interactio...		10.1016...	347	-	109
<input type="checkbox"/>	34345859	2021	Endocrine disrupting chemic...	Mattiske; Pask	Current research in toxicology	✓	10.1016...	2	-	179
<input type="checkbox"/>	34302887	2021	Proteomic profile of the effec...	Molina; Abril; Lora; Huertas-...	Food and chemical toxicolog...		10.1016...	156	-	112.



Literature tab: PubChem Articles

Literature

Google Scholar

PubMed Abstract Sifter

PubChem Articles

PubChem Patents



IRIS

Literature - PubChem Articles

PUBCHEM > BISPHENOL A > DEPOSITOR PROVIDED PUBMED CITATIONS

Links out to external source (PubChem)

Depositor Provided PubMed Citations

4,582 items View More Rows & Details

Download

SORT BY Publication Date

PMID	Publication Date	Title	Journal
34910997	2022-03-05	Bisphenol A drives di(2-ethylhexyl) phthalate promoting thyroid tumorigenesis via regulating HDAC6/PTEN and c-MYC signaling	Journal of hazardous materials
34788942	2022-01-10	BDNF as a potential mediator between childhood BPA exposure and behavioral function in adolescent boys from the INMA-Granada cohort	The Science of the total environment
34537452	2022-01-01	Maternal exposure to bisphenol A induces fetal growth restriction via upregulating the expression of estrogen receptors	Chemosphere
34627044	2021-12-15	Binding and activity of bisphenol analogues to human peroxisome proliferator-activated receptor β/δ	Ecotoxicology and environmental safety
34947998	2021-12-08	Autism-Related Transcription Factors Underlying the Sex-Specific Effects of Prenatal Bisphenol A Exposure on Transcriptome-Interactome Profiles in the Offspring Prefrontal Cortex	International journal of molecular sciences

1 2 3 ... 917 Next >



Literature tab: PubChem Patents

Literature

Google Scholar

PubMed Abstract Sifter

PubChem Articles

PubChem Patents

PPRTV

IRIS

`Literature - PubChem Patents`

PUBCHEM > BISPHENOL A > DEPOSITOR-SUPPLIED PATENT IDENTIFIERS

Depositor-Supplied Patent Identifiers

179,052 items View More Rows & Details

Download

SORT BY Priority Date

Publication Number ?	Title	Priority Date ?	Grant Date
EP-3757145-A2	Microcellular polyurethane elastomers	2020-10-27	
US-10894625-B1	Lightweight polymer bottle for wine and spirits	2020-07-29	2021-01-19
US-10906238-B1	Shape memory polymer inks and methods of printing the same	2020-06-26	2021-02-02
US-2020268558-A1	Chromism For Hemorrhage Control	2020-05-09	
US-2020268559-A1	Method For Dressing Wounds With Chromic Materials	2020-05-09	
1 2 3 ... 35,811 Next >			

PubChem



Literature tab: PPRTV

Literature

Google Scholar

PubMed Abstract Sifter

PubChem Articles

PubChem Patents

PPRTV

IRIS

Literature - Provisional Peer Reviewed Toxicity Values



Provisional Peer Reviewed To...

1 / 23



51%



1



2

*example chemical is Aniline



EPA/690/R-07/001F
Final
5-23-2007

Provisional Peer Reviewed Toxicity Values for

Aniline
(CASRN 62-53-3)

Superfund Health Risk Technical Support Center
National Center for Environmental Assessment
Office of Research and Development
U.S. Environmental Protection Agency
Cincinnati, OH 45268



Literature tab: IRIS

Literature

Google Scholar

PubMed Abstract Sifter

PubChem Articles

PubChem Patents

PPRTV

IRIS

Literature - IRIS

EPA's Integrated Risk Information System

[IRIS Home](#)

[About IRIS](#)

[IRIS Recent Additions](#)

[IRIS Calendar](#)

[IRIS Assessments](#)

[Advanced Search](#)

[IRIS Program Materials](#)

[Contact Us](#)

Bisphenol A

CASRN 80-05-7 | DTXSID7020182

- [IRIS Summary \(PDF\)](#) (8 pp, 93 K)


Key IRIS
Values

Other EPA
Information

Noncancer Assessment

[Reference Dose for Oral Exposure \(RfD\) \(PDF\)](#) (8 pp, 93 K)

Last Updated: 09/26/1988

System	RfD (mg/kg-day)	Basis	PoD	Composite UF
 Other	5×10^{-2}	Reduced mean body weight	LOAEL : 5.0×10^1 mg/kg-day	1000

Related Links

- [EPA
Chemicals
Dashboard -
Bisphenol A](#)

Chemical Structure for Bisphenol A

 Bisphenol A



External Links

Literature

Links

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 NIST Chemistry Webbook
- PubChem
- PubChem 3D conformer download
- PubChem 3D Structure Display
- PubChem: Chemical Vendors
- PubChem Safety Sheet

Toxicology

- ACToR
- ACToR PDF Report
- BindingDB
- CaIPEA OEHHHA
- 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

Analytical

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

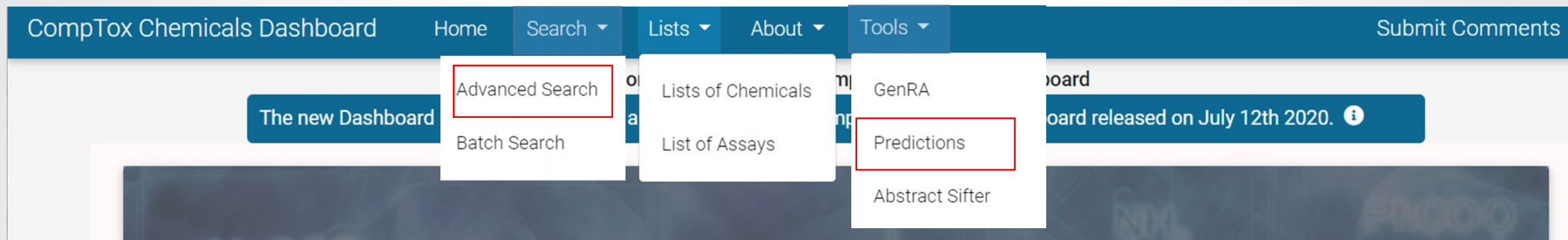
Prediction

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





Are there other ways to search?



- **Advanced Search, by**

- Mass
- Empirical formula
- Both

- **Predictions**

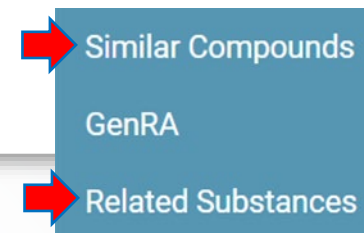
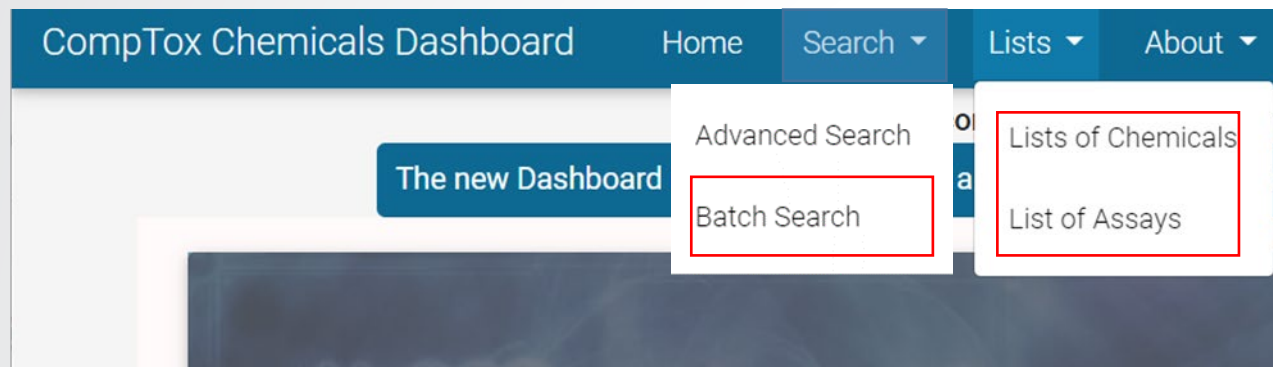
- Search or draw structure
- Predictions are based on QSAR models related to the Toxicity Estimation Software Tool (TEST)

- ✓ 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

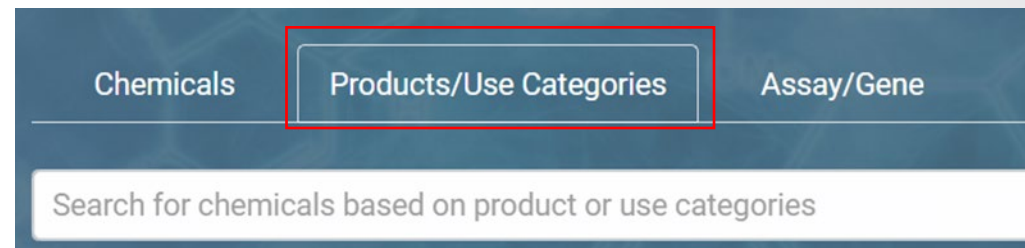
- ✓ Physical properties
 - ✓ Normal boiling point
 - ✓ Melting point
 - ✓ Flash point
 - ✓ Vapor pressure
 - ✓ Density
 - ✓ Surface tension
 - ✓ Thermal conductivity
 - ✓ Viscosity
 - ✓ Water solubility



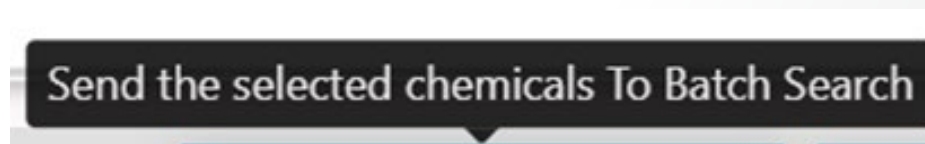
Batch Searches



*within a
chemical search



List of Chemicals
Lists of Assays
Products/Use Categories
Similar Compounds
Related Substances



Batch Search



Batch Search

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

Presence in Lists

Title	Description
<input type="checkbox"/> 40CFR1164	40 CFR 116.4 Designation of Hazardous Substances (Above Ground Storage Tanks)
<input type="checkbox"/> 40CFR355	40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities
<input type="checkbox"/> ACSREAG	LIST: ACS Reagent Chemicals
<input type="checkbox"/> AEGLVALUES	AEGLS: Acute Exposure Guideline Levels
<input type="checkbox"/> ALGALTOX	LIST: Algal Toxins
<input type="checkbox"/> ALLSURFACTANTS	CATEGORY: Surfactants
<input type="checkbox"/> AMINOACIDS	CATEGORY: Amino acids
<input type="checkbox"/> AMPHIBOLES	Amphibole minerals
<input type="checkbox"/> ANTIBIOTICS	CATEGORY PHARMACEUTICALS: Antibiotics
<input type="checkbox"/> ANTIMICROBIALS	CATEGORY WIKILIST ANTIMICROBIALS: Antimicrobials from Wikipedia
<input type="checkbox"/> AOPSTRESSORS	List of Adverse Outcome Pathway Stressors
<input type="checkbox"/> APCRARETRO	LIST: APCRA Chemicals for Retrospective Analysis
<input type="checkbox"/> ARCHEMICALS	ANDROGEN: Androgen Receptor Chemicals

Rows: 323

5

DOWNLOAD EXPORT FILE

How are data available through the CompTox Chemicals Dashboard used in the Clean Water Act programs?



Clean Water Act Programs

<https://www.epa.gov/laws-regulations/summary-clean-water-act>

EPA publishes human health criteria recommendations to protect from ingestion of aquatic organisms and for ingestion of water and the organisms.

These recommended criteria are calculated using toxicity factors, bioaccumulation factors, and exposure factors (body weight, water intake, fish consumption rate).

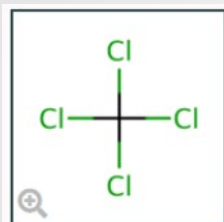
EPA often uses a cancer slope factor (carcinogens) or a reference dose (noncarcinogens) from the agency's Integrated Risk Information System (IRIS) as the toxicity factor.



Finding information on the Dashboard

Single chemical search

<https://comptox.epa.gov/dashboard/chemical/details/DTXSID8020250>



Carbon tetrachloride

56-23-5 | DTXSID8020250

Searched by Approved Name.

A chemical may be identified by more than one name or identifier (e.g., CAS – assigned by the American Chemical Society)

Synonyms

Synonyms

Search Chemical Synonyms		EXPORT
Synonym	Quality	
56-23-5 Active CAS-RN	Valid	
Carbon tetrachloride	Valid	
Methane, tetrachloro-	Valid	
Tetrachloromethane	Valid	
Carbana	Good	
Flukoids	Good	
Kohlenstofftetrachlorid	Good	



Environmental fate and transport data

Properties

Env. Fate/Transport

Hazard

Safety > GHS Data

ADME > IVIVE

Exposure

Bioactivity

EXPORT

Summary

Property ↓↑	Experimental average ↓↑	Predicted average ↓↑	Experimental median ↓↑	Predicted median ↓↑	Experimental range ↓↑	Predicted range ↓↑	Unit ↓↑
Atmos. Hydroxylation Rate	1.20e-16 (1)	1.20e-16 (1)	1.20e-16	1.20e-16	1.20e-16	1.20e-16	cm ³ /molecule*sec
Biodeg. Half-Life		19.9 (1)		19.9	-	19.9	days
Fish Biotrans. Half-Life (Km)	6.46e-2 (1)	6.47e-2 (1)	6.46e-2	6.47e-2	6.46e-2	6.47e-2	days
Soil Adsorp. Coeff. (Koc)	70.8 (1)	178 (2)	70.8	178	70.8	70.8 to 286	L/kg
Bioaccumulation Factor		18.8 (1)		18.8	-	18.8	
Bioconcentration Factor	112 (3)	19.4 (4)	30.0	18.1	7.41 to 300	7.45 to 34.2	

Measured values: EPA's ECOTOXicology Knowledgebase (ECOTOX) for studies on bioconcentration in plants and animals

EXPORT

Experimental

Source ↓↑	Result ↓↑	Experimental Details ↓↑
PhysPropNCCT	7.41	Species: undefined; Response Site: undefined
ECOTOX: aquatic	30.0	Species: Lepomis macrochirus; Response Site: Whole organism
ECOTOX: aquatic	300	Species: Chlorella fusca var. vacuolata; Response Site: Whole organ...



Toxicity values

Three ways to find toxicity values

1

Executive Summary

Regional Screening i

Class	Risk Level	Value
cancer unit risk ((ug/m3)-1)	1	6.00e-6
MCL-based SSL (mg/kg soil)	1	1.90e-3
RfDo (mg/kg-day)	1	4.00e-3
cancer slope factor ((mg/kg-day)-1)	1	7.00e-2

3

Literature

PPRTV

Literature - IRIS



United States Environmental Protection Agency

Environmental Topics | Laws & Regulations | About EPA

Search EPA.gov

Contact Us

IRIS

- IRIS Home
- About IRIS
- IRIS Recent Additions
- IRIS Calendar
- IRIS Assessments**
- Advanced Search
- IRIS Program Materials
- Contact Us

Carbon tetrachloride

CASRN 56-23-5 | DTXSID8020250

- [Toxicological Review \(PDF\)](#) (473 pp, 3.04 M)
- [IRIS Summary \(PDF\)](#) (20 pp, 363 K)

Key IRIS Values

Chemical Documents

Other EPA Information

Related Links

2

Hazard

Toxicity Value



Search Hazard

EXPORT

More	Source	Type	Risk Assessment	Qualifier	Value	Units	Exposure Route	Critical effect	Species	Year
	IRIS									
	IRIS	RfD	chronic	=	4.00e-3	mg/kg-day	oral	increased serum sdh activity	-	-
	IRIS	cancer slope factor	carcinogenicity	=	7.00e-2	(mg/kg-day)-1	oral	hepatocellular adenoma or carcinoma	-	-
	IRIS	RfC	chronic	=	0.100	mg/m3	inhalation	fatty liver	-	-



Clean Water Act Programs

The Clean Water Act requires EPA to develop criteria for surface water quality that accurately reflect the latest scientific knowledge on the impacts of pollutants on human health and the environment.

<https://www.epa.gov/wqc>

Current Water Quality Criteria Tables



- [Aquatic Life Criteria Table](#)
- [Human Health Criteria Table](#)
- [Organoleptic Effects Criteria Table](#)

Values are publicly available to be adopted by states and other authorities

Pollutant	CAS Number	Human Health for the consumption of Water + Organism (µg/L)	Human Health for the consumption of Organism Only (µg/L)	Publication Year	Notes
Acenaphthene <small>EXIT</small> (P)	83329	70	90	2015	The criterion for organoleptic (taste and odor) effects may be more stringent. Refer to National Recommended Water Quality Criteria - Organoleptic Effects .
Acrolein <small>EXIT</small> (P)	107028	3	400	2015	
					This criterion is based on carcinogenicity of 10 ⁻⁶ risk. Alternate risk



Additional Hazard Exposure Limit Info

Water quality, air quality, and occupational exposure values
e.g., EPA Office of Water, Health Canada, State-specific information

Hazard: Exposure Limit

Exposure Limit

Q

Search Hazard

human

eco

EXPORT

More	Priority	Source	Type	Subtype	Risk Assessment	Qualifier	Value	Units	Study Type	Exposure Route	Critical effect
	7	DOE Protective Action Crit...	PAC-1	PAC 1	acute	=	7.50	mg/m3	acute	inhalation	-
	7	DOE Protective Action Crit...	PAC-3	PAC 3	acute	=	2.10e+3	mg/m3	acute	inhalation	-
	4	Health Canada	TDI	-	chronic	=	7.10e-4	mg/kg-...	-	oral	hepatotoxicity
	7	Mass. Drinking Water Stan...	MCL	-	chronic	=	5.00e-3	mg/L	-	oral	-
	4	OW Drinking Water Stand...	health adv...	lifetime	drinking water standard	=	3.00e-2	mg/L	-	oral	-
	4	OW Drinking Water Stand...	health adv...	carcino...	drinking water standard	=	5.00e-2	mg/L	-	oral	-
	4	OW Drinking Water Stand...	MCL	-	chronic	=	5.00e-3	mg/L	-	oral	-
	4	OW Drinking Water Stand...	health adv...	-	drinking water standard	=	0.200	mg/L	-	oral	-
	4	OW Drinking Water Stand...	health adv...	-	drinking water standard	=	4.00	mg/L	-	oral	-
	5	Pennsylvania DEP MCLs	MCL	ground...	chronic	=	50.0	mg/L	-	oral	-

Rows: 25

Total Rows: 25

EPA Offi

Standar

<https://s/static/03/docu>

Health A

accepta

chemical

informa

enforce

a techn

and loc

EPA Office of Water Drinking Water Standards and Health Advisories (2018)

<https://19january2021snapshot.epa.gov/site/static/files/2018-03/documents/dwtable2018.pdf>

Health Advisory Levels. An estimate of acceptable drinking water levels for a chemical substance based on health effects information; an HA is not a legally enforceable Federal standard, but serves as a technical guidance to assist Federal, State, and local officials.

<https://www.epa.gov/ground-water-and-drinking-water>



I can't remember how to...

CompTox Chemicals Dashboard

Home Search ▾ Lists ▾ About ▾ Tools ▾

Submit Comments

Welcome to the new CompTox Chemicals Dashboard

The new Dashboard is a complete rebuild and is released on July 12th 2020. ⓘ

About
News
Help
Feedback
Downloads
Cite the Dashboard
Comments

CompTox Chemicals Dashboard

Chemicals Products/Use Categories Assay/Gene

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

☐ Identifier substring search

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

CCD Help Pages Introduction

Introduction

[Common Navigational Tips](#)
[Searching CCD](#)
[Batch Search](#)
[Details](#)
[Executive Summary](#)
[Properties](#)
[Env. Fate/Transport](#)
[Hazard](#)
[Safety](#)
[ADME](#)
[Exposure](#)
[Bioactivity](#)
[Similar Compounds](#)
[GenRA](#)
[Related Substances](#)
[Synonyms](#)
[Literature](#)
[Links](#)

The **CompTox Chemicals Dashboard** (hereafter the “Dashboard”) is a publicly available web-based application developed by the US Environmental Protection Agency to provide access to chemistry, toxicity, and exposure information for hundreds of thousands of chemicals. The data and predictive models within the Dashboard support the Agency’s efforts to identify bioactive chemicals to identify further testing needs, to support an Agency priority to accelerate chemical hazard assessment data acquisition and translate effects to protect human health and the environment. In addition, in silico models facilitate the prediction of hazard properties of chemicals for which in vivo data are not available.

The Dashboard is increasingly becoming a valuable resource for risk assessors tasked with the evaluation of potential human health risks associated with chemical exposures. In this context, the significant amount of information present in the Dashboard allows for:

1. Assembly of information on chemical properties, environmental fate and transport, and exposure metrics.
2. Identification of health effects from extant studies in the public domain and/or information not available in peer-reviewed literature (i.e., “grey literature”).
3. Facilitation of systematic literature searching and review for developing hazard evidence bases.
4. Access to mechanistic information that can aid or augment the analysis of experimental animal bioassay or epidemiological evidence, or potentially, serve as the primary basis for informing hazard identification and dose-response when traditional bioassay data are lacking.

Finally, in silico predictive tools developed to conduct structure-activity or read-across analyses are also available within the Dashboard. The addition of new data and curation according to [our exacting processes](#) [EXIT](#) is ongoing and [multiple publications](#) represent the data, individual modules and applications of the Dashboard to solve various problems.



Please report bugs using “Submit Comments”



Searched by DTXS

20. 

SEND 



Acknowledgments

Sipes.Nisha@epa.gov

Efforts include many more than who are listed here

Many external collaborators provided data & links

Thanks to Diane Evans (Region 6), Katie Paul Friedman (ORD), Grace Patlewicz (ORD), and Antony Williams (ORD) for allowing me to adapt some of their material



EPA/ORD/Center for Computational Toxicology and Exposure



Relevant publications

Computational Toxicology

- Kavlock RJ, et al. Toxicol Sci. 2008;103(1):14-27.
- Kleinstreuer NC, Tetko IV, Tong W. Chem Res Toxicol. 2021;34(2):171-175.

CompTox Chemicals Dashboard

- Williams AJ, et al. The CompTox Chemistry Dashboard: a community data resource for environmental chemistry. J Cheminform. 2017 Nov 28;9(1):61.
- Lowe CN and Williams AJ. Enabling High-Throughput Searches for Multiple Chemical Data Using the U.S.-EPA CompTox Chemicals Dashboard. J. Chem. Inf. Model. 2021, 61, 2, 565–570. Publication Date: January 22, 202
- Williams AJ, et al. Sourcing data on chemical properties and hazard data from the US-EPA CompTox Chemicals Dashboard: A practical guide for human risk assessment. Environ Int. 2021 Sep;154:106566.

Chemistry – related references

- Grulke CM, et al. EPA's DSSTox database: History of development of a curated chemistry resource supporting computational toxicology research. Comput Toxicol. 2019 Nov 1;12:10.1016/j.comtox.2019.100096.
- Helman G, Shah I, Williams AJ, Edwards J, Dunne J, Patlewicz G. Generalized Read-Across (GenRA): A workflow implemented into the EPA CompTox Chemicals Dashboard. ALTEX. 2019;36(3):462-465.



Relevant publications

Ecotoxicology

- Olker JH, et al The ECOTOXicology Knowledgebase: A Curated Database of Ecologically Relevant Toxicity Tests to Support Environmental Research and Risk Assessment. Environ Toxicol Chem. 2022 Mar 9. doi: 10.1002/etc.5324. Epub ahead of print. PMID: 35262228.
- LaLone CA, et al. Editor's Highlight: Sequence Alignment to Predict Across Species Susceptibility (SeqAPASS): A Web-Based Tool for Addressing the Challenges of Cross-Species Extrapolation of Chemical Toxicity. Toxicol Sci. 2016 Oct;153(2):228-45.

In Vitro to In Vivo Extrapolation (IVIVE)

- Wambaugh JF, et al. High throughput heuristics for prioritizing human exposure to environmental chemicals. Environmental science & technology. 2014;48(21):12760–7.
- Wambaugh, JF et al., 2015. Toxicokinetic Triage for Environmental Chemicals. Toxicol Sci., 147(1):55-67.
- Wetmore, BA, et al. 2015. Quantitative in vitro-in vivo extrapolation in a high-throughput environment. Toxicol. 332:94-101
- Pearce RG, Setzer RW, Strobe CL, et al. htk: R Package for High-Throughput Toxicokinetics. J Stat Softw. 2017;79(4):1-26
- Rotroff, DM et al., 2010. Incorporating Human Dosimetry and Exposure into High-Throughput In Vitro Toxicity Screening. Toxicol. Sci., 117 (2):348-358.
- Wilkinson RG, and Shand DG (1975). A physiological approach to hepatic drug clearance. Clin. Pharmacol. Ther. 18, 377–389.

EPA's Toxics Release Inventory: https://awsedap.epa.gov/public/extensions/TRINA_dashboard_2020/TRINA_dashboard_2020.html



Relevant publications

Exposure

- Dionisio KL, et al. Exploring consumer exposure pathways and patterns of use for chemicals in the environment. Toxicol Rep. 2015 Jan 2;2:228-237.
- Isaacs KK, et al. Characterization and prediction of chemical functions and weight fractions in consumer products. Toxicol Rep. 2016 Sep 1;3:723-732.
- Phillips KA, et al. High-throughput screening of chemicals as functional substitutes using structure-based classification models. Green Chem. 2017;19(4):1063-1074.
- Dionisio KL, et al. The Chemical and Products Database, a resource for exposure-relevant data on chemicals in consumer products. Sci Data. 2018 Jul 10;5:180125.
- Isaacs KK, et al. Establishing a system of consumer product use categories to support rapid modeling of human exposure. J Expo Sci Environ Epidemiol. 2020 Jan;30(1):171-183.
- EPA's Toxics Release Inventory: https://awsedap.epa.gov/public/extensions/TRINA_dashboard_2020/TRINA_dashboard_2020.html
- Ring CI et. al. Consensus Modeling of Median Chemical Intake for the U.S. Population Based on Predictions of Exposure Pathways. Environ Sci Technol. 2019 Jan 15;53(2):719-732.