

# Going for Your First Drive in Toxicology: Using the Comptox Chemicals Dashboard



**CDI**  
**Baltimore MD**  
**March 10, 2019**

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**Antony J Williams BSc PhD**  
**National Center for Computational Toxicology**  
**Office of Research and Development**  
**US Environmental Protection Agency**

# Regulatory Agencies Make a Broad Range of Decisions on Chemicals...



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## Harmful algal bloom initiative funds additional research

Written by J. Patrick Eaken  
February 16, 2018  
Hits: 472

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The Ohio Department of Higher Education (ODHE) has awarded \$3.5 million in funding for 21 additional projects in its ongoing Harmful Algal Bloom Research Initiative.

HABRI is a statewide response to the threat of harmful algal blooms that arose out of the 2014 Toledo drinking water crisis, where elevated levels of the algal toxin microcystin in Lake Erie threatened water supplies for more than 500,000 people in Northwest Ohio.

"I am proud of the work that is being done, and that researchers from our public and private higher education institutions continue to work together to address this issue," said Ohio Department of Higher Education Chancellor John Carey. "Using the talent of Ohio's researchers and students to solve pressing environmental problems is a top priority."

## Montana preparing to take over after \$600M EPA asbestos cleanup near Libby

Associated Press Sep 21, 2017

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Widespread asbestos contamination has killed an estimated 400 people in

## The Intelligencer

### Congress budget deal sets table for \$7M PFAS study

By Kyle Bagenstose

Posted Feb 9, 2018 at 3:18 PM

Updated Feb 9, 2018 at 3:18 PM

But the nationwide health study, which could well include Bucks and Montgomery County residents exposed to toxic chemicals in drinking water, isn't a done deal.

## ChemicalWatch

GLOBAL RISK & REGULATION NEWS

### ToxCast and Tox21 high-throughput data identify potential EDCs

Fifra SAP set to discuss androgen receptor model

23 November 2017 / Alternative approaches to testing, EDCs, United States

ToxCast<sup>1</sup> and Tox21<sup>2</sup> high-throughput screening data provide a "rapid and effective resource" for identifying substances with the potential to activate human oestrogen (estrogen) receptors (ERs), according to a top US Environmental Protection Agency (EPA) official.

Stan Barone, acting director of the EPA's Office of Chemical Safety and Pollution Prevention, was describing progress in using ER high-throughput assays for tier 1 of the Endocrine Disruptor Screening Program (EDSP) at a workshop on toxicity



The New York Times | <https://nyti.ms/KIDgRu>

u.s|

## Thousands Without Water After Spill in West Virginia

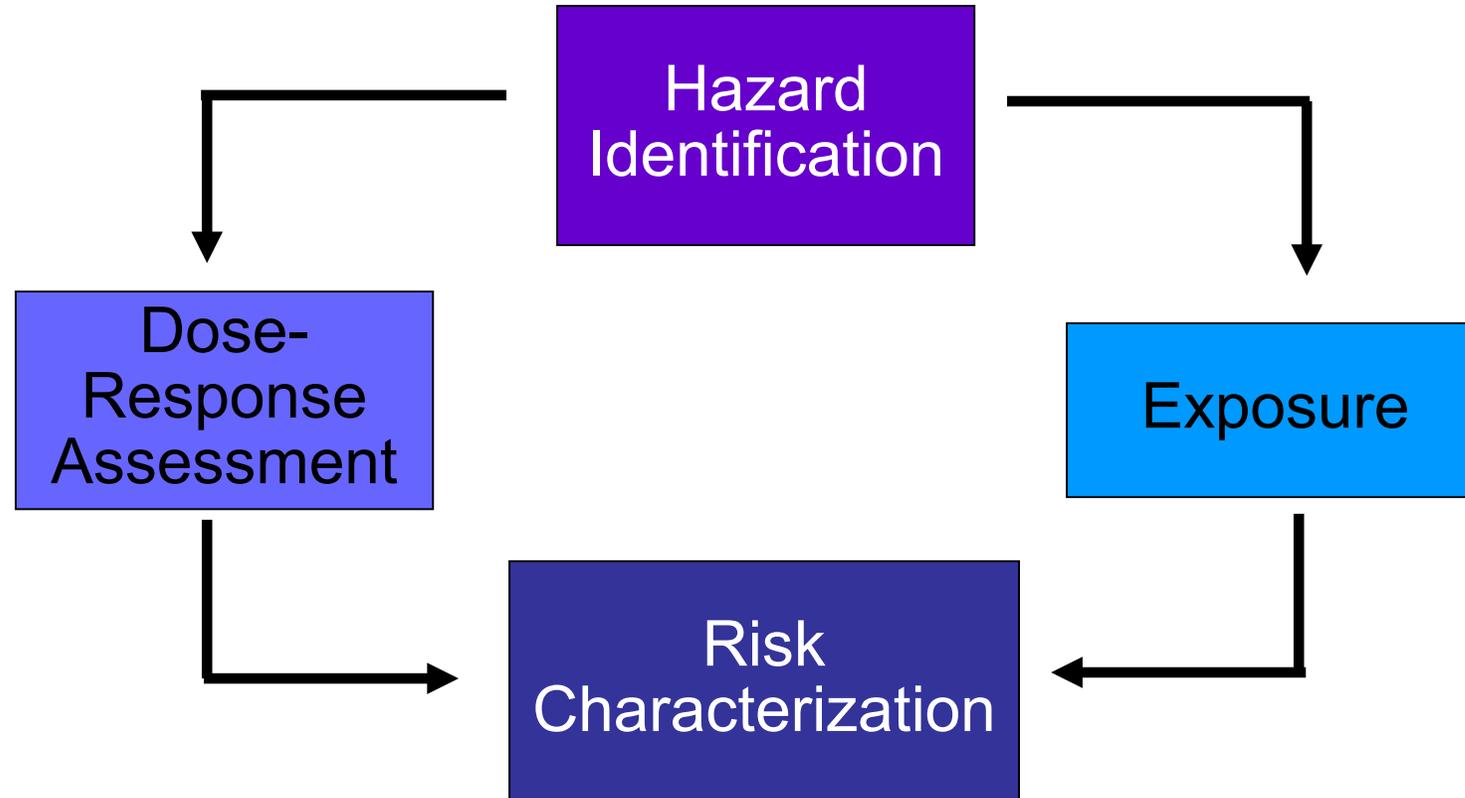
By TRIP GABRIEL JAN. 10, 2014

CHARLESTON, W.Va. — As 300,000 people awoke on Friday to learn that their tap water was unsafe for brushing teeth, brewing coffee or showering, residents and businesses expressed a mix of anger and anxiety in coping with an industrial accident with no clear end in sight.

Schools were closed, restaurants locked their doors and hotels refused reservations. Store shelves were quickly stripped of bottled water, and traffic snarled as drivers waited to fill jugs from tankers delivered by the National Guard.

## The Risk Assessment Paradigm: The “Red Book”

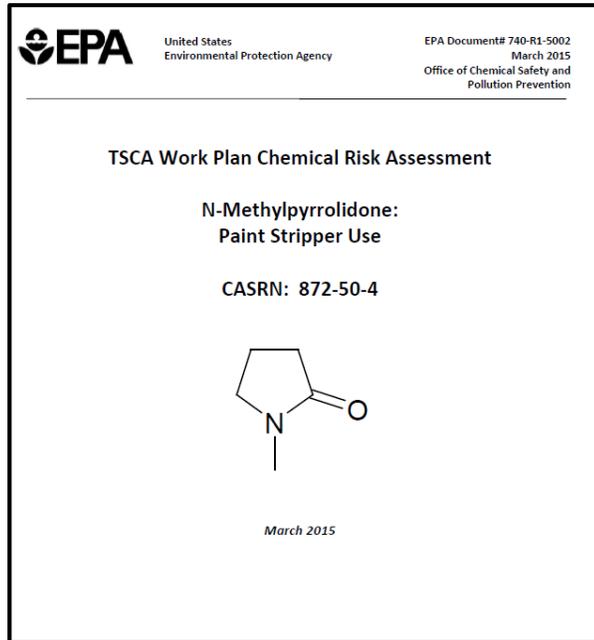
Follow the National Academy of Sciences (NAS) four-step risk assessment paradigm



National Research Council's *Risk Assessment in the Federal Government: Managing the Process*, 1983.

<http://books.nap.edu/books/030904894X/html/1.html>

# Covering All the Components of a 21<sup>st</sup> Century Risk Assessment



**EPA** United States Environmental Protection Agency  
EPA Document# 740-R1-5002  
March 2015  
Office of Chemical Safety and Pollution Prevention

**TSCA Work Plan Chemical Risk Assessment**

**N-Methylpyrrolidone:  
Paint Stripper Use**

CASRN: 872-50-4

CN1CCCC1=O

March 2015

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Variability ✓

Risk Summary ✓

Uncertainty ✓

Phys Chem ✓

Exposure ✓

Hazard ✓

Dose Response ✓

PK, and PODs ✓

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

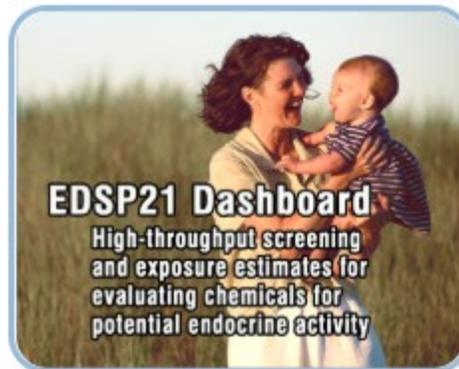
# Provide Data Through Support Dashboards The CompTox Portal (<http://comptox.epa.gov>)

Environmental Topics

Laws & Regulations

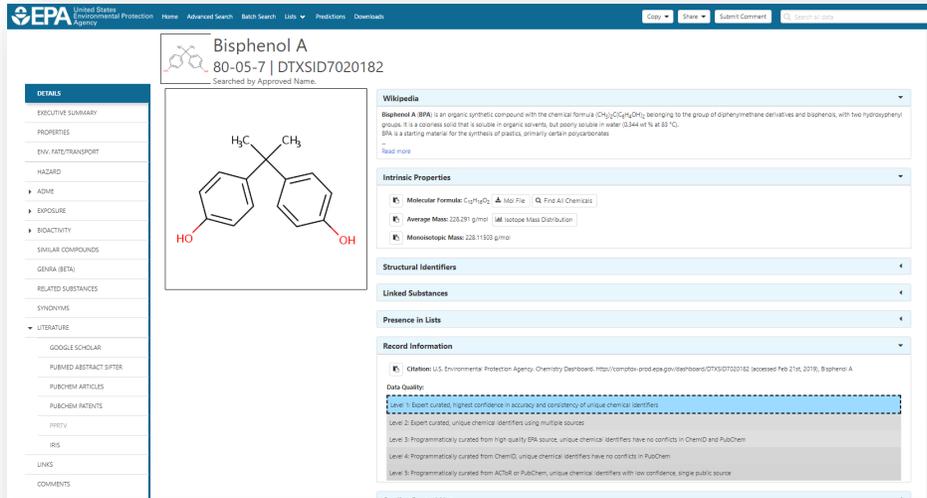
About EPA

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# The CompTox Chemicals Dashboard:

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



**Bisphenol A**  
80-05-7 | DTXSID7020182

Wikipedia: Bisphenol A (BPA) is an organic synthetic compound with the chemical formula (C<sub>15</sub>H<sub>16</sub>O<sub>2</sub>) belonging to the group of diphenylmethane derivatives and bisphenols, with two hydroxyl groups. It is a colorless solid that is soluble in organic solvents, but poorly soluble in water (3.34 wt % at 25 °C). BPA is a starting material for the synthesis of plastics, primarily certain polycarbonates.

Intrinsic Properties

- Molecular Formula: C<sub>15</sub>H<sub>16</sub>O<sub>2</sub> | Mol. Fz. | Find All Chemicals
- Average Mass: 228.291 g/mol | Mol. Weight Distribution
- Monoisotopic Mass: 228.1153 g/mol

Structural Identifiers

Linked Substances

Presence in Lists

Record Information

Citation: U.S. Environmental Protection Agency. Chemistry Dashboard. <https://comptox.epa.gov/dashboard/DTXSID7020182> (accessed Feb 15th, 2018). Bisphenol A

Data Quality

- Level 1: Expert curated, highest confidence in accuracy and consistency of unique chemical identifiers
- Level 2: Expert curated, unique chemical identifiers using multiple sources
- Level 3: Programmatically curated from high quality EPA source, unique chemical identifiers have no conflicts in ChemID and PubChem
- Level 4: Programmatically curated from ChemID, unique chemical identifiers have no conflicts in PubChem
- Level 5: Programmatically curated from ACToR or PubChem, unique chemical identifiers with low confidence, single public source



Chemical Activity Summary

TOXCAST DATA

ASSAY DETAILS

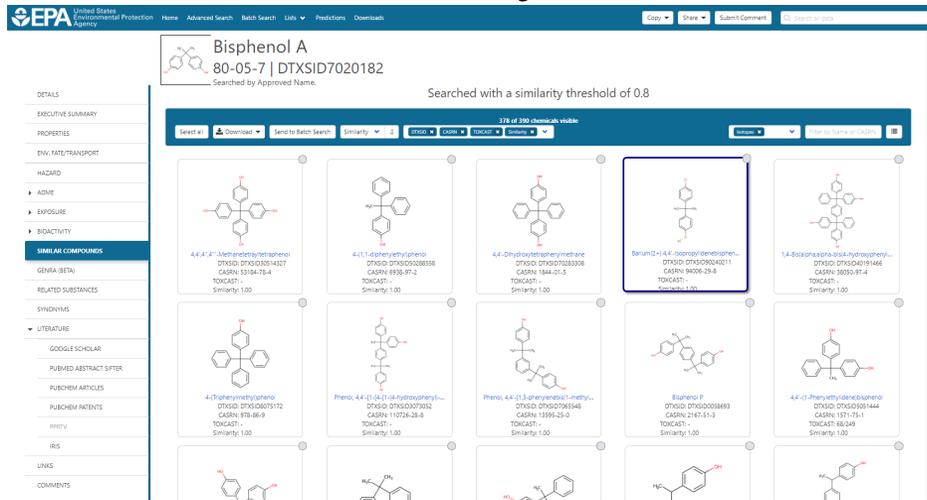
ACSU LHM: 17937  
Scaled log: 11.9

Assay Endpoint Name: TOX21\_POC\_ER\_Artemisinin  
Gene Symbol: ESRRA  
Organism: human  
Tissue: kidney  
Assay Format Type: cell-based  
Biological Process: target regulation of transcription factor activity  
Detection Technology: luminescence-coupled ATP quantifier  
Analysis Direction: positive  
Intended Target Family: nuclear receptor  
Description: Data from the assay component TOX21\_POC\_ER\_Artemisinin was analyzed into 3 assays endpoints. This assay endpoint, TOX21\_POC\_ER\_Artemisinin, was analyzed in the positive firing direction relative to DMSO as the negative control and baseline of activity.  $\log_{10}(\text{AC}_{50})$  using a type of inducible reporter, loss-of-signal activity can be used to understand changes in the reporter gene as they relate to the gene ESRRA.  $\log_{10}(\text{AC}_{50})$  Furthermore, this assay endpoint can be referred to as a primary readout, because this assay has produced multiple assay endpoints where this one serves a receptor gene function.  $\log_{10}(\text{AC}_{50})$  To generate the intended target to other available targets, this assay endpoint is annotated to the nuclear receptor intended target family.

Name	Model	Description	SeqPass	AOP	Event	Hit (Cell)	Top	AC50	logAC50	Emad	MaxMod	MaxModConc	Cutoff	Flags	ModAC50	ModAC10	ModAC5	Stock Concentration	Intended Target Family
ACSL_ER_Bhr	2	NP_000162	200	151	ACTIVE	112	0.373	-0.428	8.96	113	0.301	26.9		-0.66	113	-0.66	20		nuclear receptor
AHR_HO2C2_Cell_Loss_H4I_oh	-	-	-	-	ACTIVE	1.06	1.20	2.02	6.63e-1	1.20	2.30	0.663		2.04	1.20	1.94	20		cell cycle
AHR_HO2C2_Cell_Loss_H4I_oh	-	-	-	-	ACTIVE	0.874	1.09	2.04	4.95e-1	0.874	1.30	0.456		0.98	1.20	1.94	20		cell cycle

## Chemistry Data

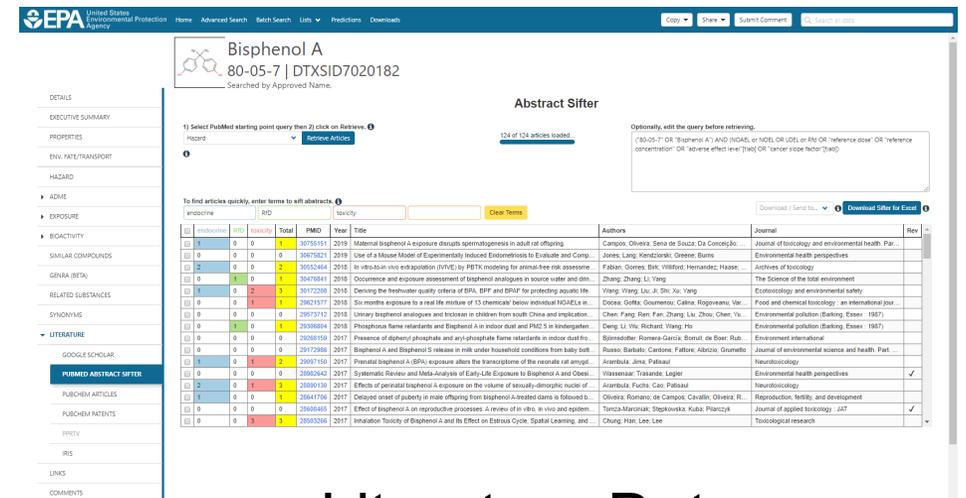
## Bioactivity Data



Similar Compounds

178 of 390 chemicals visible

Similarity	Chemical Name	Chemical ID	Similarity
0.8	4,4'-[4,4'-Methylenedioxy]bisphenol	DTXSID: DTKSD0354427 CASRN: 33304-75-4 TOXCAST: - Similarity: 1.00	0.8
0.8	4,4'-[3,3'-Ethylenedioxy]bisphenol	DTXSID: DTKSD0268559 CASRN: 9509-97-2 TOXCAST: - Similarity: 1.00	0.8
0.8	4,4'-Dihydroxydiphenylmethane	DTXSID: DTKSD0283206 CASRN: 106421-9-4 TOXCAST: - Similarity: 1.00	0.8
0.8	Belum-2-(4'-[4'-Isopropylidene]phenyl)-2-(4'-[4'-Isopropylidene]phenyl)ethane	DTXSID: DTKSD0240211 CASRN: 30009-29-8 TOXCAST: - Similarity: 1.00	0.8
0.8	1,4-Bis(4-hydroxyphenyl)butane	DTXSID: DTKSD0491466 CASRN: 30009-29-8 TOXCAST: - Similarity: 1.00	0.8
0.8	4-(3-hydroxyphenyl)phenol	DTXSID: DTKSD0373932 CASRN: 10725-24-8 TOXCAST: - Similarity: 1.00	0.8
0.8	Phenol	DTXSID: DTKSD0373932 CASRN: 10725-24-8 TOXCAST: - Similarity: 1.00	0.8
0.8	4-(3-phenylethoxy)phenol	DTXSID: DTKSD0088893 CASRN: 1099-23-0 TOXCAST: - Similarity: 1.00	0.8
0.8	Bisphenol P	DTXSID: DTKSD0301444 CASRN: 1971-76-1 TOXCAST: 66-249 Similarity: 1.00	0.8
0.8	4-(1-Phenylethoxy)phenol	DTXSID: DTKSD0301444 CASRN: 1971-76-1 TOXCAST: 66-249 Similarity: 1.00	0.8



Abstract Sifter

124 of 124 articles loaded

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Optional, edit the query before retrieving.

["80-05-7" OR "Bisphenol A"] AND (NCBI, or NCI, or NLM, or DOI, or PMID, or Epub, or Reference date, OR reference concentration, OR "adverse effect level" [EPA]) OR "toxicology" [EPA]

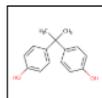
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Pubmed ID	Year	Title	Authors	Journal	Rev			
0	0	0	3597591	2018	Maternal bisphenol A exposure disrupts spermatogenesis in adult rat offspring	Campos, Olaya; Sena de Sauci, Da Conceição	Journal of toxicology and environmental health. Part A	
0	0	0	3597623	2019	Use of a Mouse Model of Experimentally Induced Endometriosis to Evaluate and Comp...	Jones, Lang; Kenedrick, Dreene; Burns	Environmental health perspectives	
2	0	0	3595244	2018	In vitro-to in vivo extrapolation (IVIVE) by PBTK modeling for animal-free risk assessme...	Faban, Gomes; Birk; Wilford; Hernandez; Haase...	Archives of toxicology	
0	0	1	3547684	2018	Occurrence and exposure assessment of bisphenol analogues in source water and drin...	Zhang, Zhang; Li; Yang	The Science of the Total Environment	
0	0	0	3477202	2018	Deriving the reproductive quality index of BPA, BPF and BPAF for protecting aquatic life...	Yang, Yang; Liu, S; Shi, Yu; Yang	Ecotoxicology and environmental safety	
0	0	1	2962157	2016	Six-months exposure to a real-life mixture of 13 chemicals' below individual NOAELs in...	Dorea, Giffa; Guemene, Celine; Roggenauer, W...	Food and chemical toxicology: an international journal...	
0	0	0	2957312	2016	Urinary bisphenol analogues and bisphenol in children from south China and implicatio...	Chen, Fang; Fan, Zhang, Liu, Zhou, Chen, Yu...	Environmental pollution (Basing, Essex, 1987)	
0	0	1	2936934	2016	Phosphoric flame retardants and Bisphenol A in indoor dust and PM2.5 in kindergarten...	Deng, Li; Wu; Richard; Wang; Fu	Environmental pollution (Basing, Essex, 1987)	
0	0	0	2817202	2017	Presence of diphenylmethane and arylphenylethane flame retardants in indoor dust fr...	Sponheimer, Roman; Garcia, Ramon; de Paor, Ru...	Environmental international	
0	0	0	2917268	2017	Bisphenol A and Bisphenol S release in milk under household conditions from baby bott...	Russo, Barbara; Carboni, Fabrizio; Abate, Diletto	Journal of environmental science and health. Part A	
1	0	1	2909710	2017	Prenatal bisphenol A (BPA) exposure alters the transcription of the neonatal rat amygd...	Atanasiu, Aneta; Palau	Neurotoxicology	
0	0	0	2892642	2017	Systematic Review and Meta-Analysis of Early-Life Exposure to Bisphenol A and Obese...	Vassanati, Tiziana; Legler	Environmental health perspectives	✓
2	0	0	2891010	2017	Effects of prenatal bisphenol A exposure on the release of sexually-dimorphic neurotr...	Amadori, Fabio; Cui; Palau	Neurotoxicology	
1	0	0	2841708	2017	Delayed onset of puberty in male offspring from bisphenol A-treated dams is followed b...	Oliveira, Ronaldo; de Campos, Cavalli; Oliveira, R...	Reproduction, fertility, and development	
0	0	0	2808486	2017	Effect of bisphenol A on reproductive processes: A review of in vitro, in vivo and epidem...	Tanica-Marciniak, Szeplowska; Kubla; Piaczyk	Journal of applied toxicology: JAT	✓
0	0	0	2805206	2017	Inhalation Toxicity of Bisphenol A and Its Effect on Estrogen Cycle, Spinal Learning, and...	Chung; Han; Lee; Lee	Toxicological research	

## Literature Data

# The CompTox Chemicals Dashboard

## Toxicity Data harvested from multiple databases



Bisphenol A

80-05-7 | DTXSID7020182

Searched by Approved Name.

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

### Hazard

Data Type

Toxicity Value

Human Eco

Download

Columns

Search query

More	Priority	Type	Subtype	Risk assessment class	Value	Units	Study type	Exposure route	Species	Subsource	Source
	7	MEG	Short-term Critical Air	short-term	500	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Short-term Marginal Air	short-term	100	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Short-term Negligible Air	short-term	15	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Soil Negligible Soil	chronic	106000	mg/kg	-	soil	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Long-Term, SU/d Negligible Water	chronic	7	mg/L	-	oral	-	TG 230 Military Exposure Guidelines Table	DOD
	6	RfD	-	chronic	0.05	mg/kg-day	-	oral	rat	Wignall	Wignall
	5	RfD	-	chronic	0.05	mg/kg-day	-	-	-	MSC Table 5	Pennsylvania DEP Tox/Values
	4	RfD	-	chronic	0.05	mg/kg-day	-	oral	-	EPA NCEA	Chiu
	3	RfD	-	chronic	0.05	mg/kg-day	-	oral	-	EPA NCEA	HEAST
	1	RfD	-	chronic	0.05	mg/kg-day	-	oral	-	EPA NCEA	IRIS

10 records



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# Example Exec Summary

## Quantitative Risk Assessment Values

- ✔ IRIS values available [↗](#)
- ✘ No PPRTV values
- ✔ EPA RSL values available [↗](#)
- ✔ Minimum RfD: 0.050 mg/kg-day (chronic, IRIS, oral, 8) [↗](#)
- ✘ No RfC calculated
- ✘ IVIVE POD not calculated

## Quantitative Hazard Values

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

## Cancer Information

- ✘ No cancer slope factor
- ✘ No inhalation unit risk value
- ✔ Carcinogenicity data available: University of Maryland carcinogenicity warning; [↗](#)
- ✘ No genotoxicity findings reported

## Reproductive Toxicology

- ✔ 200 Reproductive toxicity PODs available [↗](#)

## Chronic Toxicology

- ✔ 340 Chronic toxicity PODs available [↗](#)

## Subchronic Toxicology

- ✔ 12 Subchronic toxicity PODs available [↗](#)

## Developmental Toxicology

- ✔ 6 Developmental toxicity PODs available [↗](#)

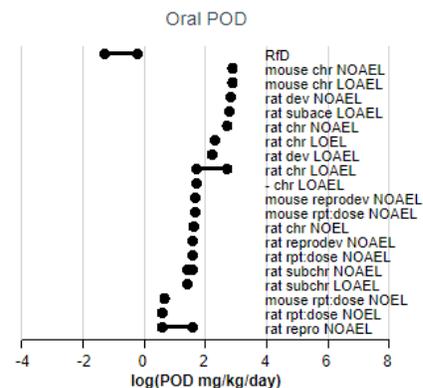
## Acute Toxicology

- ✔ 391 Acute toxicity PODs available [↗](#)

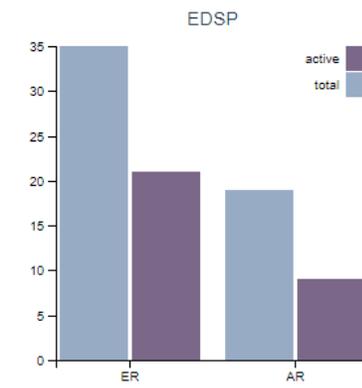
## Subacute Toxicology

- ✔ 1 subacute toxicity PODs available [↗](#)

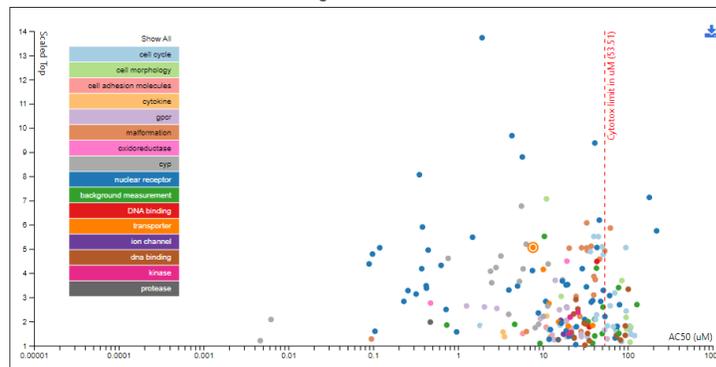
## POINT-OF-DEPARTURE PLOTS



## ASSAY PLOTS



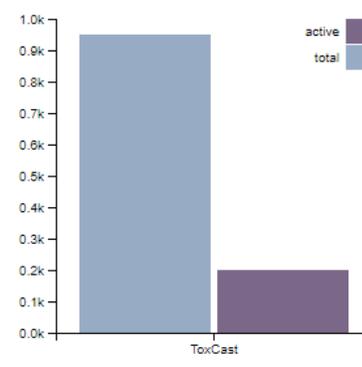
## TOXCAST DATA



## ASSAY DETAILS

ACS0 (uM): 7.64  
Scaled top: 5.06  
Assay Endpoint Name: NVS\_TR\_hDAT  
Gene Symbol: SLC6A3  
Organism: human  
Tissue: NA  
Assay Format Type: biochemical  
Biological Process Target: receptor binding  
Detection Technology: Filter-based radiodetection  
Analysis Direction: positive  
Intended Target Family: transporter  
Description: Data from the assay component NVS\_TR\_hDAT was analyzed into 1 assay endpoint. This assay endpoint, NVS\_TR\_hDAT, was analyzed in the positive fitting direction relative to DMISO as the negative control and baseline of activity, \_x000D\_x000D\_. Using a type of binding reporter, loss-of-signal activity can be used to understand changes in the binding as they relate to the gene SLC6A3\_x000D\_x000D\_. Furthermore, this assay endpoint can be referred to as a primary readout, because the performed assay has only produced 1 assay endpoint, \_x000D\_x000D\_. To generalize the intended target to other related targets, this assay endpoint is annotated to the "transporter" intended target family, where the subfamily is "neurotransmitter transporter".

## ToxCast



# Thank You for Your Attention!



**EPA's National Center for Computational Toxicology**