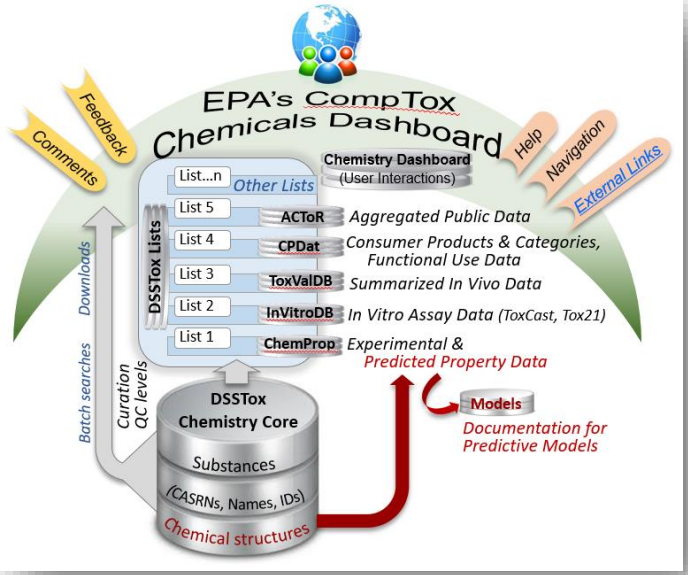
http://www.orcid.org/0000-0002-2668-4821

EPA CompTox Chemicals Dashboard as a Data Integration Hub for Environmental Chemistry Data



Antony Williams

Center for Computational Toxicology and Exposure,
U.S. Environmental Protection Agency, RTP, NC

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

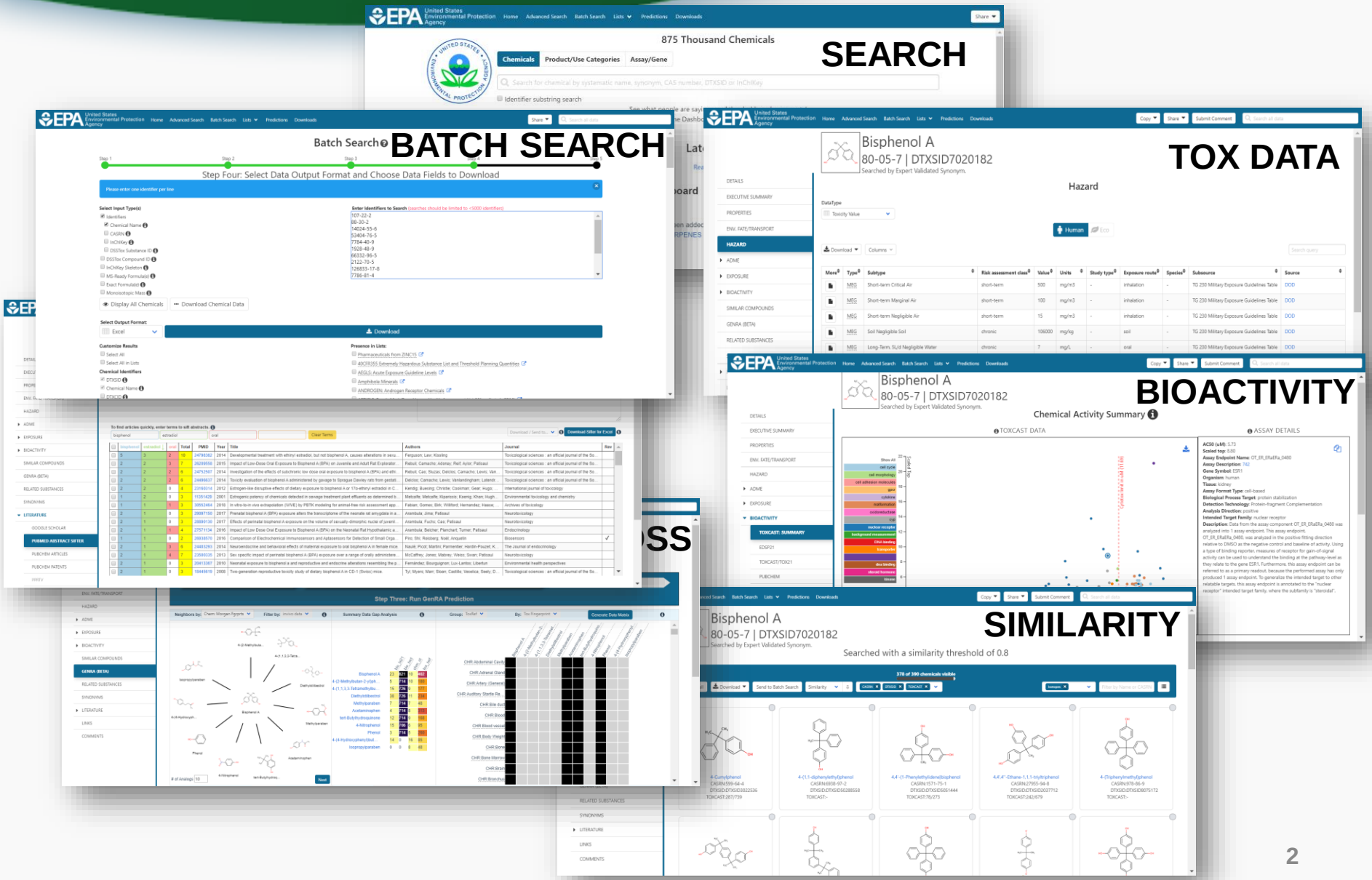
November 2019
Decontamination Conference, Norfolk, VA

CompTox Chemicals Dashboard

https://comptox.epa.gov/dashboard

- Freely accessible website and integration hub
  - Chemical substances – the majority with structures
  - Searchable by chemical, product use and gene
  - Experimental and predicted physicochemical property data
  - Experimental and predicted fate and transport data
  - Bioactivity data for the ToxCast/Tox21 project
  - Literature searches for chemicals using public resources
  - Links to other agency websites and public data resources
  - Batch searching for *thousands* of chemicals
  - Chemical lists of interest – pesticides, leachables, PFAS

A single application integrating…



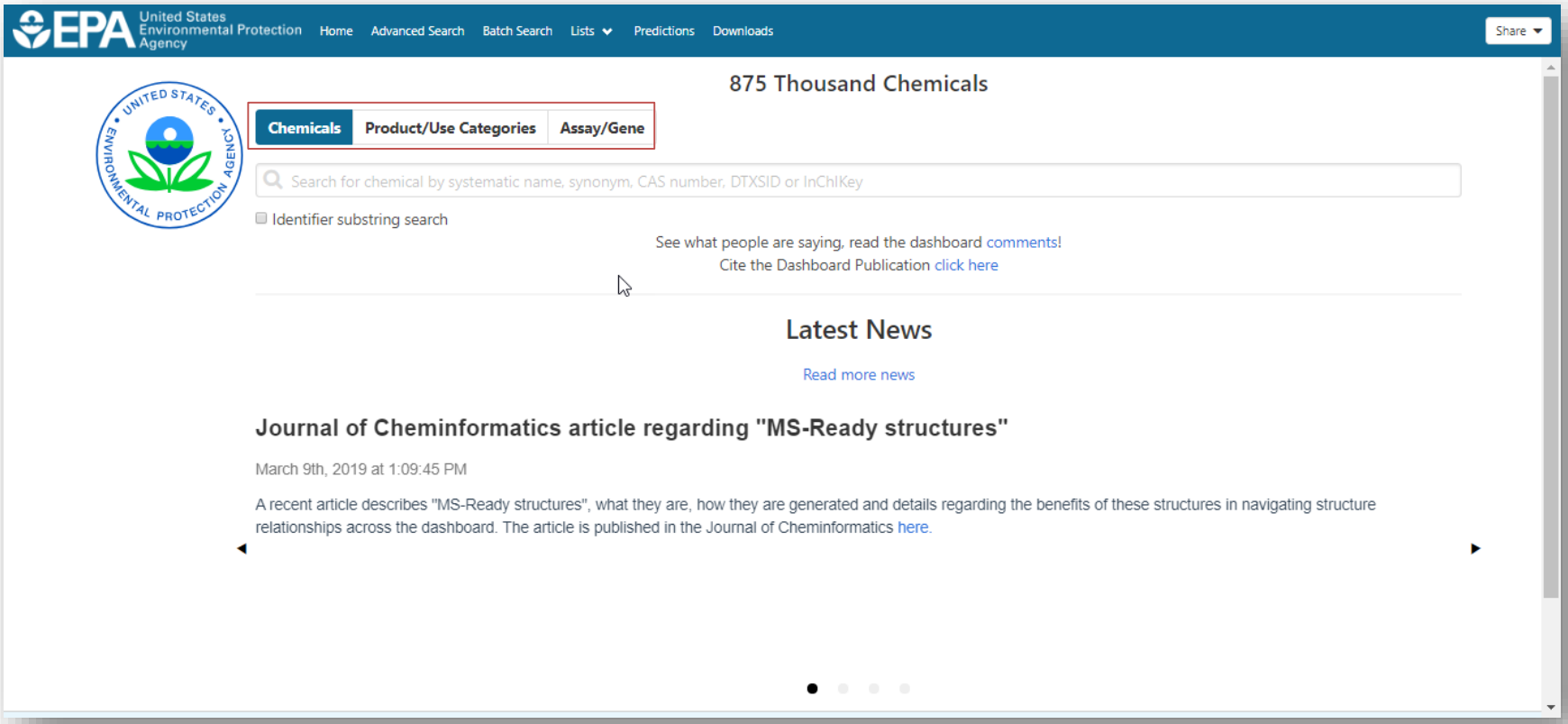
A data integration hub
LOTS of data!

- >875,000 chemicals curated over 20 years
- >700,000 toxicity data points from >30 sources
- Millions of synonyms and identifiers
- Tens of thousands of experimental data points
- Millions of QSAR prediction reports
- Millions of bioactivity data points for >4000 chemicals and hundreds of assay end points
- Searching of Pubmed's 29 million abstracts

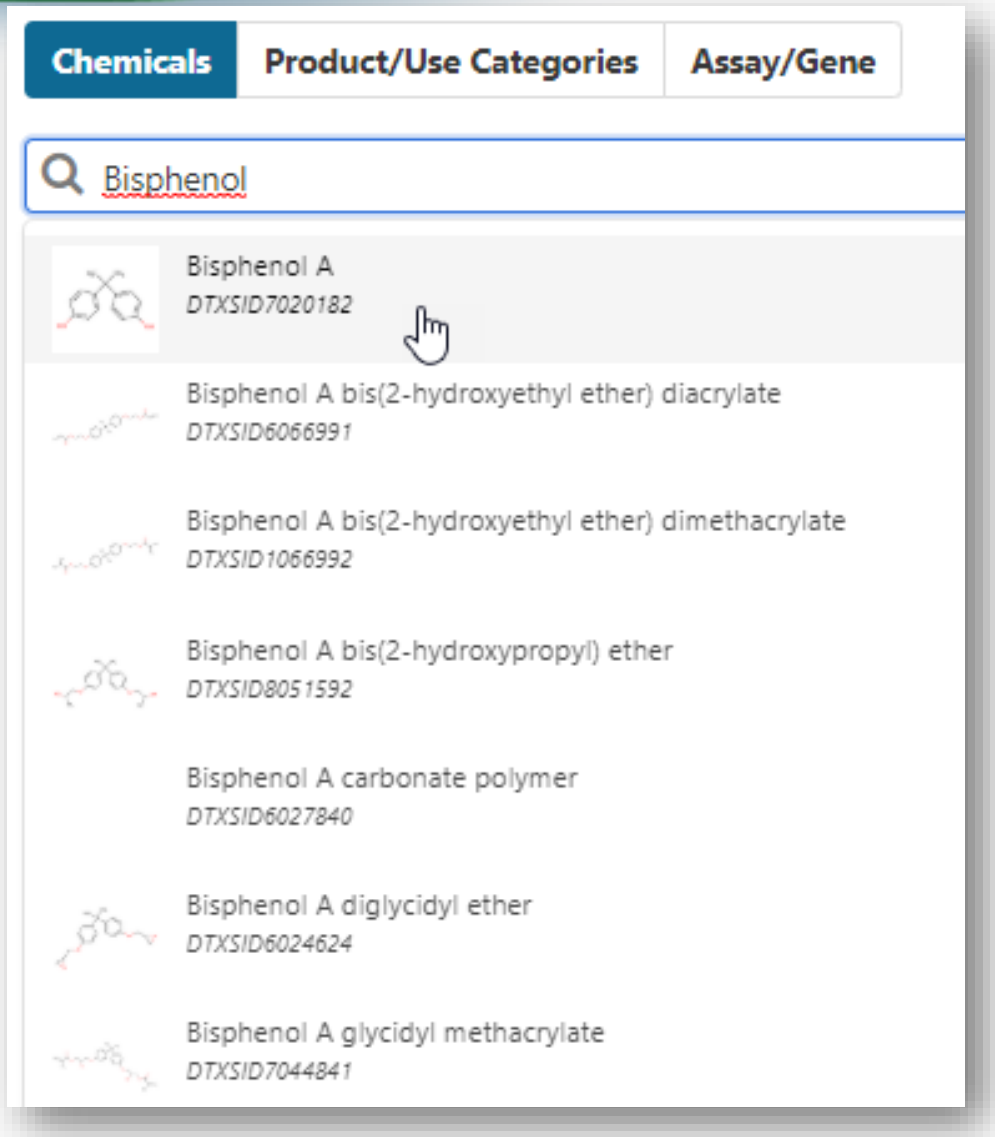
CompTox Chemicals Dashboard

https://comptox.epa.gov/dashboard

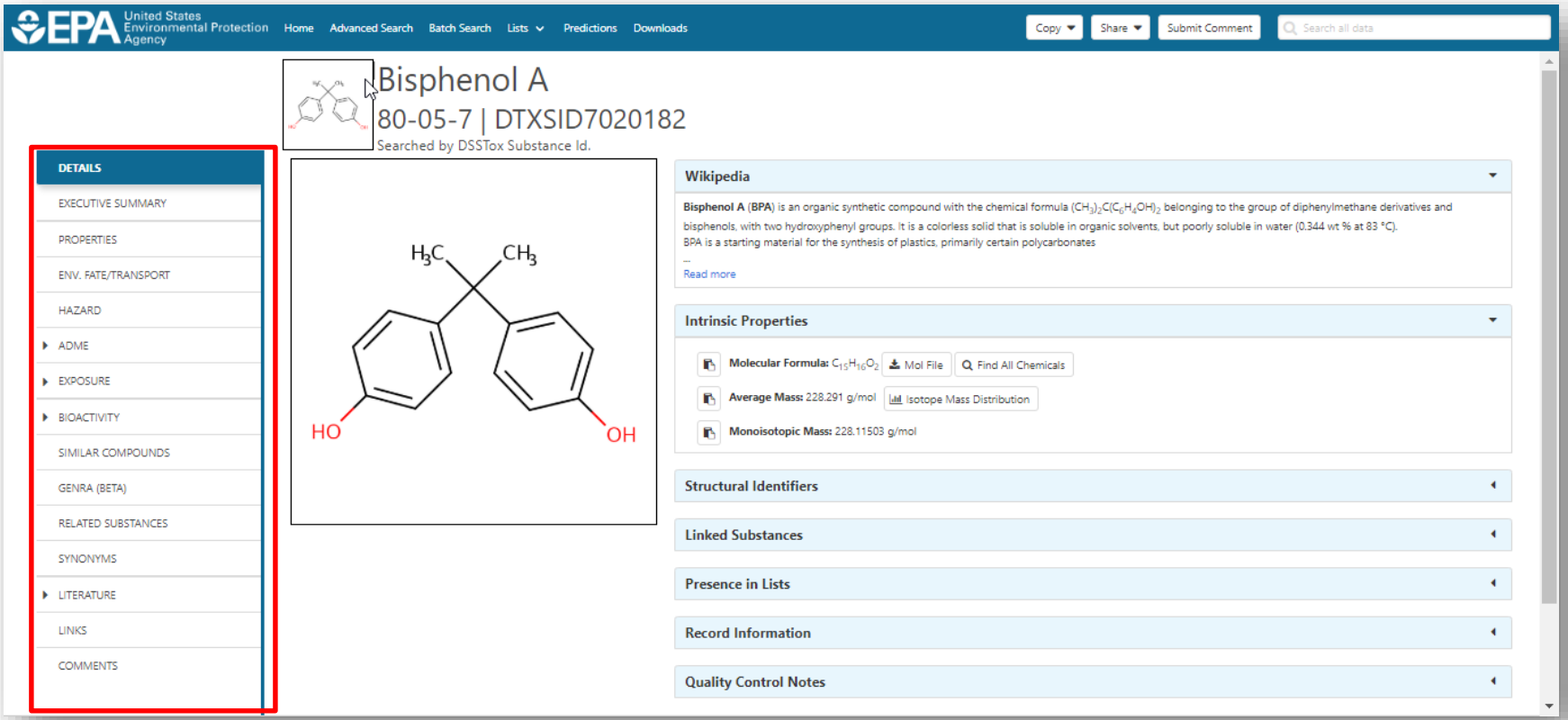
875k Chemical Substances



BASIC Search



Detailed Chemical Pages



An “Executive Summary” Quick Look Tox Info

EPA United States Environmental Protection Agency

Executive Summary

Quantitative Risk Assessment Values
- IRIS values available
- No PPRTV values
- EPA RSL values available
- Minimum RfD: **0.050 mg/kg-day** (chronic, IRIS, oral, 8)
- 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

Neurotoxicology
- No neurotoxicology data available.

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

ADME
- HTTK Css data are available

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

Exposure
- Exposure estimates are available based on NHANES and SEEM

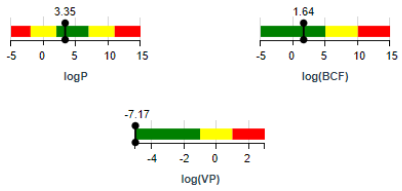
AOP Information
- AOP Links: 13, 33, 36, 58, 60, 61, 66, 107, 124, 150, 163, 175, 187, 200

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

REGIONAL SCREENING

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

PHYSCHEM PARAMETERS



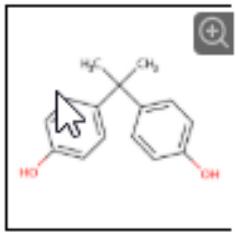
POINT-OF-DEPARTURE PLOTS

ASSAY PLOTS

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, NR1I3, PPARA, NR1I2, Cyp2c11, MMP3, Esr1

Experimental and Predicted Data



Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

Property

Summary

Download Columns

Property	Experimental average	Predicted average
LogP: Octanol-Water	3.32 (1)	3.29
Melting Point	155 (7)	139
Boiling Point	200 (1)	363
Water Solubility	5.26e-4 (1)	9.62e-4
Vapor Pressure	-	8.37e-7
Flash Point	-	190

Transparency for prediction models

EPA United States Environmental Protection Agency

Predicted

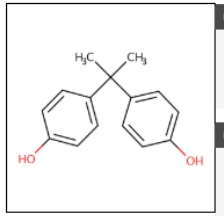
Download Predicted Data

Source	Result	Calculation Details	QMRF
EPISUITE	3.64	Not Available	Not Available
NICEATM	2.40	Not Available	Available
ACD/Labs Consensus	3.63	Not Available	Not Available
ACD/Labs	3.43	Not Available	Not Available
OPERA	3.35	OPERA Model Report [Inside AD]	Available

OPERA Models: LogP: Octanol-Water

Bisphenol A

80-05-7 | DTXSID7020182

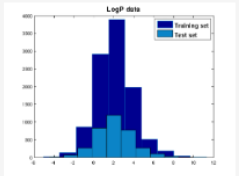


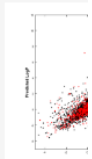
Print PDF

Model Results

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

Model Performance



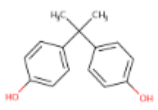


QMRF

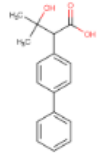
Weighted KNN model

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

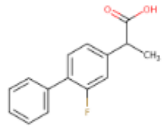
Nearest Neighbors from the Training Set



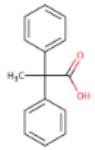
Bisphenol A
Measured:3.32
Predicted: 3.35076



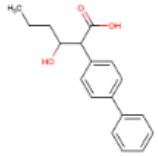
BUTANOIC ACID,2-(4-BIPHENYLYL)-3-HYDROXY-3-METHY
Measured:3.25
Predicted: 3.39062



Flurbiprofen
Measured:4.16
Predicted: 3.94445

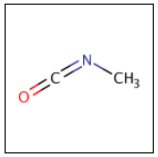


2,2-Diphenylpropionic acid
Measured:2.69
Predicted: 2.84603



3-OH-2-(4-BIPHENYLYL)HEXANOIC ACID
Measured:3.75
Predicted: 3.70322

Access to Chemical Hazard Data



Methyl isocyanate

624-83-9 | DTXSID1023786

Searched by DSSTox Substance Id.

Hazard

DataType

Toxicity Value

Human | Eco

Download | Columns | 10 | Search query

More	Type	Risk assessment class	Value	Units	Exposure route	Subsource	Source
	RfC	chronic	0.001	mg/m3	-	MSC Table 5	Pennsylvania DEP ToxValues
	AEGL 2 - 8 hr (final)	acute	0.008	ppm	inhalation	EPA OW	EPA AEGL
	MEG	short-term	0.016	mg/m3	inhalation	TG 230 Military Exposure Guidelines Table	DOD
	MEG	chronic	0.016	mg/m3	inhalation	TG 230 Military Exposure Guidelines Table	DOD
	AEGL 2 - 4 hr (final)	acute	0.017	ppm	inhalation	EPA OW	EPA AEGL
	MEG	short-term	0.02	mg/m3	inhalation	TG 230 Military Exposure Guidelines Table	DOD
	MEG	short-term	0.02	mg/m3	inhalation	TG 230 Military Exposure Guidelines Table	DOD
	AEGL 3 - 8 hr (final)	acute	0.025	ppm	inhalation	EPA OW	EPA AEGL
	AEGL 3 - 4 hr (final)	acute	0.05	ppm	inhalation	EPA OW	EPA AEGL
	MEG	short-term	0.058	mg/m3	inhalation	TG 230 Military Exposure Guidelines Table	DOD

<< < 1 2 3 > >>

Showing 1 to 10 of 24 records

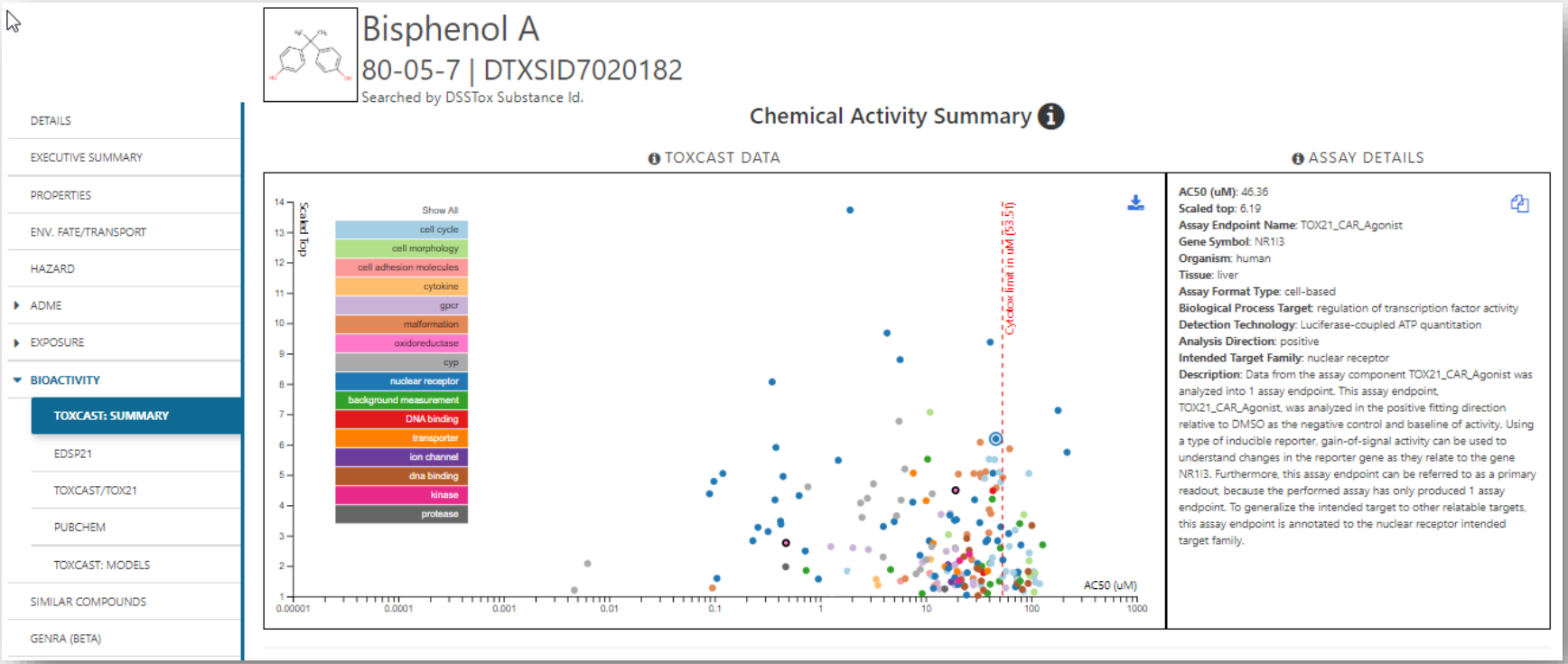
Hazard Data from “ToxVal_DB”

- ToxVal Database contains following data:
  - ~800,000 toxicity values
  - ~30 sources of data
  - ~22,000 sub-sources
  - ~5000 journals cited
  - ~70,000 literature citations

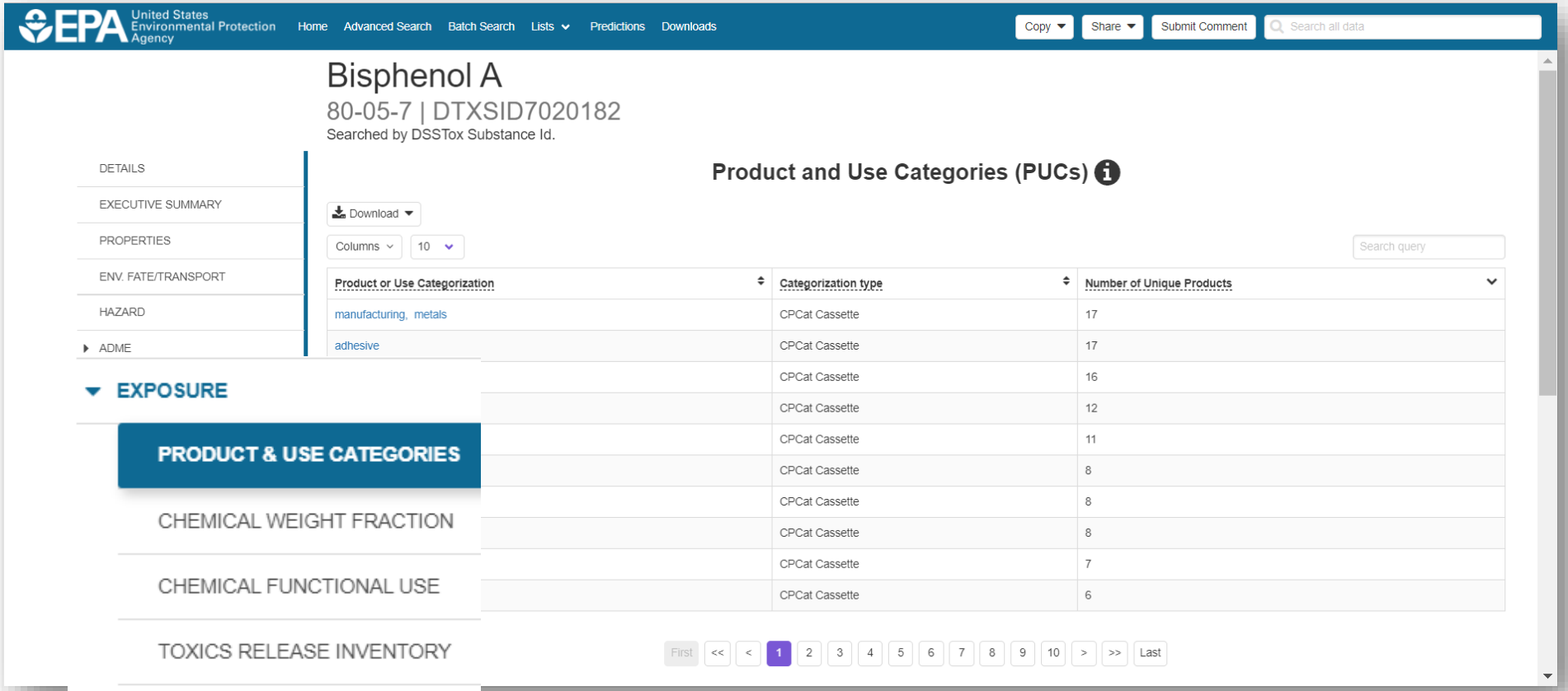
In Vitro Bioassay Screening

ToxCast and Tox21

EPA United States Environmental Protection Agency



Sources of Exposure to Chemicals



Sources of Exposure to Chemicals

EPA United States Environmental Protection Agency

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

Bisphenol A

80-05-7 | DTXSID7020182

Searched by DSSTox Substance Id.

- DETAILS
- EXECUTIVE SUMMARY
- PROPERTIES
- ENV. FATE/TRANSPORT
- HAZARD
- ADME
- **EXPOSURE**
  - PRODUCT & USE CATEGORIES
  - CHEMICAL WEIGHT FRACTION
  - CHEMICAL FUNCTIONAL USE
  - **TOXICS RELEASE INVENTORY**
  - MONITORING DATA
  - EXPOSURE PREDICTIONS
  - PRODUCTION VOLUME
- BIOACTIVITY

Toxics Release Inventory

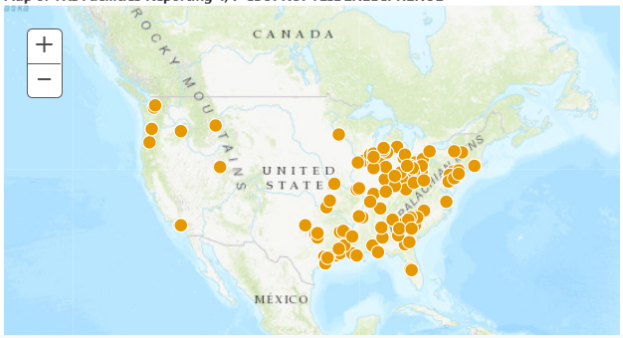
Print Page

2015 TRI Factsheet: Chemical - 4,4'-ISOPROPYLIDENEDIPHENOL, 000080057

Data Source: 2016 Dataset (released March 2018)

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.

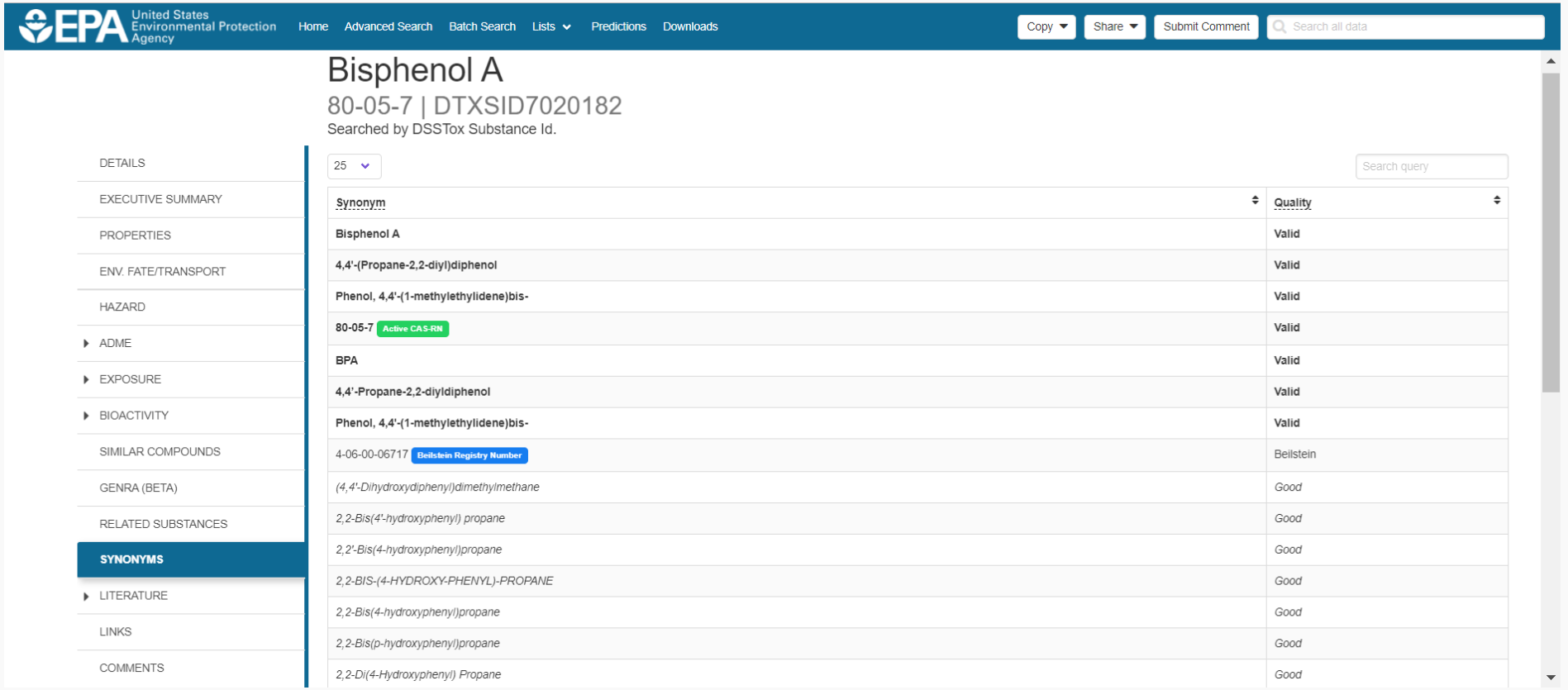
Map of TRI Facilities Reporting 4,4'-ISOPROPYLIDENEDIPHENOL



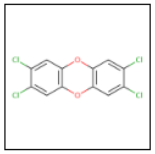
Quick Facts for 2015

	Chemical	United States
Number of TRI Facilities:	120	22,130
Total Production-Related Waste Managed:	15.8 million lbs	27.1 billion lbs
Total On-site and Off-site Disposal or Other Releases:	2.5 million lbs	3.4 billion lbs
Total On-site:	39.4 thousand lbs	2.9 billion lbs
• Air:	28.7 thousand lbs	686.4 million lbs
• Water:	4.4 thousand lbs	198.2 million lbs
• Land:	6.2 thousand lbs	2.0 billion lbs

Identifiers to Support Searches



What if we have nothing for you? "EXTERNAL LINKS"



2,3,7,8-Tetrachlorodibenzo-p-dioxin

1746-01-6 | DTXSID2021315

Searched by DSSTox Substance Id.

General

- EPA Substance Registry Service
- Household Products Database
- PubChem
- Chemspider
- CPCat
- DrugBank
- Wikipedia
- MSDS Lookup
- ChEMBL
- Chemical Vendors
- ToxPlanet
- ACS Reagent Chemicals
- ChemHat: Hazards and Alternatives Toolbox
- Wolfram Alpha
- ECHA Infocard
- ChemAgora
- ChEBI
- NIST Chemistry Webbook

Toxicology

- ACToR
- DrugPortal
- CCRIS
- ChemView
- CTD
- eChemPortal
- Gene-Tox
- HSDB
- ToxCast Dashboard 2
- LactMed
- ATSDR Toxic Substances Portal
- ACToR PDF Report
- CREST
- National Air Toxics Assessment
- Superfund Chemical Data matrix
- ECOTOX
- NIOSH IDLH Values
- International Toxicity Estimates for Risk

Publications

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

Analytical

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

Prediction

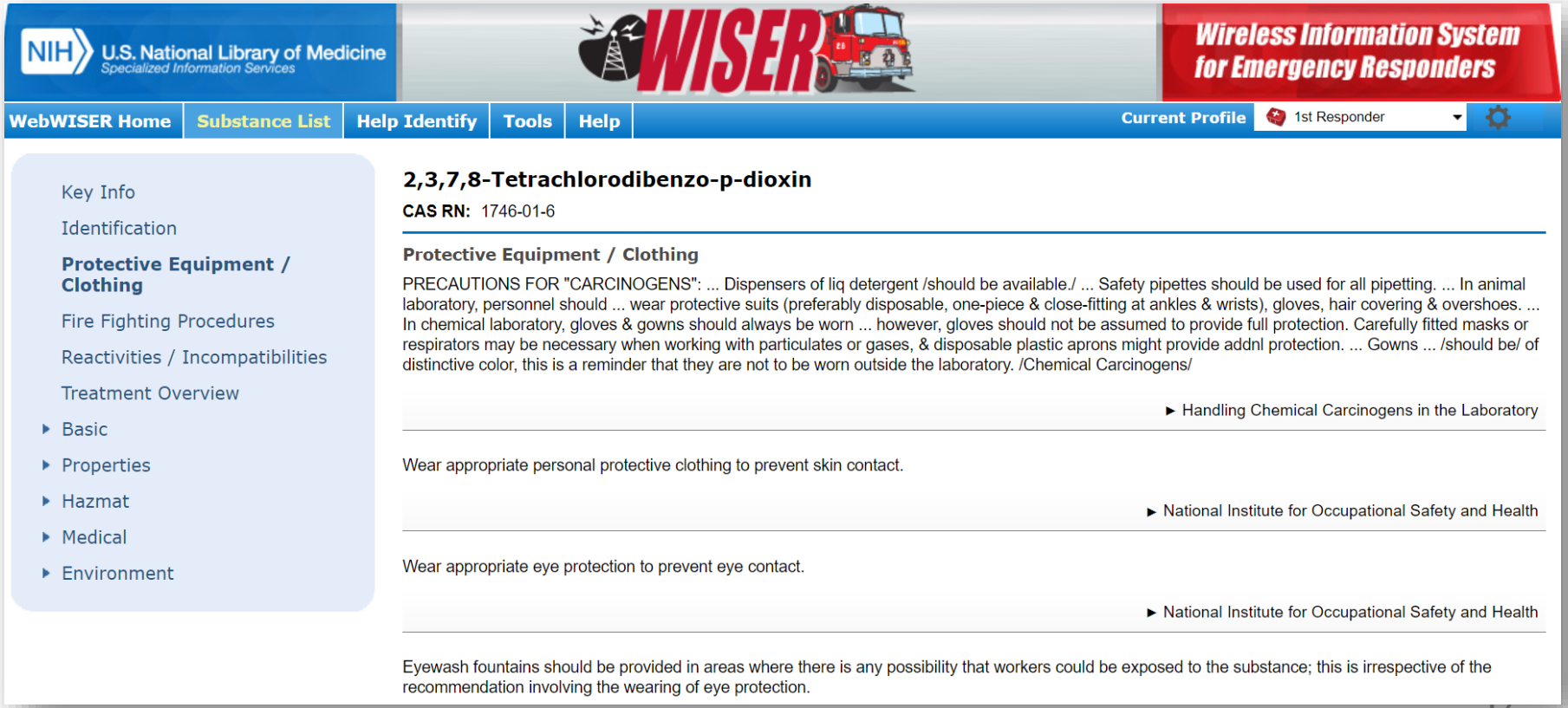
- 2D NMR HSQC/HMBC Prediction
- Carbon-13 NMR Prediction
- Proton NMR Prediction
- LSERD

External Links

WEBWISER

PubChem Safety Sheet

NIOSH Chemical Safety Cards



External Links

WEBWISER

PubChem Safety Sheet

NIOSH Chemical Safety Cards

PUBCHEM > 2,3,7,8-TETRACHLOROD... > GHS CLASSIFICATION

CID 15625

2,3,7,8-Tetrachlorodibenzo-P-dioxin

GHS Classification

Showing 3 of 3

Pictogram(s)	 Acute Toxic, Irritant, Environmental Hazard
Signal	Danger
GHS Hazard Statements	Aggregated GHS information provided by 23 companies from 1 notifications to the ECHA C&L Inventory. Each notification may be associated with multiple companies. H300 (100%): Fatal if swallowed [Danger Acute toxicity, oral] H319 (100%): Causes serious eye irritation [Warning Serious eye damage/eye irritation] H400 (100%): Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard] H410 (100%): Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard] Information may vary between notifications depending on impurities, additives, and other factors. The percentage value in parenthesis indicates the notified classification ratio from companies that provide hazard codes. Only hazard codes with percentage values above 10% are shown.

External Links

WEBWISER

PubChem Safety Sheet

NIOSH Chemical Safety Cards

« back to the search result list

English - EN

2,3,7,8-TETRACHLORODIBENZO-p-DIOXIN **ICSC: 1467**

Dibenzo [b,e] [1,4]dioxin, 2,3,7,8-tetrachloro-
2,3,7,8-TCDD **November 2003**
2,3,7,8-Tetrachloro-1,4-dioxin

CAS #: 1746-01-6
UN #: 2811
EC Number: 217-122-7

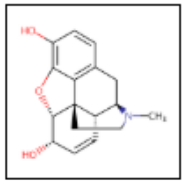
	ACUTE HAZARDS	PREVENTION	FIRE FIGHTING
FIRE & EXPLOSION	Gives off irritating or toxic fumes (or gases) in a fire.		In case of fire in the surroundings, use appropriate extinguishing media.

AVOID ALL CONTACT! IN ALL CASES CONSULT A DOCTOR!			
	SYMPTOMS	**PREVENTION**	**FIRST AID**
Inhalation	Symptoms may be delayed.	Use appropriate engineering controls.	Fresh air, rest. Refer for medical attention.
Skin	MAY BE ABSORBED! See Inhalation. Redness. Pain.	Protective gloves. Protective clothing.	Remove contaminated clothes. Rinse and then wash skin with water and soap. Refer for medical attention .
Eyes	Redness. Pain.	Wear face shield or eye protection in combination with breathing protection.	First rinse with plenty of water for several minutes (remove contact lenses if easily possible), then refer for medical attention.
Ingestion	See Inhalation.	Do not eat, drink, or smoke during work. Wash hands before eating.	Give a slurry of activated charcoal in water to drink. Induce vomiting (ONLY IN CONSCIOUS PERSONS!). Refer for medical attention .

SPILLAGE DISPOSAL	CLASSIFICATION & LABELLING
Evacuate danger area! Consult an expert! Personal protection: chemical protection suit including self-contained breathing apparatus.	**According to UN GHS Criteria**
STORAGE	
Separated from food and feedstuffs.	**Transportation** **UN Classification** UN Hazard Class: 6.1; UN Pack Group: I
PACKAGING	

Built in "Modules"

Literature Searching



Morphine

57-27-2 | DTXSID9023336

Searched by Approved Name.

Abstract Sifter

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

Select a Query Term

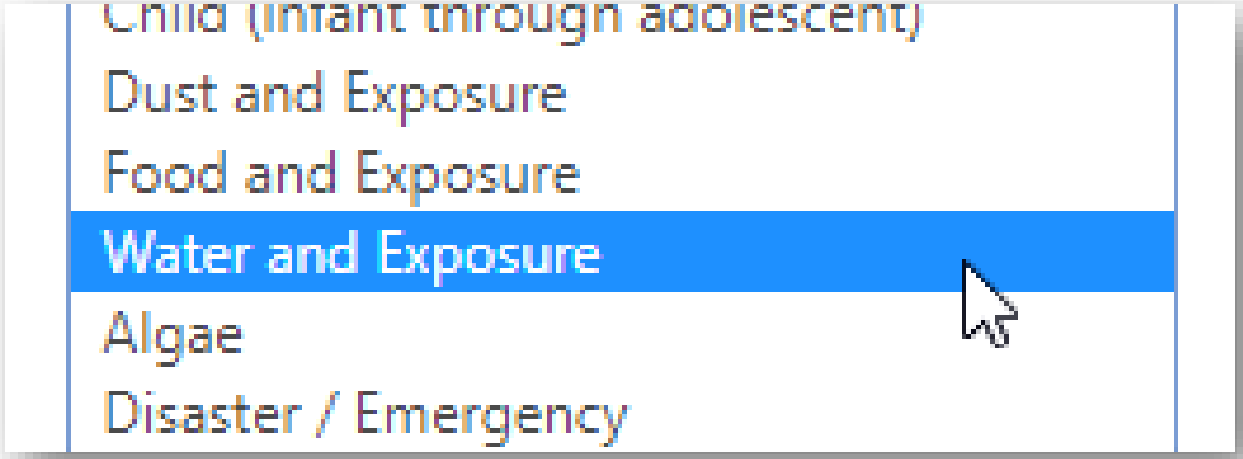
Retrieve Articles

- Select a Query Term
- Hazard
- Fate and Transport
- Metabolism/PK/PD
- Chemical Properties
- Exposure
- Mixtures
- Male Reproduction
- Androgen Disruption
- Female Reproduction
- GeneTox
- Cancer
- Clinical Trials
- Embryo and embryonic development
- Child (infant through adolescent)
- Dust and Exposure
- Food and Exposure
- Water and Exposure
- Algae
- Disaster / Emergency

Optionally, edit the query before retrieving.

"57-27-2" OR "Morphine"

Literature Searching



Optionally, edit the query before retrieving.

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

Literature Searching

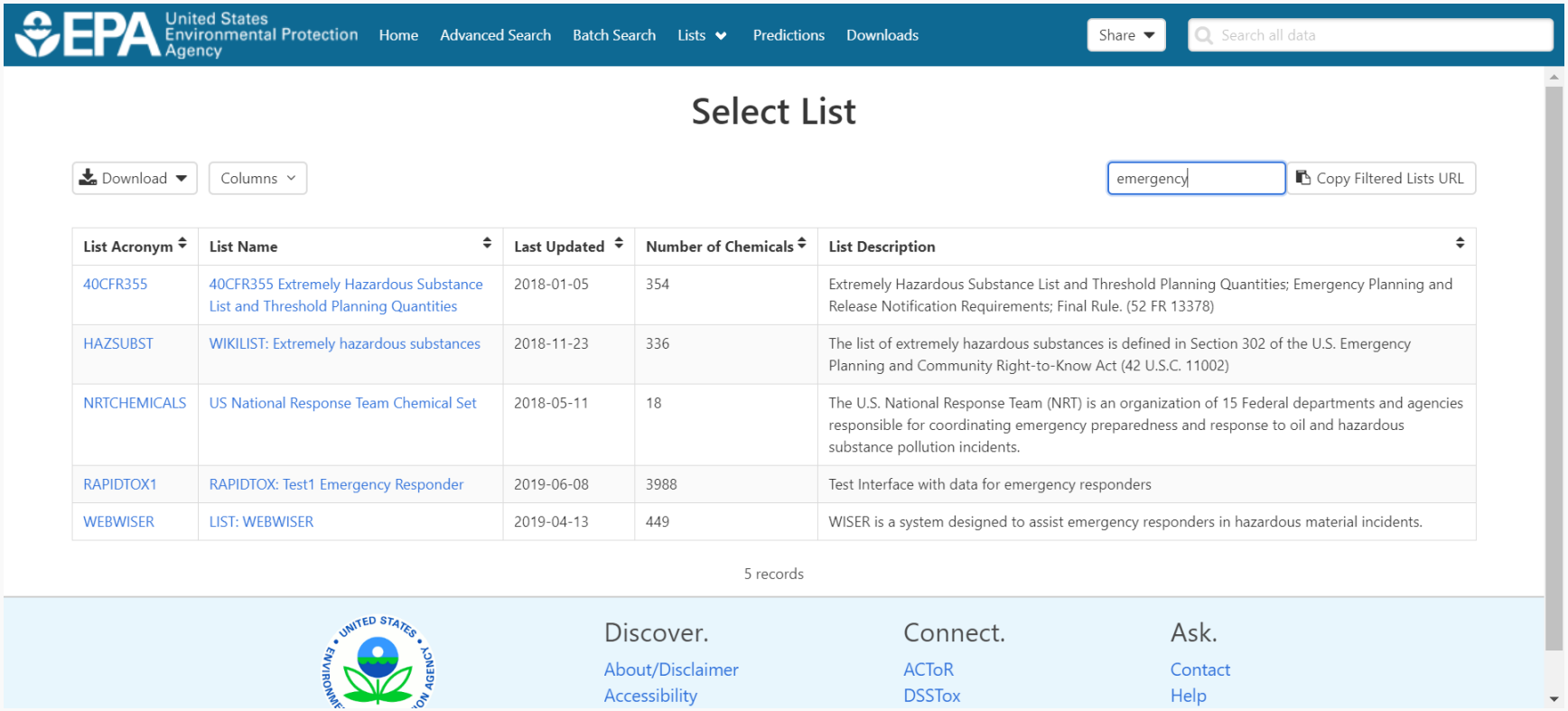
To find articles quickly, enter terms to sift abstracts.

wastewater | Spectrometry | EPA | Clear Terms | Download / Send to... | Download Sifter for Excel

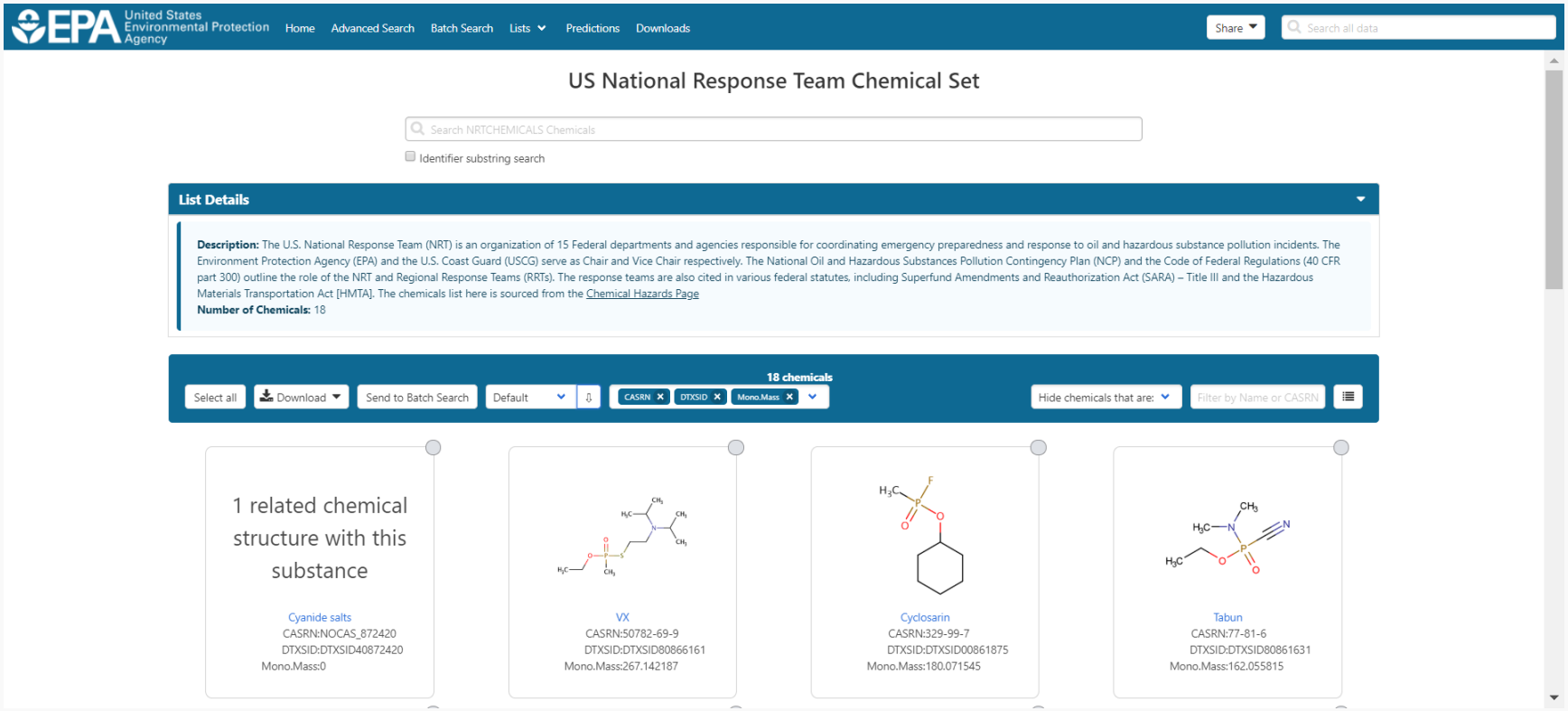
	wastewater	Spectrometry	EPA	Total	PMID	Year	Title	Authors	Journal	Rev
	4	2	0	6	29274731	2017	Simultaneous analysis of opioid analgesics and thei...	Krizman-Matasic; Kostanjevecki; Ahel; Terzic	Journal of chromatography. A	
	0	1	0	1	25768972	2015	Evaluating external contamination of polybrominate...	Poon;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

Chemical Lists

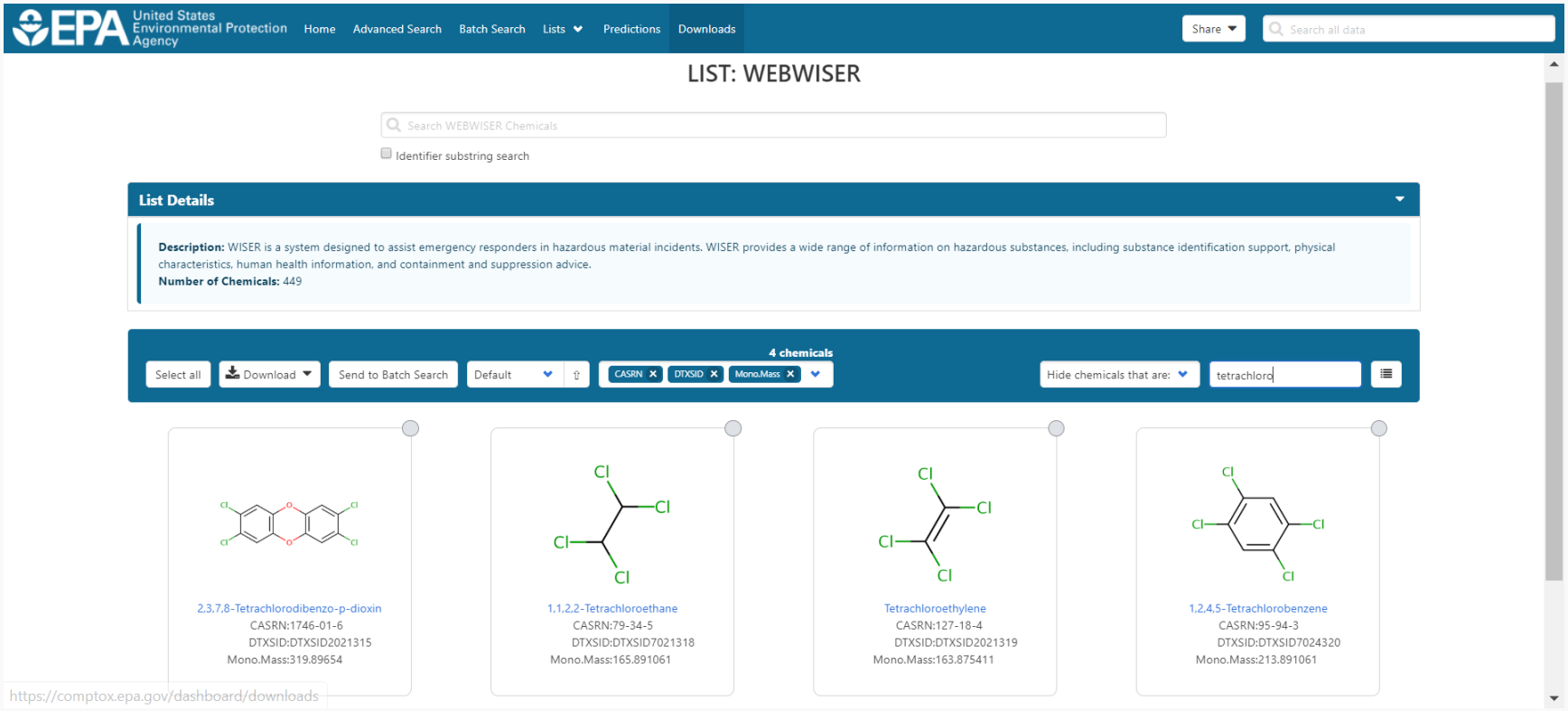
EPAHFR: Hydraulic Fracturing



Emergency Response List



WebWISER List



Batch Searching

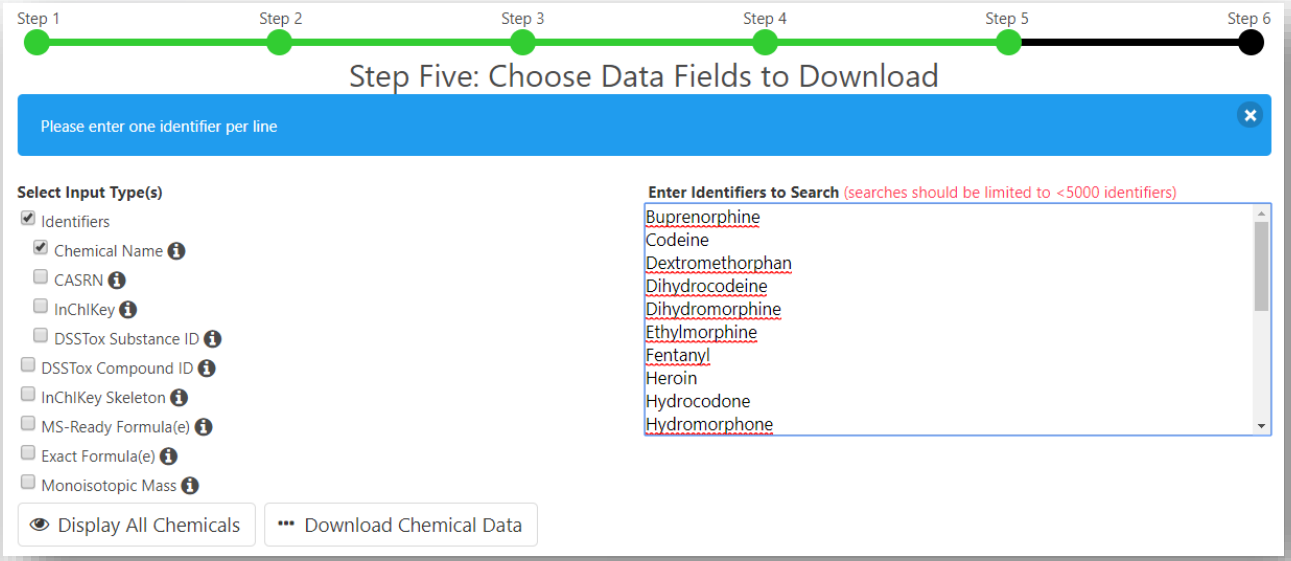
Batch Searching

- Singleton searches are useful but people generally want data on LOTS of chemicals!

- Typical questions
  - What is the list of chemicals for the formula $C_xH_yO_z$
  - What is the list of chemicals for a mass +/- error
  - Can I get chemical lists in Excel files? In SDF files?
  - Can I include properties in the download file?

Batch Search Names

Buprenorphine
Codeine
Dextromethorphan
Dihydrocodeine
Dihydromorphine
Ethylmorphine
Fentanyl
Heroin
Hydrocodone
Hydromorphone
Ketamine
Meperidine
Methadone
Morphine
Morphinone
Naloxone
Naltriben
Oxycodone
Oxymorphone
Propoxyphene
Sufentanil
Tramadol

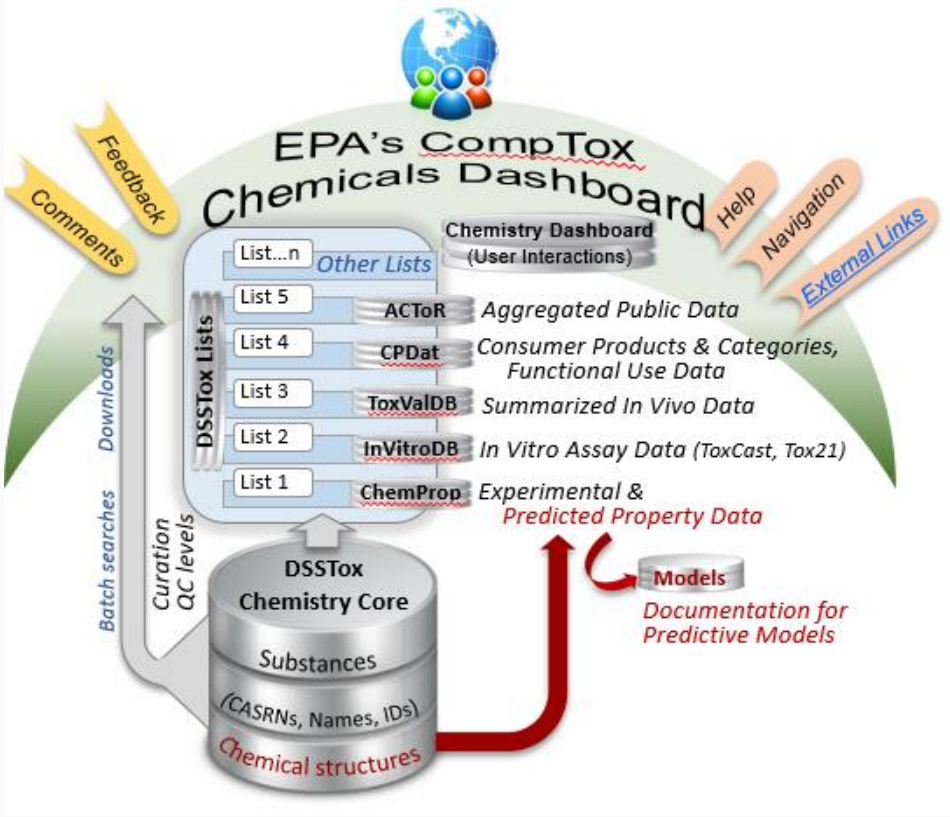


Excel Download

INPUT	FOUND_BY	DTXSID
Buprenorphine	Approved Name	DTXSID2022705
Codeine	Approved Name	DTXSID2020341
Dextromethorphan	Approved Name	DTXSID3022908
Dihydrocodeine	Approved Name	DTXSID5022936
Dihydromorphine	Approved Name	DTXSID7048908
Ethylmorphine	Approved Name	DTXSID1046760
Fentanyl	Approved Name	DTXSID9023049
Heroin	Synonym	DTXSID6046761
Hydrocodone	Approved Name	DTXSID8023131
Hydromorphone	Approved Name	DTXSID8023133
Ketamine	Approved Name	DTXSID8023187
Meperidine	Approved Name	DTXSID9023253
Methadone	Approved Name	DTXSID7023273
Morphine	Approved Name	DTXSID9023336

Conclusion

- An integrated hub for environmental chemistry data to serve computational toxicology
- Serving multiple use cases and needs – let's talk!



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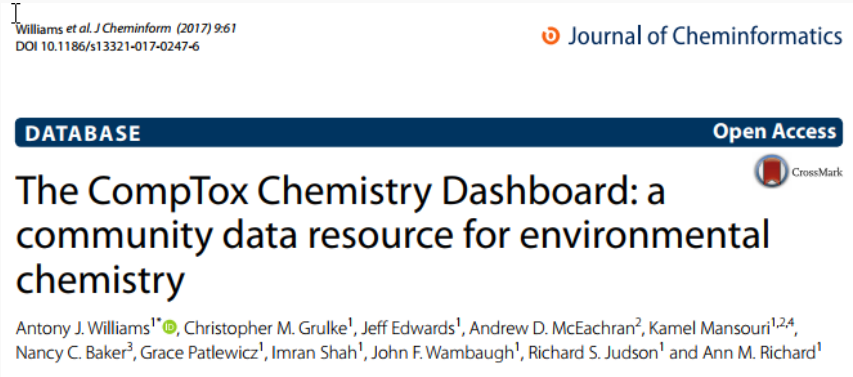

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