EPA Tools and Resources Webinar

CompTox Chemicals Dashboard:
Data and Tools to Support Chemical and Environmental Risk Assessment

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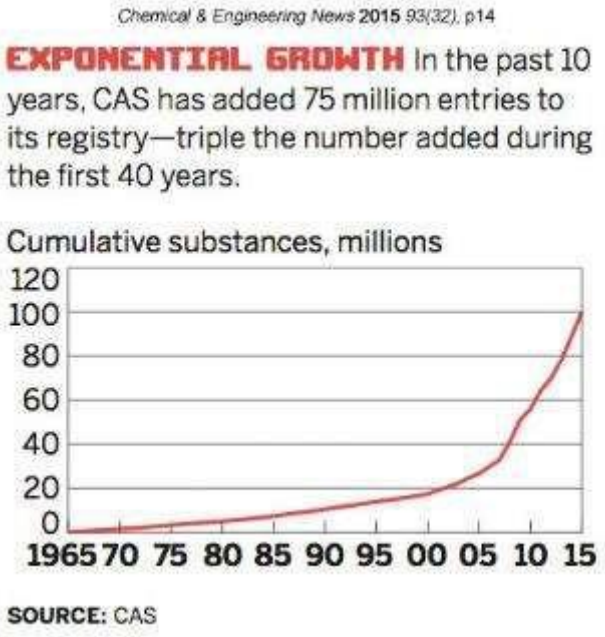
US EPA Office of Research and Development

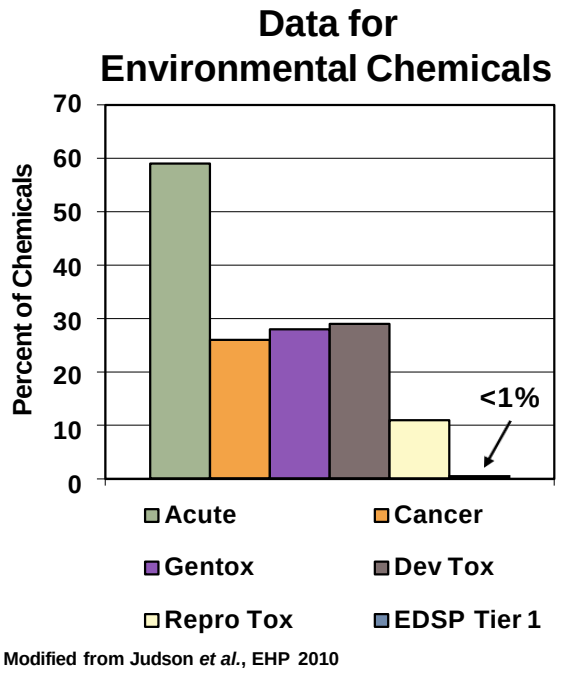
September 11, 2019

Problem: Too Many Chemicals, Too Few Resources

- **Timely characterization of human and ecological risk posed by thousands of existing and emerging chemicals is a critical challenge to protect public health and the environment**



*CAS – Chemical Abstracts Service



Modified from Judson *et al.*, EHP 2010

Approach

- **Develop a "first-stop-shop" for data as an integration node for environmental chemical data to support EPA and partner decision-making:**
  - Centralized location for relevant chemical data
  - Chemistry, exposure, hazard, dosimetry
  - Combination of existing data and predictive models
  - Publicly accessible, periodically updated, curated
- **Ease of access to data results in efficiency and accelerates chemical risk assessment**

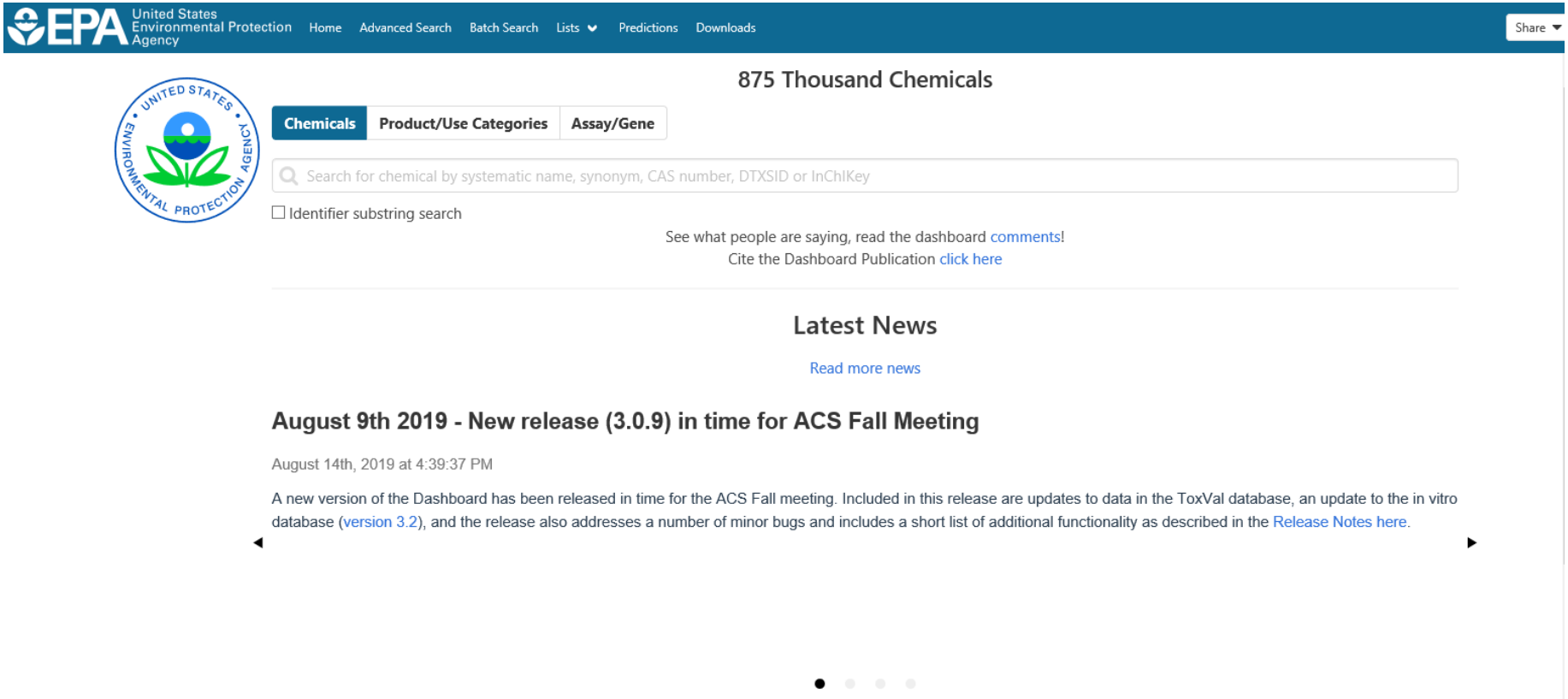
EPA's CompTox Chemicals Dashboard

A publicly accessible website delivering:

- ~875,000 chemicals with related property data
- Experimental and predicted physicochemical property data
- Integration to "biological assay data" for 1000's of chemicals
- Information regarding consumer products containing chemicals
- Links to other agency websites and public data resources
- "Literature" searches for chemicals using public resources
- "Batch searching" for thousands of chemicals
- Downloadable Open Data for reuse and repurposing
- Many features (only highlighting a few)
- Access to multiple tools (direct data interpolation and predictive) for multiple disciplines

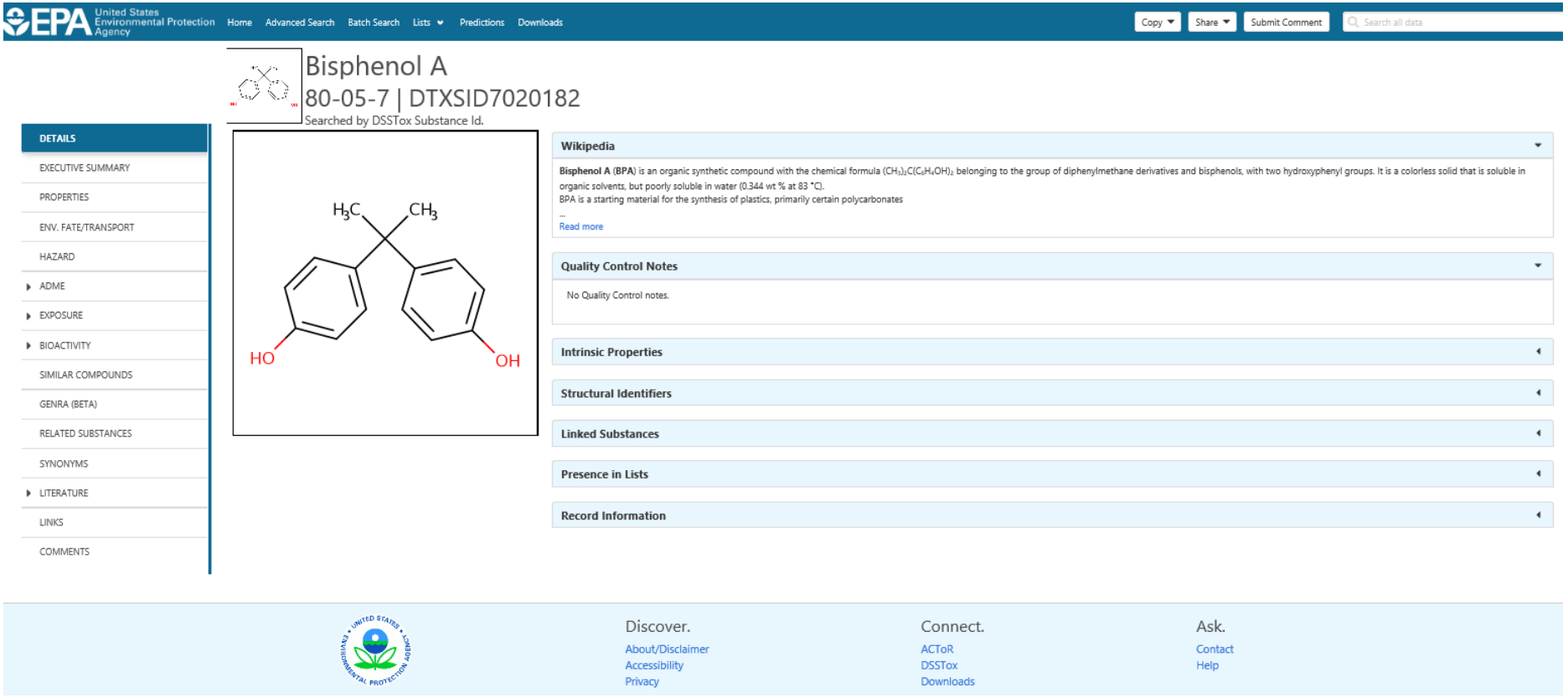
https://www.epa.gov/chemical-research/comptox-chemicals-dashboard

EPA CompTox Chemicals Dashboard

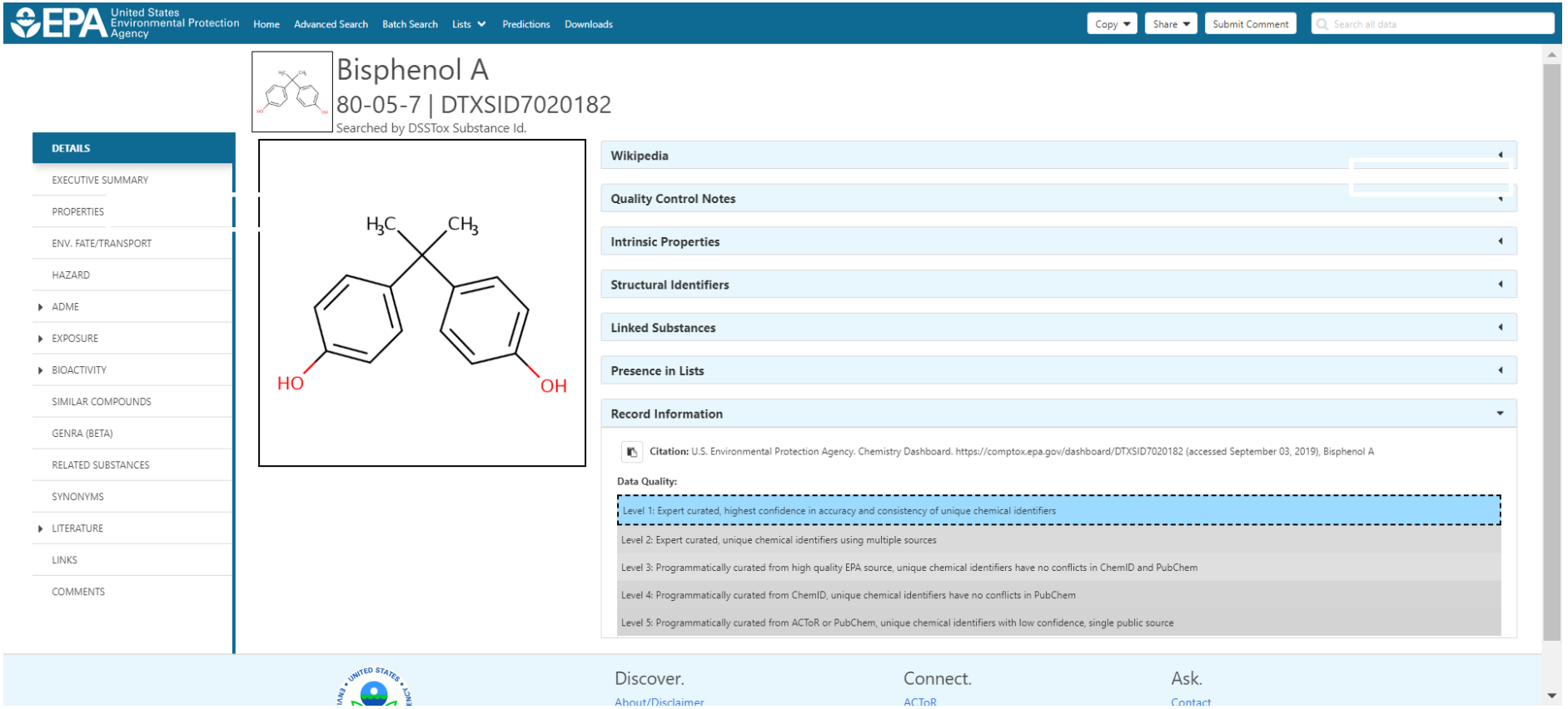


https://comptox.epa.gov/dashboard

Detailed Chemical Pages

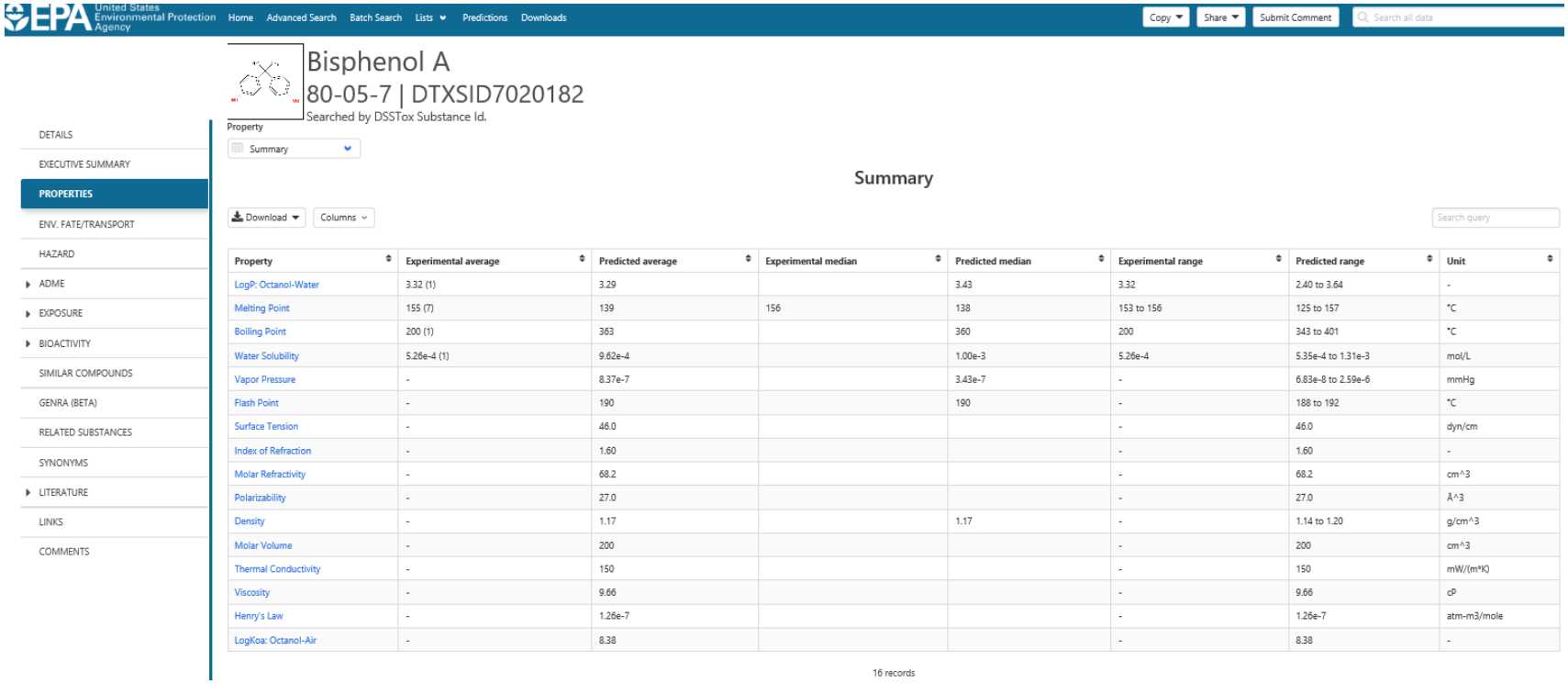


Data Quality



Grulke et al. Computational Toxicology 12 (2019) 100096

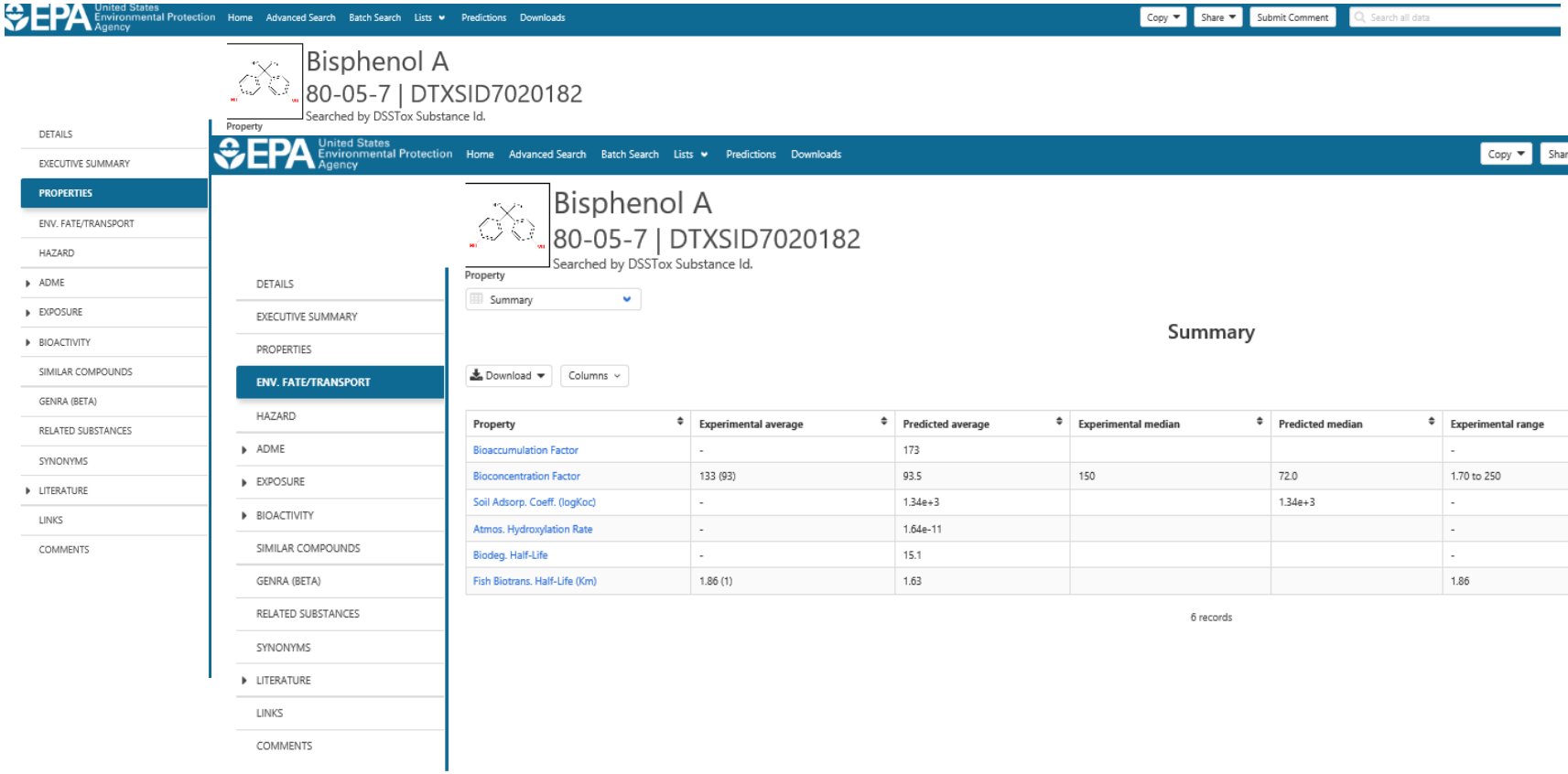
Properties



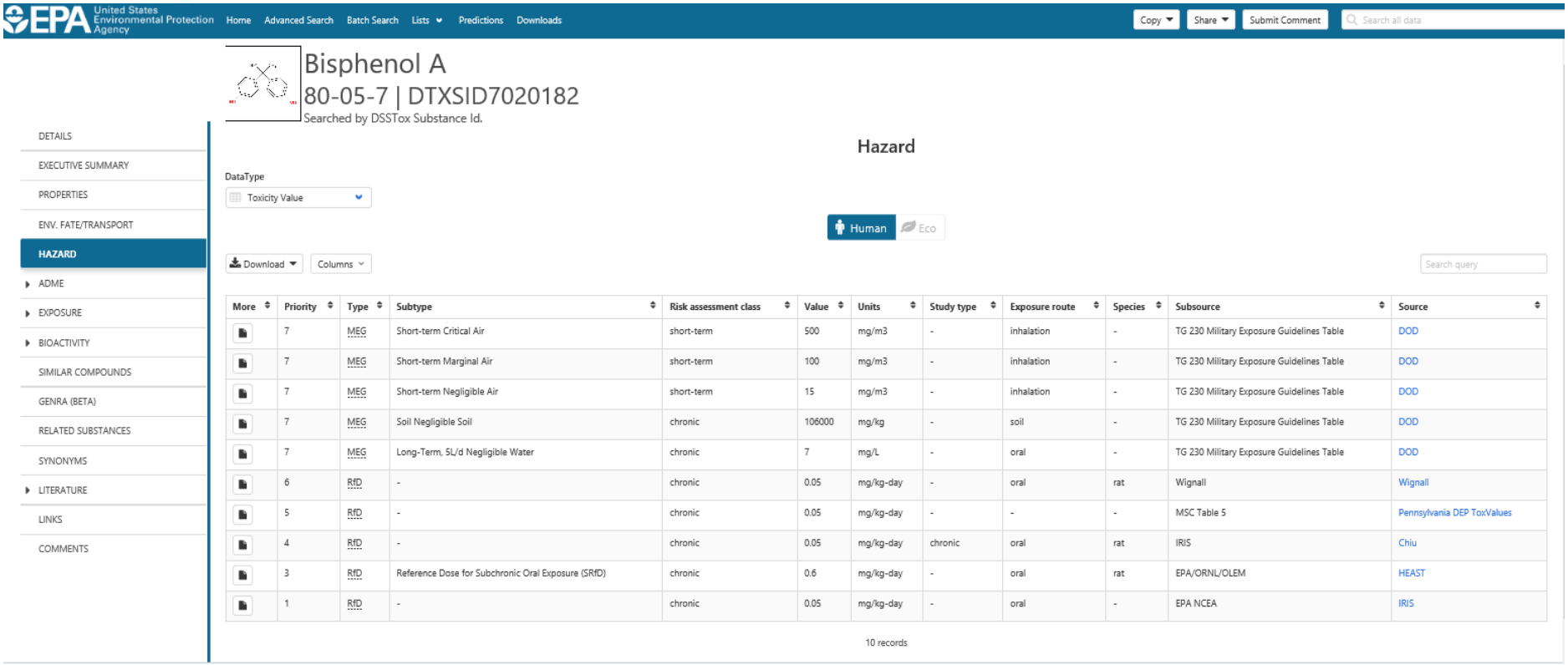
Property	Experimental average	Predicted average	Experimental median	Predicted median	Experimental range	Predicted range	Unit
LogP: Octanol-Water	3.32 (1)	3.29		3.43	3.32	2.40 to 3.64	-
Melting Point	155 (7)	139	156	138	153 to 156	125 to 157	°C
Boiling Point	200 (1)	363		360	200	343 to 401	°C
Water Solubility	5.26e-4 (1)	9.62e-4		1.00e-3	5.26e-4	5.35e-4 to 1.31e-3	mol/L
Vapor Pressure	-	8.37e-7		3.43e-7	-	6.83e-8 to 2.59e-6	mmHg
Flash Point	-	190		190	-	188 to 192	°C
Surface Tension	-	46.0			-	46.0	dyn/cm
Index of Refraction	-	1.60			-	1.60	-
Molar Refractivity	-	68.2			-	68.2	cm^3
Polarizability	-	27.0			-	27.0	Å^3
Density	-	1.17		1.17	-	1.14 to 1.20	g/cm^3
Molar Volume	-	200			-	200	cm^3
Thermal Conductivity	-	150			-	150	mW/(m*K)
Viscosity	-	9.66			-	9.66	cP
Henry's Law	-	1.26e-7			-	1.26e-7	atm-m3/mole
LogKoa: Octanol-Air	-	8.38			-	8.38	-

16 records

Properties, Environmental Fate and Transport

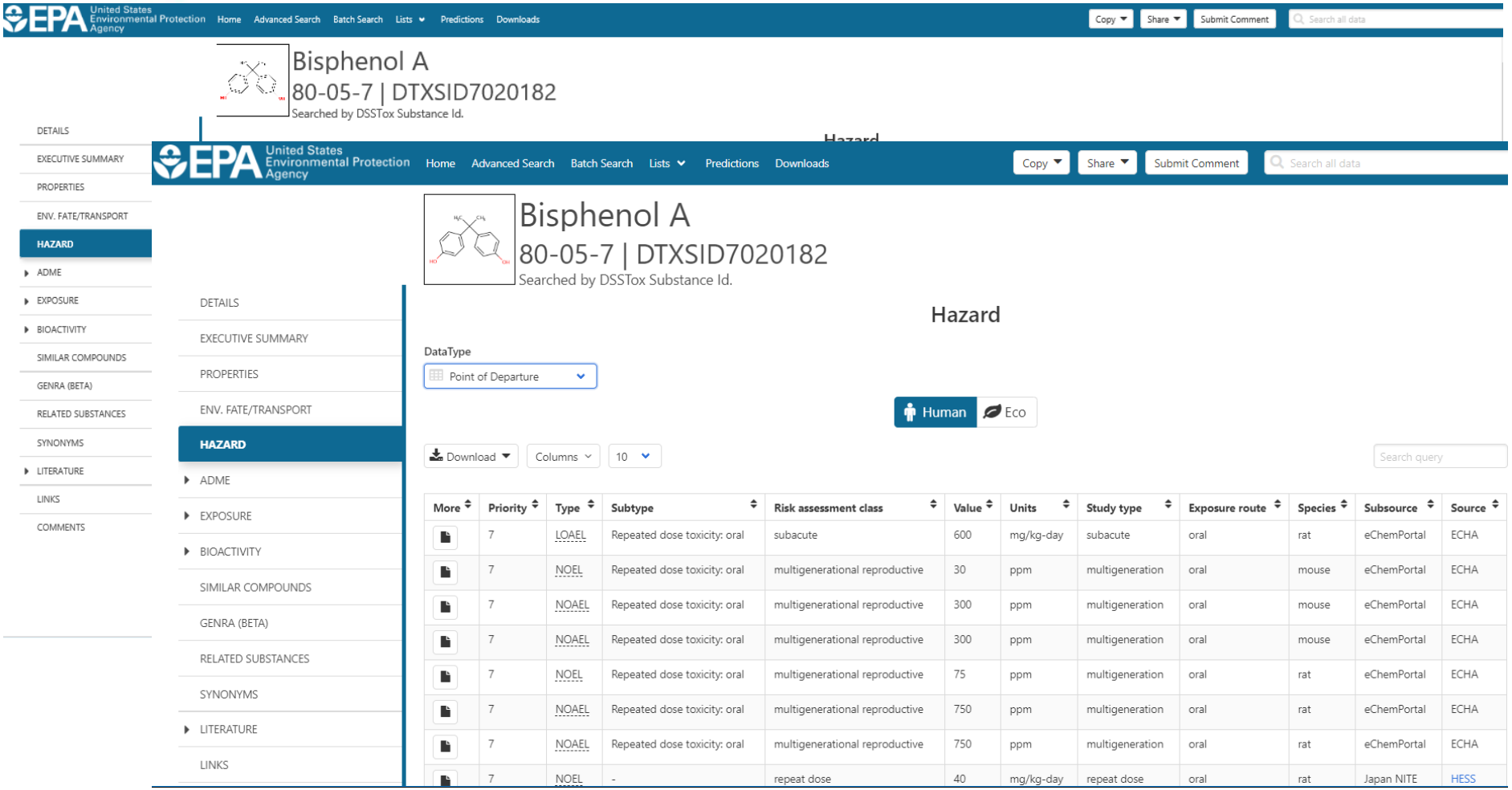


Chemical Hazard Data

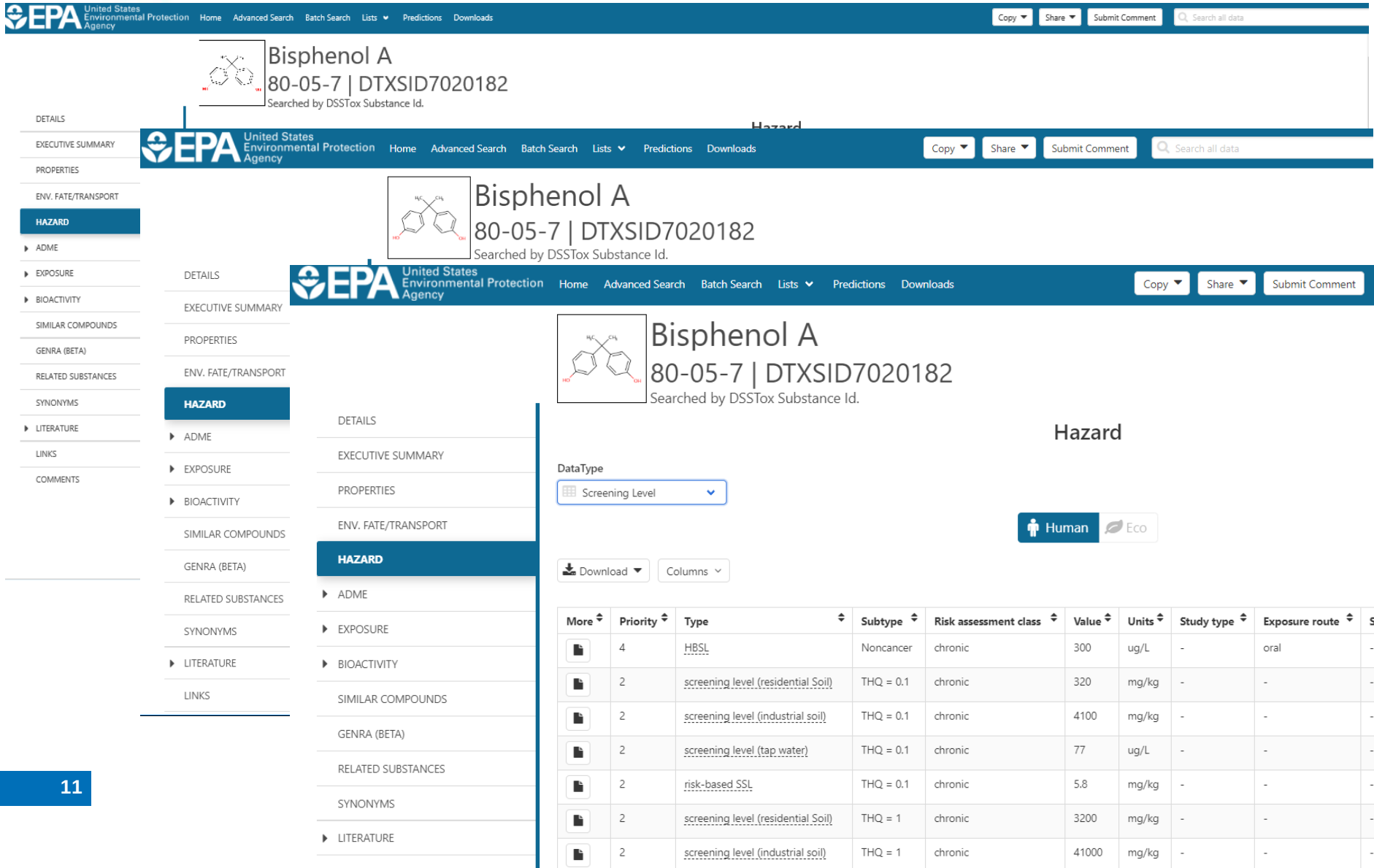


More	Priority	Type	Subtype	Risk assessment class	Value	Units	Study type	Exposure route	Species	Subsource	Source
	7	MEG	Short-term Critical Air	short-term	500	mg/m3	-	inhalation	-	TG 230 Military Exposure Guidelines Table	DOD
	7	MEG	Short-term Marginal Air	short-term	100	mg/m3	-	inhalation	-	TG 230 Military 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, 5L/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 ToxValues
	4	RfD	-	chronic	0.05	mg/kg-day	chronic	oral	rat	IRIS	Chiu
	3	RfD	Reference Dose for Subchronic Oral Exposure (SRfD)	chronic	0.6	mg/kg-day	-	oral	rat	EPA/ORNL/OLEM	HEAST
	1	RfD	-	chronic	0.05	mg/kg-day	-	oral	-	EPA NCEA	IRIS

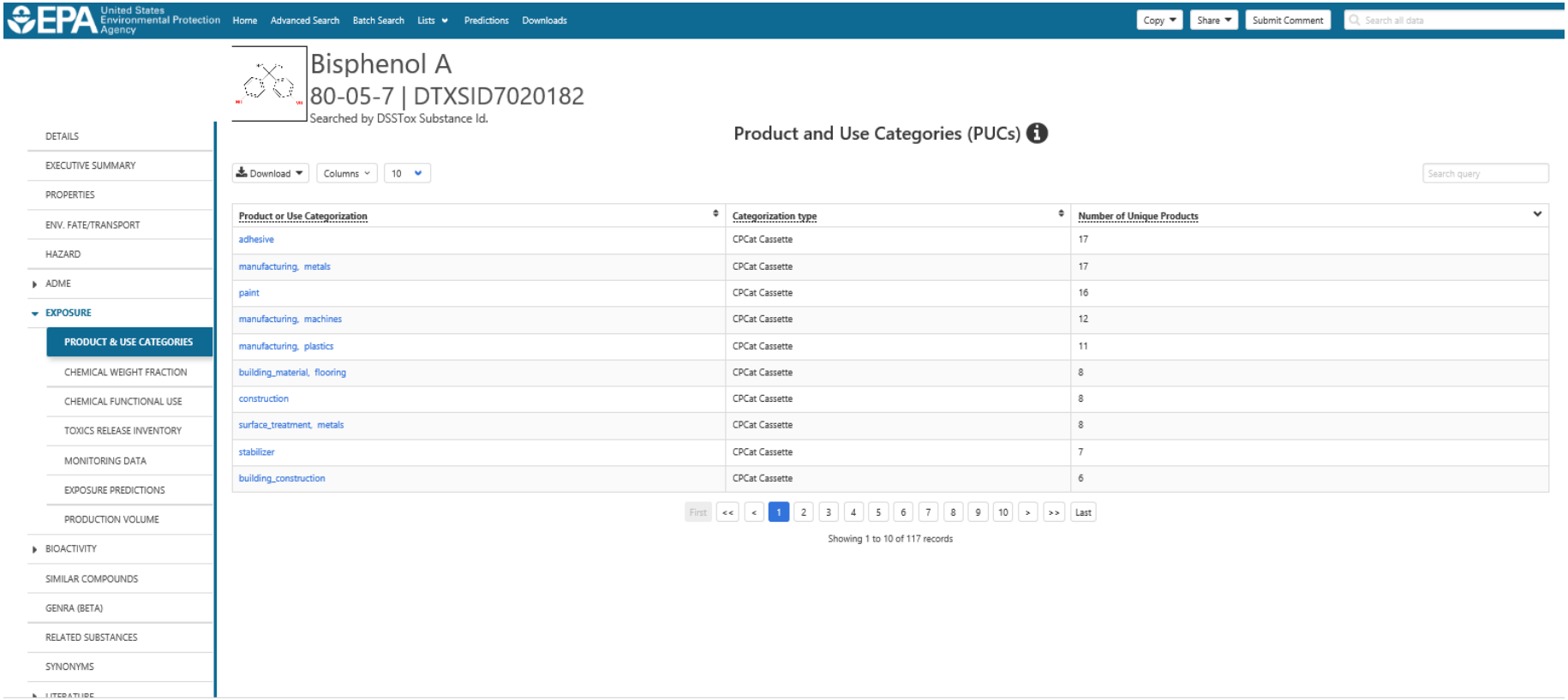
Chemical Hazard Data



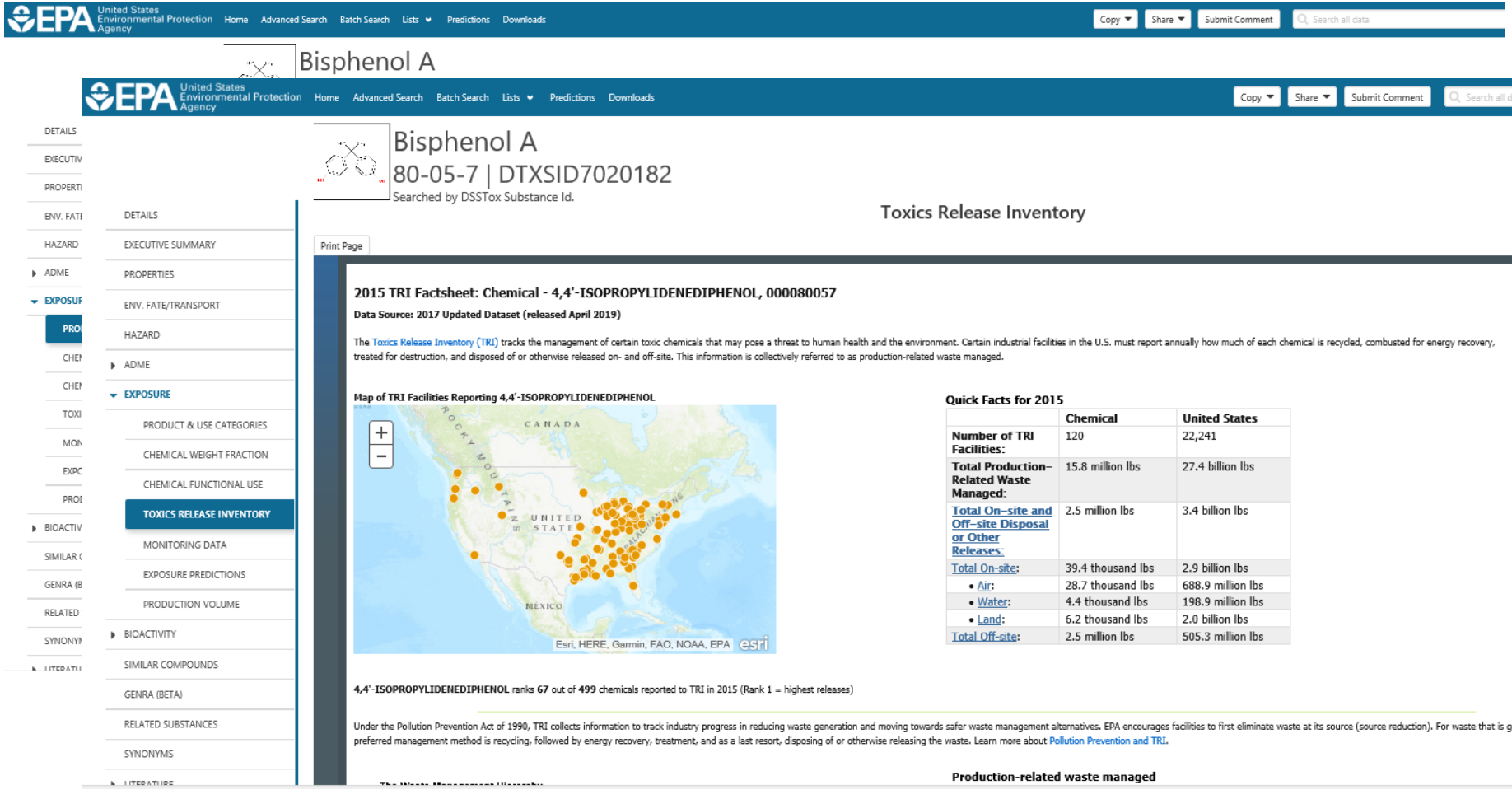
Chemical Hazard Data



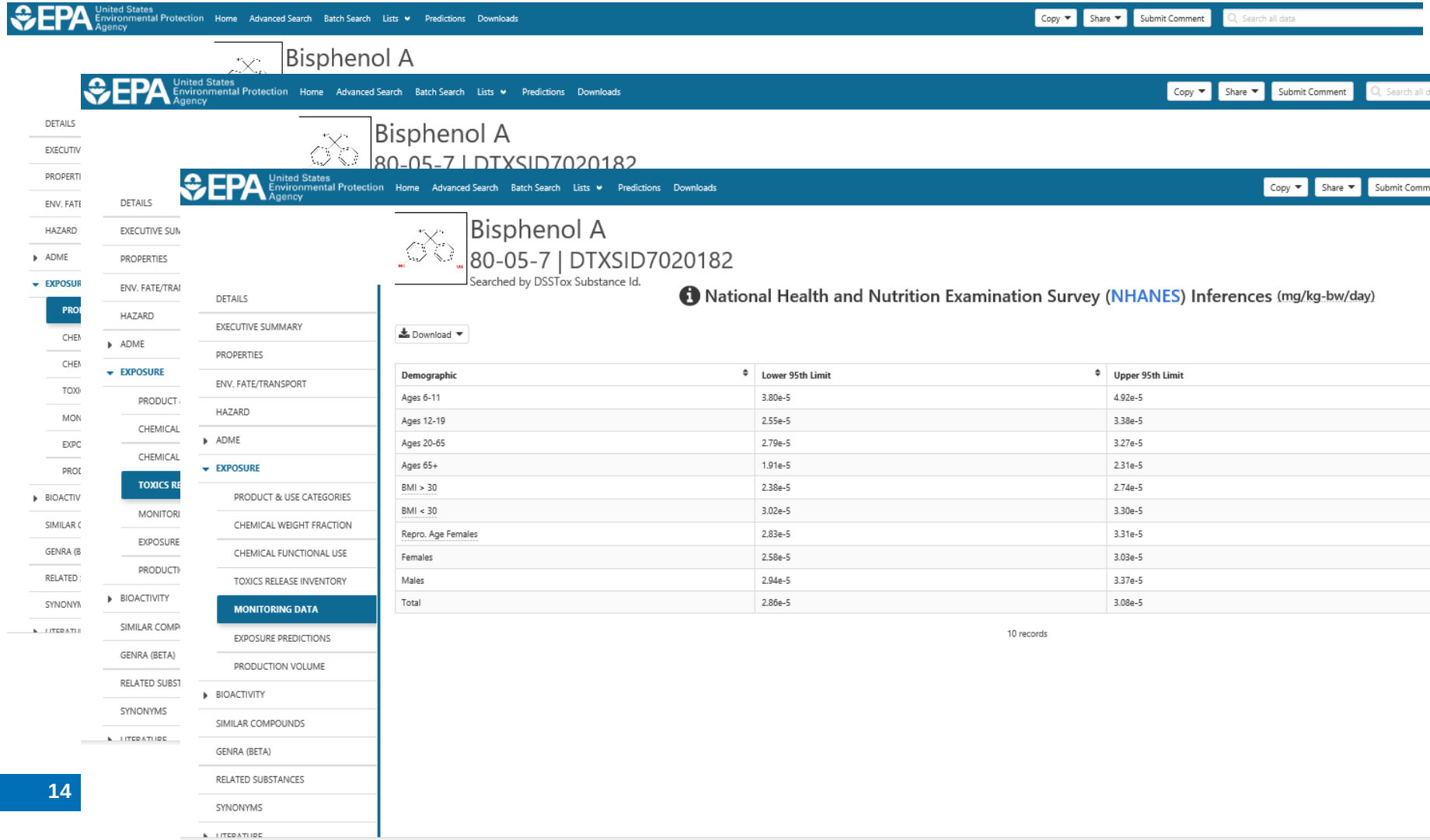
Sources of Exposure to Chemicals



Sources of Exposure to Chemicals

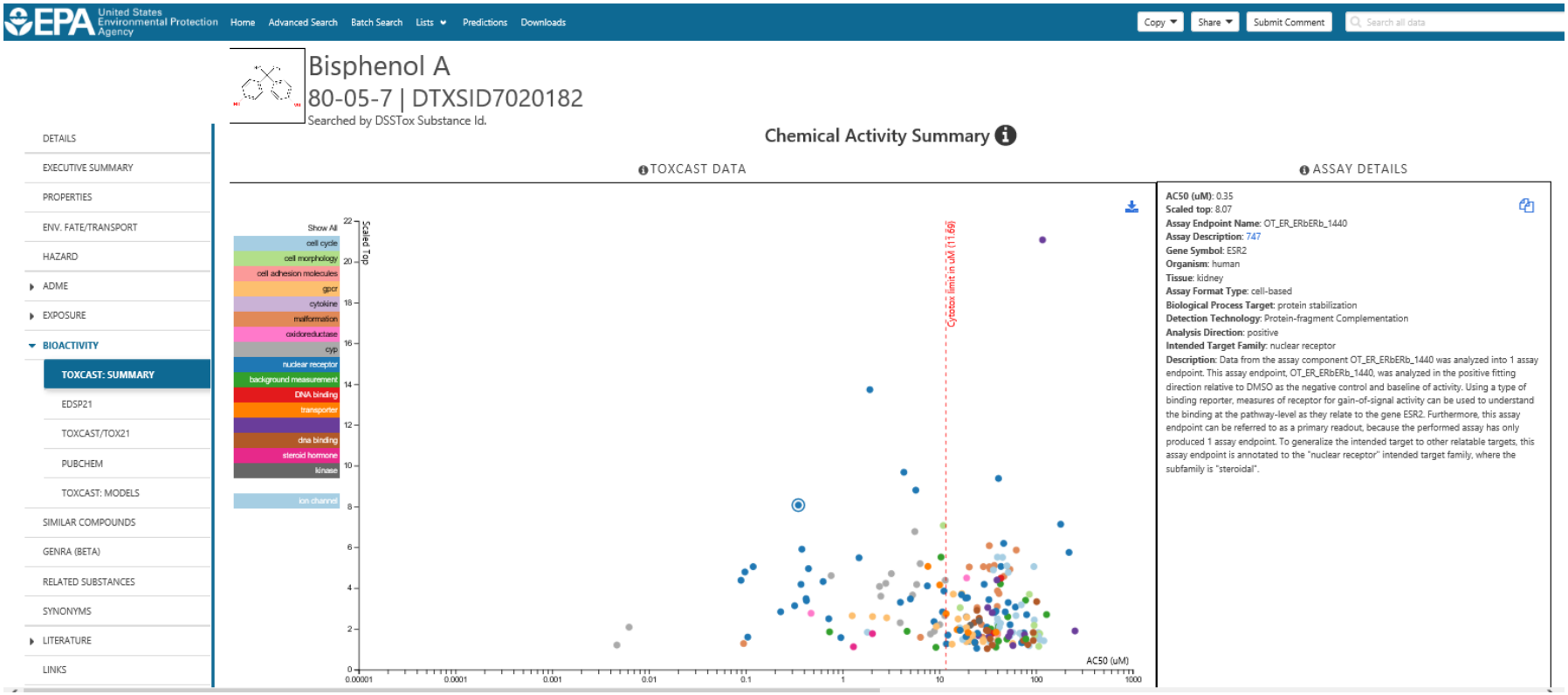


Sources of Exposure to Chemicals

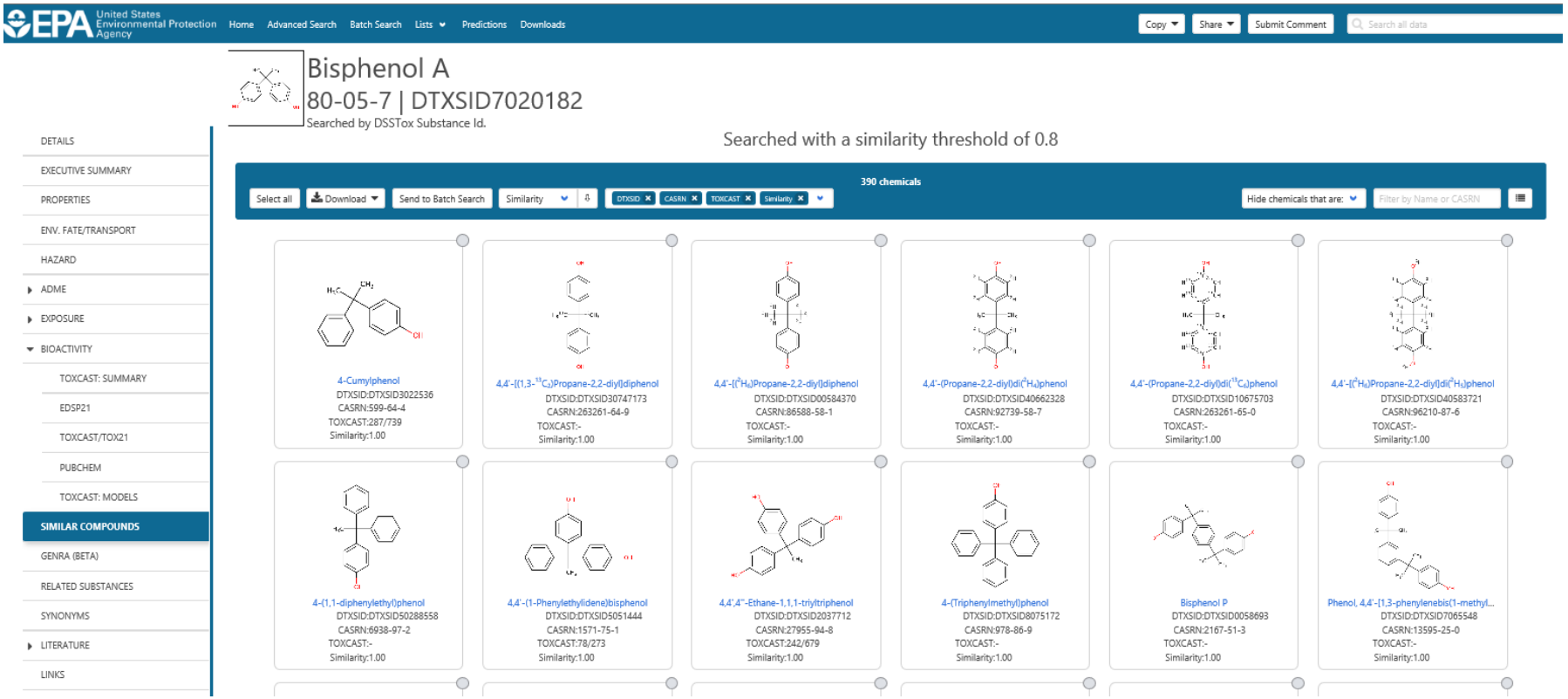


In Vitro Bioassay Screening

ToxCast Summary



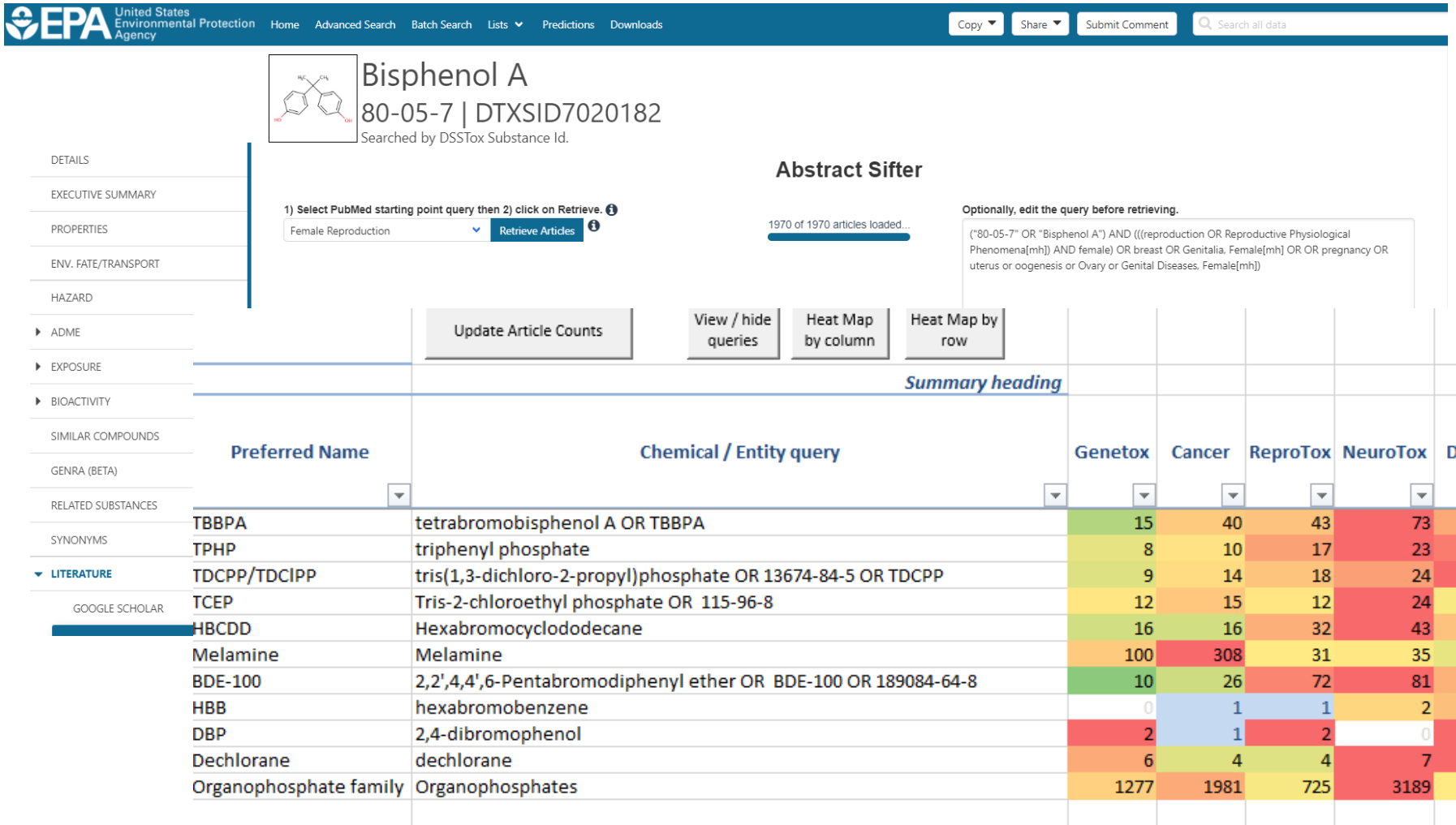
Similar Compounds



Literature

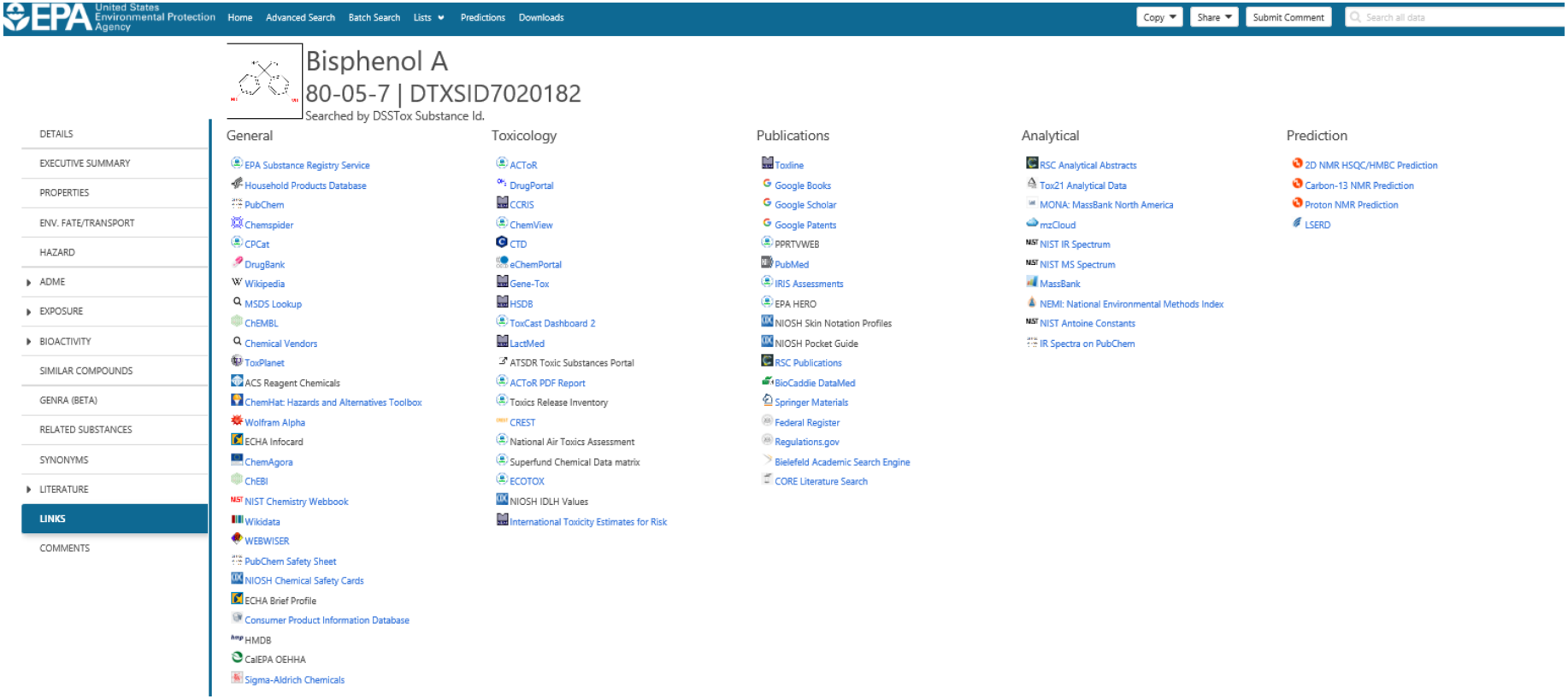
PMID	Year	Title	Authors	Journal	Rev
31471387	2019	Bisphenol A: A Concise Review of Literature and a Discussion of Health and Regulatory …	Wazir; Mokbel	In vivo (Athens, Greece)	✓
31470855	2019	Association of urinary concentrations of early pregnancy phthalate metabolites and bisp…	Chin; Jukic; Wilcox; Weinberg; Ferguson; Calafat; …	Environmental health : a global access science sou…	
31468552	2019	Association between peri-conceptional bisphenol A exposure in women and men and ti…	Yeum; Ju; Cox; Zhang; Stanford; Porucznik	Paediatric and perinatal epidemiology	
31455712	2019	Early Life Exposure in Mexico to ENvironmental Toxicants (ELEMENT) Project.	Perng; Tamayo-Ortiz; Tang; Sánchez; Cantoral; Me…	BMJ open	
31424210	2019	Phthalate and BPA Exposure in Women and Newborns through Personal Care Product …	Fisher; Arbuckle; MacPherson; Braun; Feeley; Gau…	Environmental science & technology	
31393043	2019	Differences between male and female prostates in terms of physiology, sensitivity to che…	Sanches; Carvalho; Maldarine; Biancardi; Santos; …	Cell biology international	✓
31374317	2019	Bisphenol A affects estradiol metabolism by targeting CYP1A1 and CYP19A1 in human …	Xu; Zhang; Ye; Li	Toxicology in vitro : an international journal publishe…	
31373935	2019	An Empirical Validation of the Within-subject Biospecimens Pooling Approach to Minimiz…	Vernet; Philippat; Agier; Calafat; Ye; Lyon-Caen; Ha…	Epidemiology (Cambridge, Mass.)	
31362658	2019	Neuro-toxic and reproductive effects of BPA.	Santoro; Chianese; Troisi; Richards; Nori; Fasano; …	Current neuropharmacology	
31362131	2019	Bisphenol A and bisphenol S exposures during pregnancy and gestational age - A longit…	Huang; Li; Xu; Zhao; Li; Zhou; Fang; Liao; Cai; Xia	Chemosphere	
31357276	2019	Development and validation of an LC-MS/MS method for the simultaneous determinatio…	Venisse; Cambien; Robin; Rouillon; Nadeau; Charle…	Talanta	

Literature

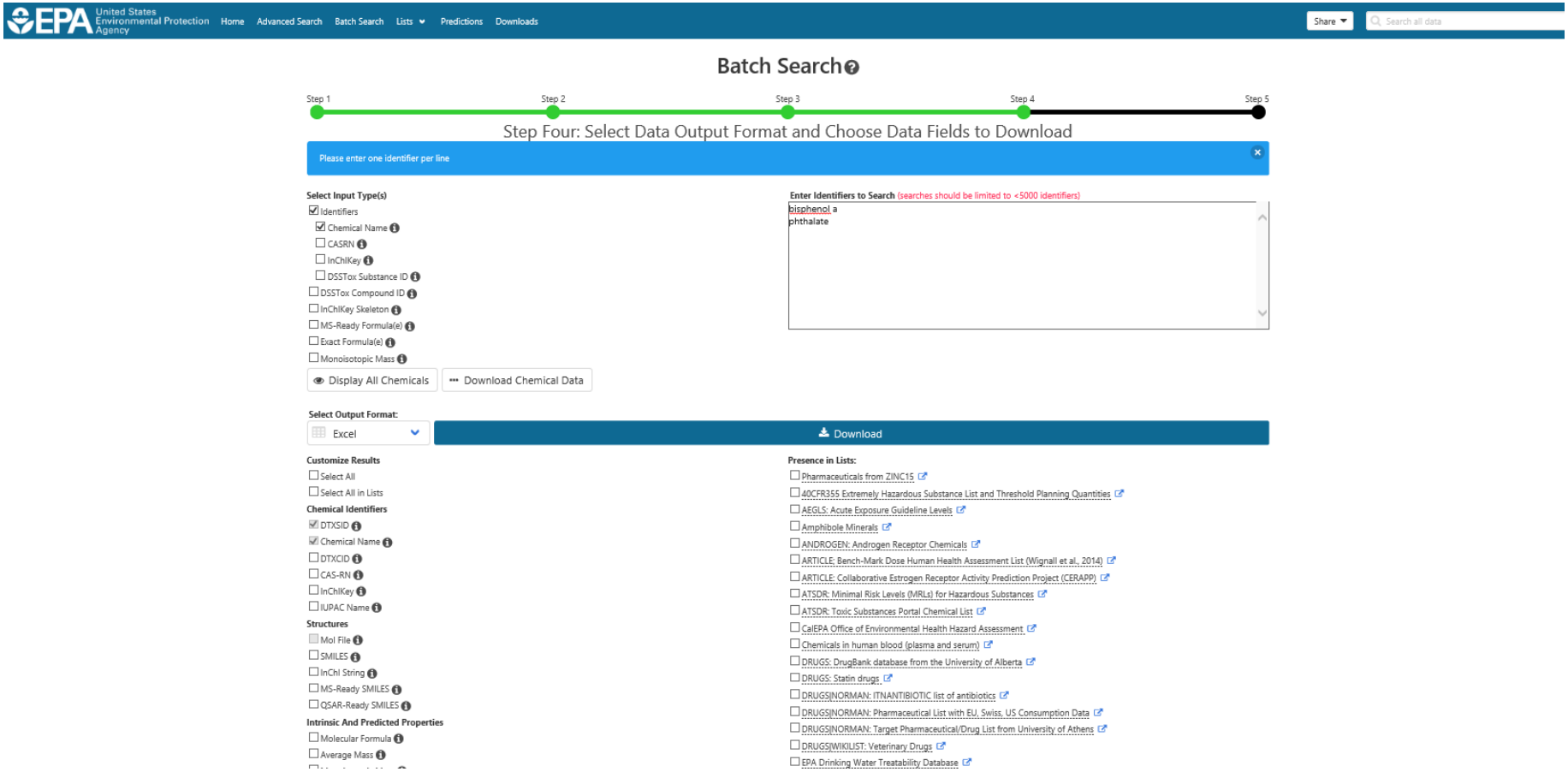


Preferred Name	Chemical / Entity query	Genetox	Cancer	ReproTox	NeuroTox	DevTox
TBBPA	tetrabromobisphenol A OR TBBPA	15	40	43	73	52
TPHP	triphenyl phosphate	8	10	17	23	21
TDCPP/TDCIPP	tris(1,3-dichloro-2-propyl)phosphate OR 13674-84-5 OR TDCPP	9	14	18	24	33
TCEP	Tris-2-chloroethyl phosphate OR 115-96-8	12	15	12	24	11
HBCDD	Hexabromocyclododecane	16	16	32	43	29
Melamine	Melamine	100	308	31	35	23
BDE-100	2,2',4,4',6-Pentabromodiphenyl ether OR BDE-100 OR 189084-64-8	10	26	72	81	57
HBB	hexabromobenzene	0	1	1	2	3
DBP	2,4-dibromophenol	2	1	2	0	2
Dechlorane	dechlorane	6	4	4	7	7
Organophosphate family	Organophosphates	1277	1981	725	3189	796

Links


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
BIOACTIVITY
SIMILAR COMPOUNDS
GENRA (BETA)
RELATED SUBSTANCES
SYNONYMS
LITERATURE
LINKS
COMMENTS
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
Wikidata
WEBWISER
PubChem Safety Sheet
NIOSH Chemical Safety Cards
ECHA Brief Profile
Consumer Product Information Database
HMDB
CalEPA OEHHA
Sigma-Aldrich Chemicals
Toxicology
ACToR
DrugPortal
CCRIS
ChemView
CTD
eChemPortal
Gene-Tox
HSDB
ToxCast Dashboard 2
LactMed
ATSDR Toxic Substances Portal
ACToR PDF Report
Toxics Release Inventory
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
Prediction
2D NMR HSQC/HMBC Prediction
Carbon-13 NMR Prediction
Proton NMR Prediction
LSERD

Searching for more than one Chemical: Batch Searching



Lists

Select List

Download | Columns | 10 | Search query | Copy page URL

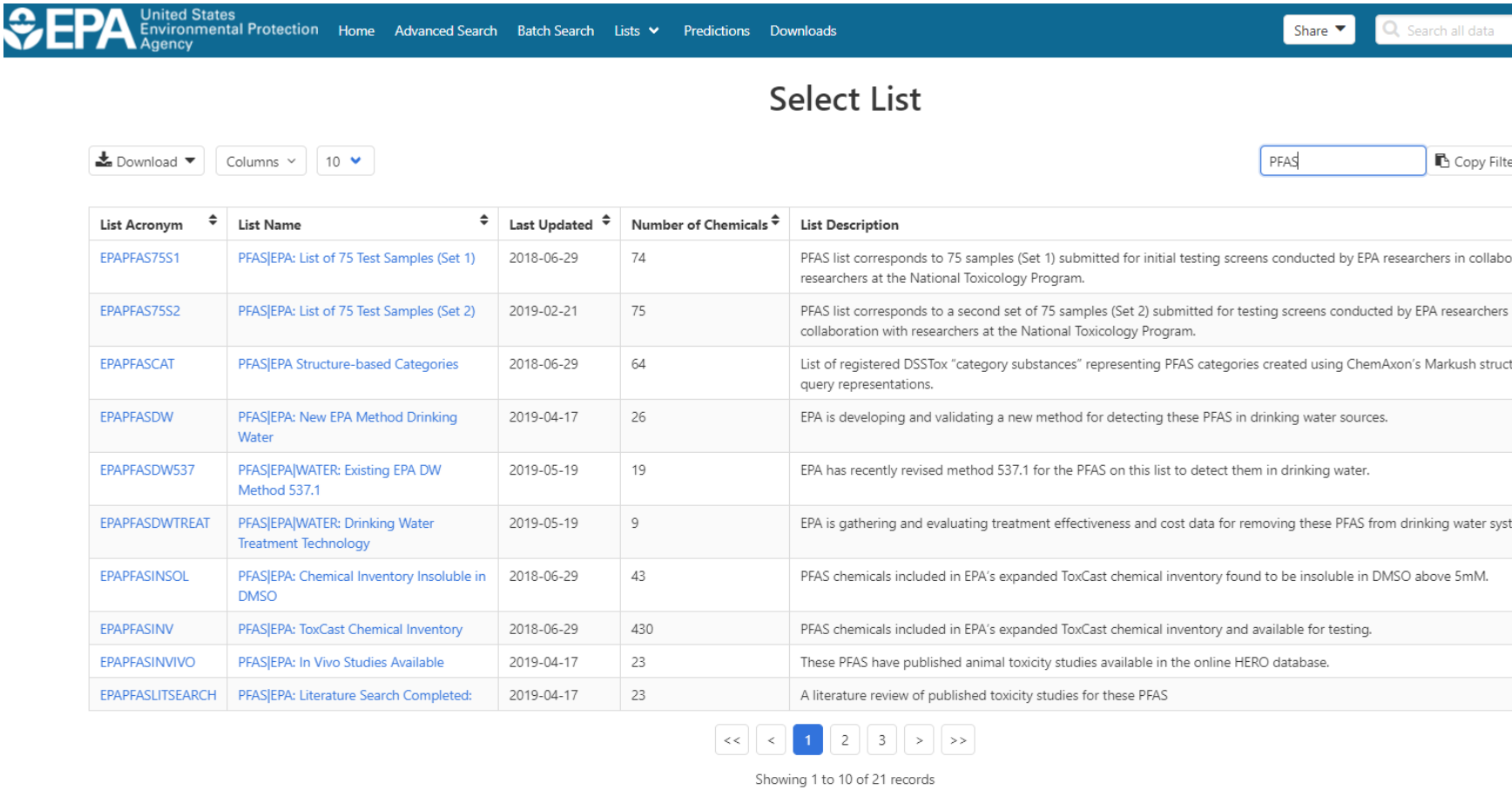
List Acronym	List Name	Last Updated	Number of Chemicals	List Description
40CFR355	40CFR355 Extremely Hazardous Substance List and Threshold Planning Quantities	2018-01-05	354	Extremely Hazardous Substance List and Threshold Planning Quantities; Emergency Planning and Release Notification Requirements; Final Rule. (52 FR 13378)
ACSREAG	LIST: ACS Reagent Chemicals	2017-04-14	405	The ACS Committee on Analytical Reagents sets purity specifications for almost 500 reagent chemicals and over 500 standard-grade reference materials.
AEGLVALUES	AEGLS: Acute Exposure Guideline Levels	2018-04-20	174	Acute exposure guideline levels (AEGLs) describe the human health effects from once-in-a-lifetime, or rare, exposure to airborne chemicals.
ALGALTOX	LIST: Algal Toxins	2018-05-04	54	A list of Algal Toxins of potential interest
AMINOACIDS	LIST: Amino Acids	2019-03-05	20	Amino acids are organic compounds containing amine (-NH2) and carboxyl (-COOH) functional groups, along with a side chain (R group) specific to each amino acid.
AMPHIBOLES	Amphibole Minerals	2019-03-26	4	Amphiboles are an important group of inosilicate minerals.
ANTIBIOTICS	LIST: Antibiotics	2019-06-01	170	List of antibiotics and related compounds
ARCHEMICALS	ANDROGEN: Androgen Receptor Chemicals	2018-11-16	110	The list of chemicals used to identify references with in vitro AR binding . From Kleinstreuer et al http://pubs.acs.org/doi/abs/10.1021/acs.chemrestox.6b00347
ATHENSSUS	WATER: Univ. Athens Surfactant and Suspect List	2017-07-14	60	ATHENSSUS is a compilation of suspects, predicted transformation products and surfactants screened in wastewater by University of Athens, as described in Gago-Ferrero et al 2015, DOI: 10.1021/acs.est.5b03454
ATSDRLST	ATSDR: Toxic Substances Portal Chemical List	2017-03-11	200	The Agency for Toxic Substances and Disease Registry (ATSDR)is a federal public health agency of the U.S. Department of Health and Human Services.

First << < 1 2 3 4 5 6 7 8 9 10 > >> Last

Showing 1 to 10 of 196 records

Lists

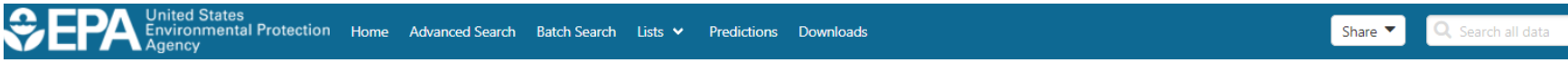
Select List



List Acronym	List Name	Last Updated	Number of Chemicals	List Description
EPAPFAS75S1	PFAS|EPA: List of 75 Test Samples (Set 1)	2018-06-29	74	PFAS list corresponds to 75 samples (Set 1) submitted for initial testing screens conducted by EPA researchers in collabo researchers at the National Toxicology Program.
EPAPFAS75S2	PFAS|EPA: List of 75 Test Samples (Set 2)	2019-02-21	75	PFAS list corresponds to a second set of 75 samples (Set 2) submitted for testing screens conducted by EPA researchers collaboration with researchers at the National Toxicology Program.
EPAPFASCAT	PFAS|EPA Structure-based Categories	2018-06-29	64	List of registered DSSTox "category substances" representing PFAS categories created using ChemAxon's Markush struct query representations.
EPAPFASDW	PFAS|EPA: New EPA Method Drinking Water	2019-04-17	26	EPA is developing and validating a new method for detecting these PFAS in drinking water sources.
EPAPFASDW537	PFAS|EPA|WATER: Existing EPA DW Method 537.1	2019-05-19	19	EPA has recently revised method 537.1 for the PFAS on this list to detect them in drinking water.
EPAPFASDWTREAT	PFAS|EPA|WATER: Drinking Water Treatment Technology	2019-05-19	9	EPA is gathering and evaluating treatment effectiveness and cost data for removing these PFAS from drinking water syst
EPAPFASINSOL	PFAS|EPA: Chemical Inventory Insoluble in DMSO	2018-06-29	43	PFAS chemicals included in EPA's expanded ToxCast chemical inventory found to be insoluble in DMSO above 5mM.
EPAPFASINV	PFAS|EPA: ToxCast Chemical Inventory	2018-06-29	430	PFAS chemicals included in EPA's expanded ToxCast chemical inventory and available for testing.
EPAPFASINVIVO	PFAS|EPA: In Vivo Studies Available	2019-04-17	23	These PFAS have published animal toxicity studies available in the online HERO database.
EPAPFASLITSEARCH	PFAS|EPA: Literature Search Completed:	2019-04-17	23	A literature review of published toxicity studies for these PFAS

Lists

Select List



Select List

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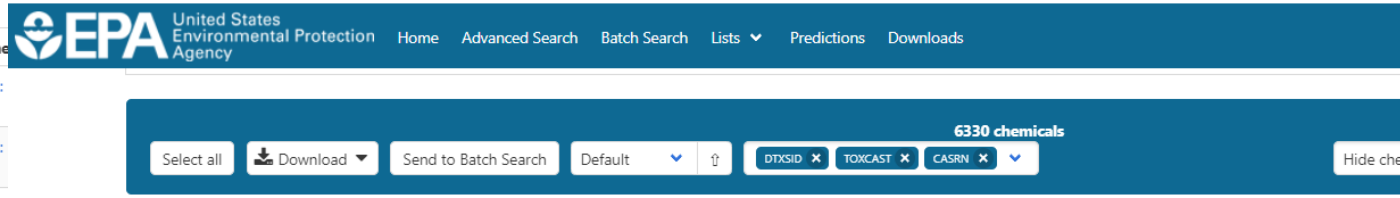
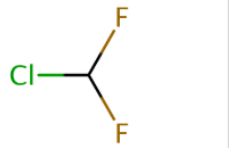
List Acronym	List Name
EPAPFAS75S1	PFAS|EPA:
EPAPFAS75S2	PFAS|EPA:
EPAPFASCAT	PFAS|EPA S
EPAPFASDW	PFAS|EPA: Water
EPAPFASDW537	PFAS|EPA| Method 53
EPAPFASDWTREAT	PFAS|EPA| Treatment
EPAPFASINSOL	PFAS|EPA: DMSO
EPAPFASINV	PFAS|EPA:
EPAPFASINVIVO	PFAS|EPA:
EPAPFASLITSEARCH	PFAS|EPA:

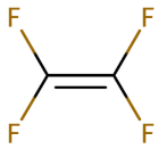


6330 chemicals

Select all | Download | Send to Batch Search | Default | DTXSID | TOXCAST | CASRN | Hide che



Chlorodifluoromethane
DTXSID:DTXSID6020301
TOXCAST:-
CASRN:75-45-6



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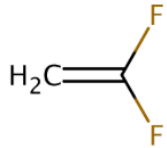

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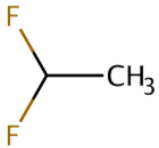
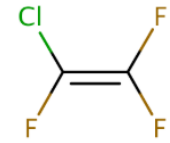
CASRN:75-38-7

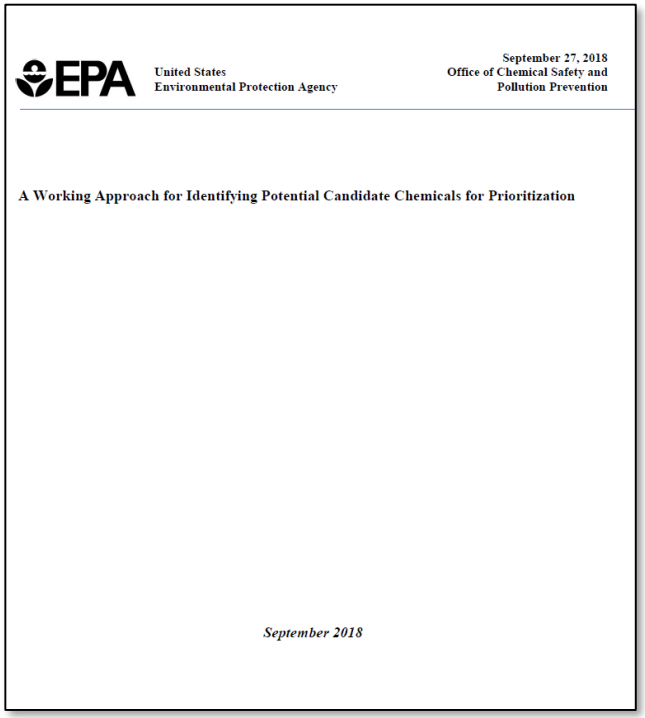




Impact

- **Challenge:** Need to identify a subset of both data rich and data poor compounds as possible candidates for prioritization under Toxic Substances Control Act (TSCA).
- **Solution:** CompTox Chemicals Dashboard integrates chemical data including human and ecological hazard, exposure and chemical properties that can be used to inform chemical screening and assessment.
- **Example:** TSCA's Working Approach for Identifying Potential Candidate Chemicals for Prioritization proposed tiered decision workflows for scientific domains of interest as part of a longer-term risk-based approach for managing the larger TSCA chemical landscape.

Example: TSCA's Working Approach for Identifying Potential Candidate Chemicals for Prioritization


EPA United States Environmental Protection Agency

September 27, 2018
Office of Chemical Safety and Pollution Prevention

A Working Approach for Identifying Potential Candidate Chemicals for Prioritization

September 2018

Impact: Evaluating chemicals for health effects in California

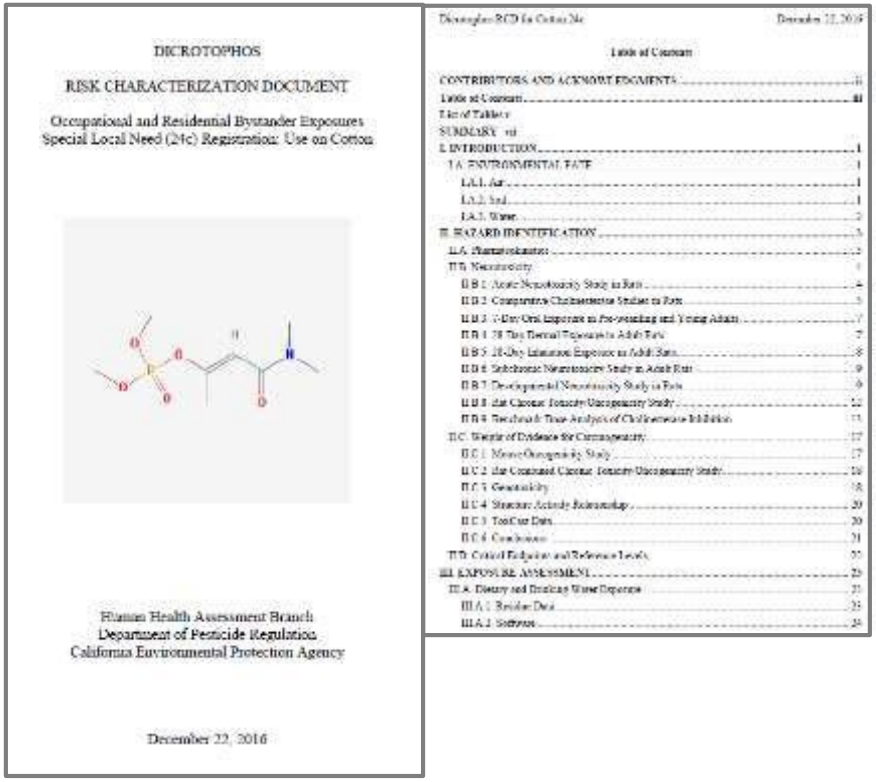
Challenge: Need to make informed decisions about the potential health effects of chemicals, and determine safer and more sustainable uses of chemicals found in products that consumers buy and use.

Solution: ORD researchers provided CalEPA staff training on the use and interpretation of chemical testing data in the CompTox Chemicals Dashboard.

CalEPA uses ToxCast data to:

- Provide insight into how chemicals cause toxicity
- Perform various state efforts using the lifecycle analytic and exposure modeling and monitoring

Example: CalEPA Pesticide Assessments


DICROTOPHOS

RISK CHARACTERIZATION DOCUMENT

Occupational and Residential Bystander Exposures
Special Local Need (24c) Registration: Use on Cotton

Human Health Assessment Branch
Department of Pesticide Regulation
California Environmental Protection Agency

December 22, 2016

Table of Contents

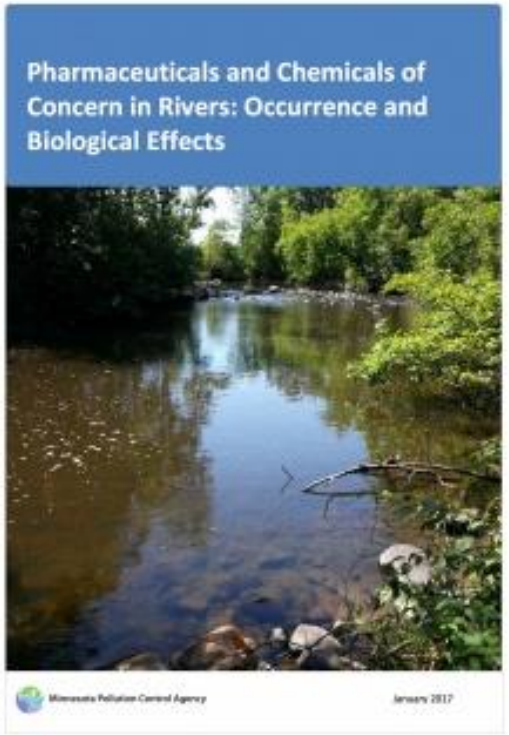
- ToxCast data used for weight of evidence decisions regarding health effects for pesticides

Potential Impact: Evaluating risk of aquatic contaminants in Minnesota

Challenge: Characterizing potential effects for a wide variety of contaminants which there exists limited information.

Solution: The Minnesota Pollution Control Agency (MPCA) used a suite of EPA tools, including those available under the CompTox Chemicals Dashboard, to prioritize chemicals based on toxicity effects and hazard characterization.

- Estimation Programs Interface (EPI) Suite
- ECOTOX
- Web-ICE



Using these tools, MPCA develops toxicity profiles to:

- Screen contaminants that have been detected in the state
- Monitor chemicals and prevent pollution
- Communicate the potential hazards associated with individual contaminants

Example: MPCA used tools available on the CompTox Chemicals Dashboard to identify triclocarban, an antibacterial agent commonly in soaps and lotions, as a high priority contaminant for monitoring in systems with effluent input.

Conclusion

- EPA's CompTox Chemicals Dashboard provides access to data for ~875,000 chemicals
- Dashboard is an integration hub for multiple "modules" and tools to support multiple environmental applications
- Data releases twice a year (at present) and supported with ongoing manual curation efforts
- Updates released in both March and August 2019
  - New bioassay data in the InvitroDBv3.1 release
  - New toxicity data added - ~800,000 toxicity data points
  - Focused data efforts for PFAS chemical lists and properties

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