EPA United States Environmental Protection Agency

EPA Tools and Resources Webinar CompTox Chemicals Dashboard:

Data and Tools to Support Chemical and Environmental Risk Assessment

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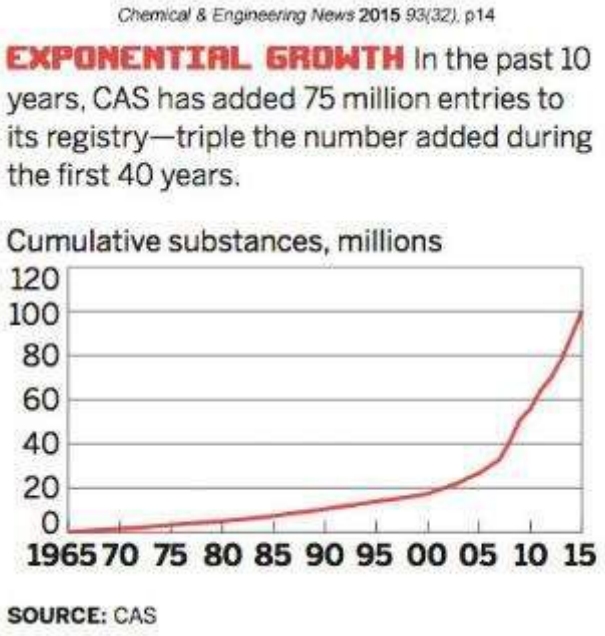
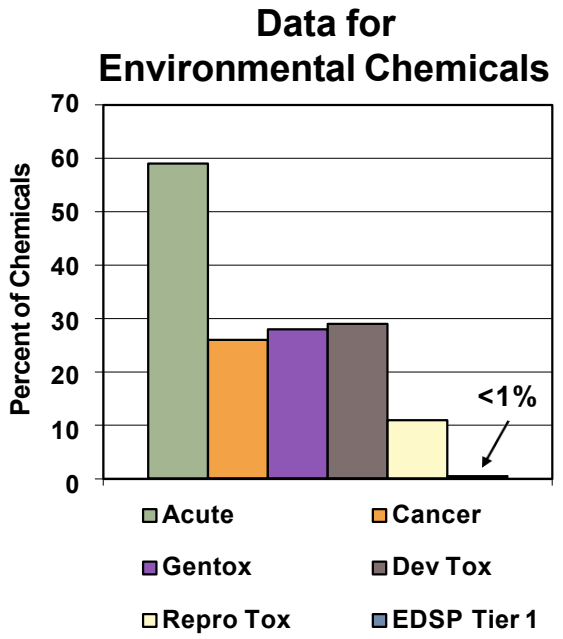
The views expressed in this presentation are those of the author and do not necessarily reflect the views or policies of the US EPA

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**



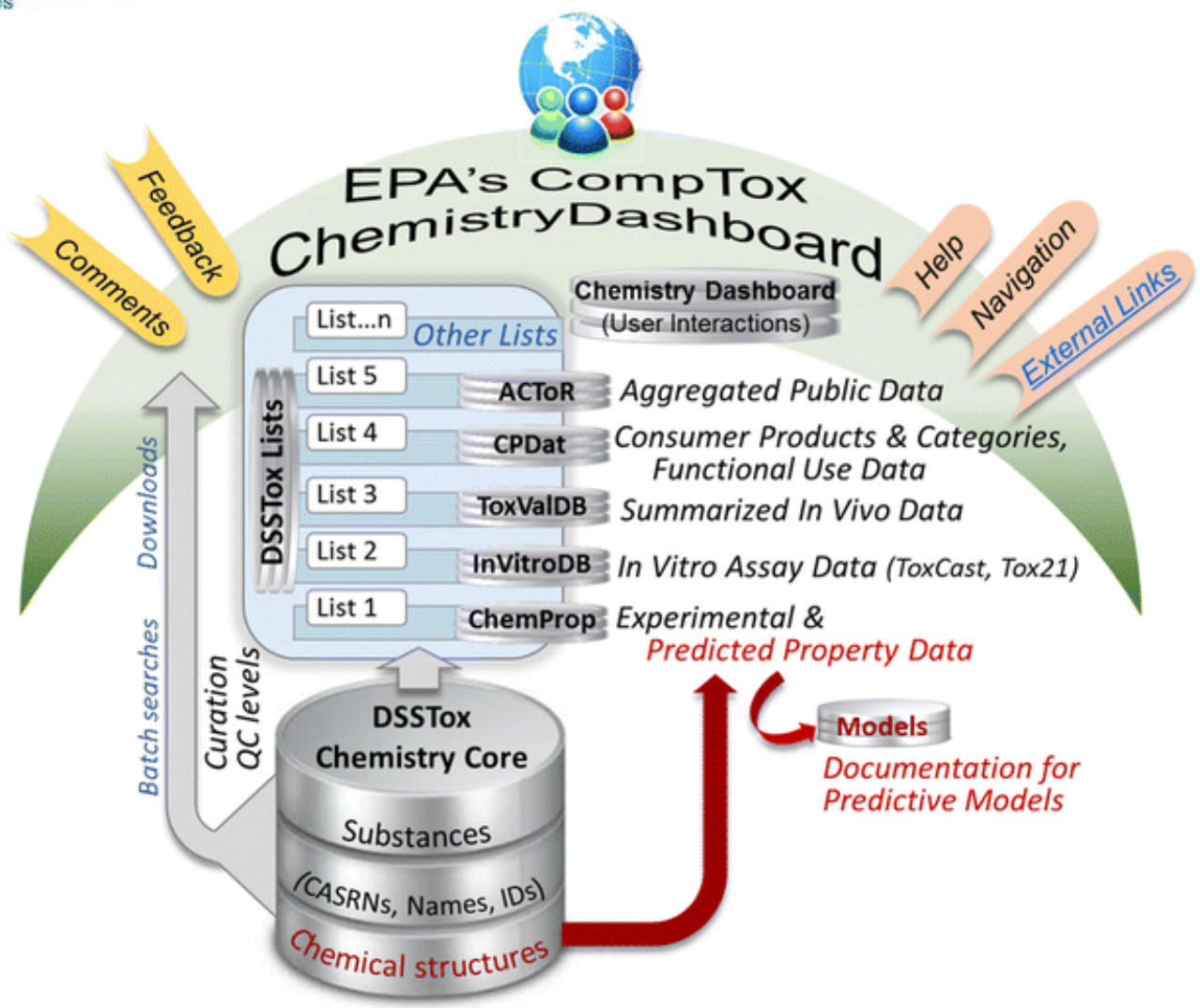


Modified from Judson *et al.*, EHP 2010

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**

Approach



Williams et al. J of Cheminformatics **9**: 61 (2017)
https://jcheminf.biomedcentral.com/articles/10.1186/s13321-017-0247-6

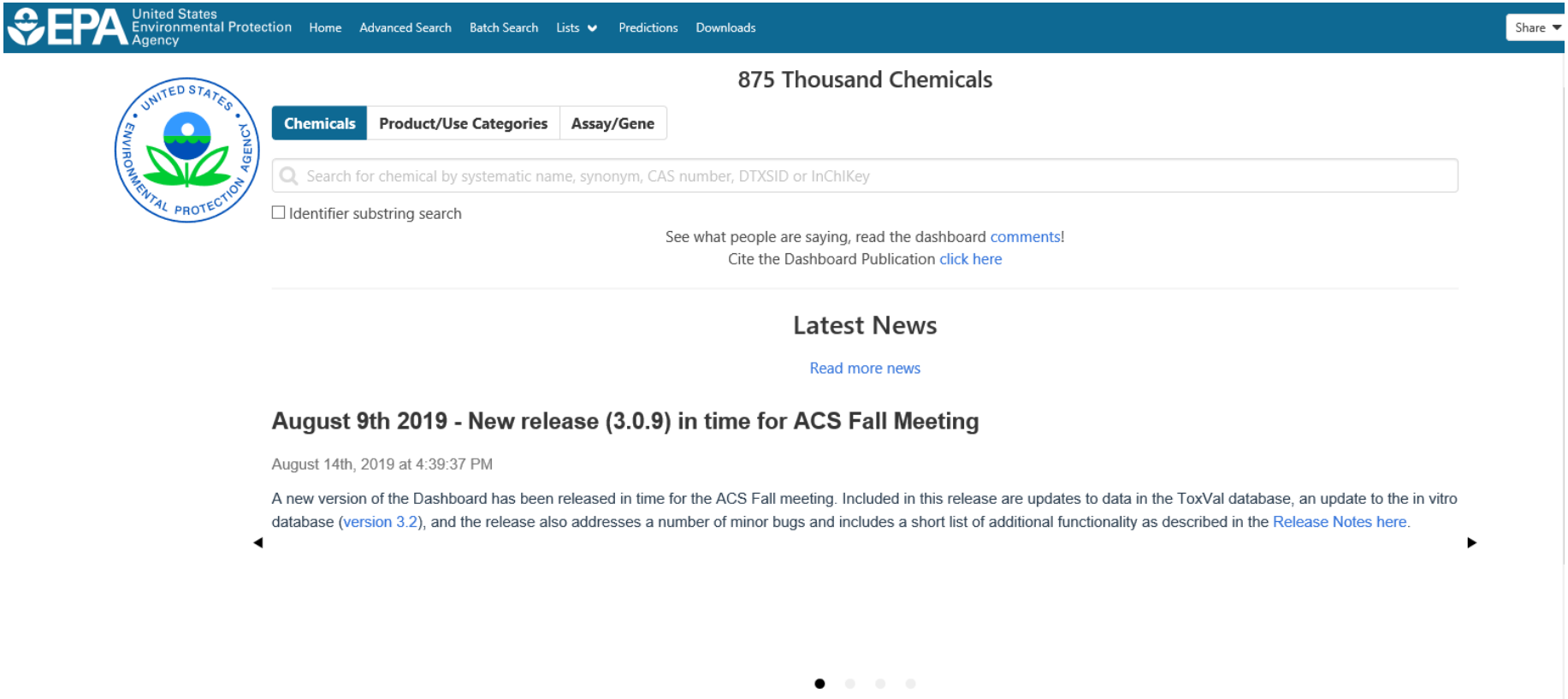
EPA's CompTox Chemicals Dashboard

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

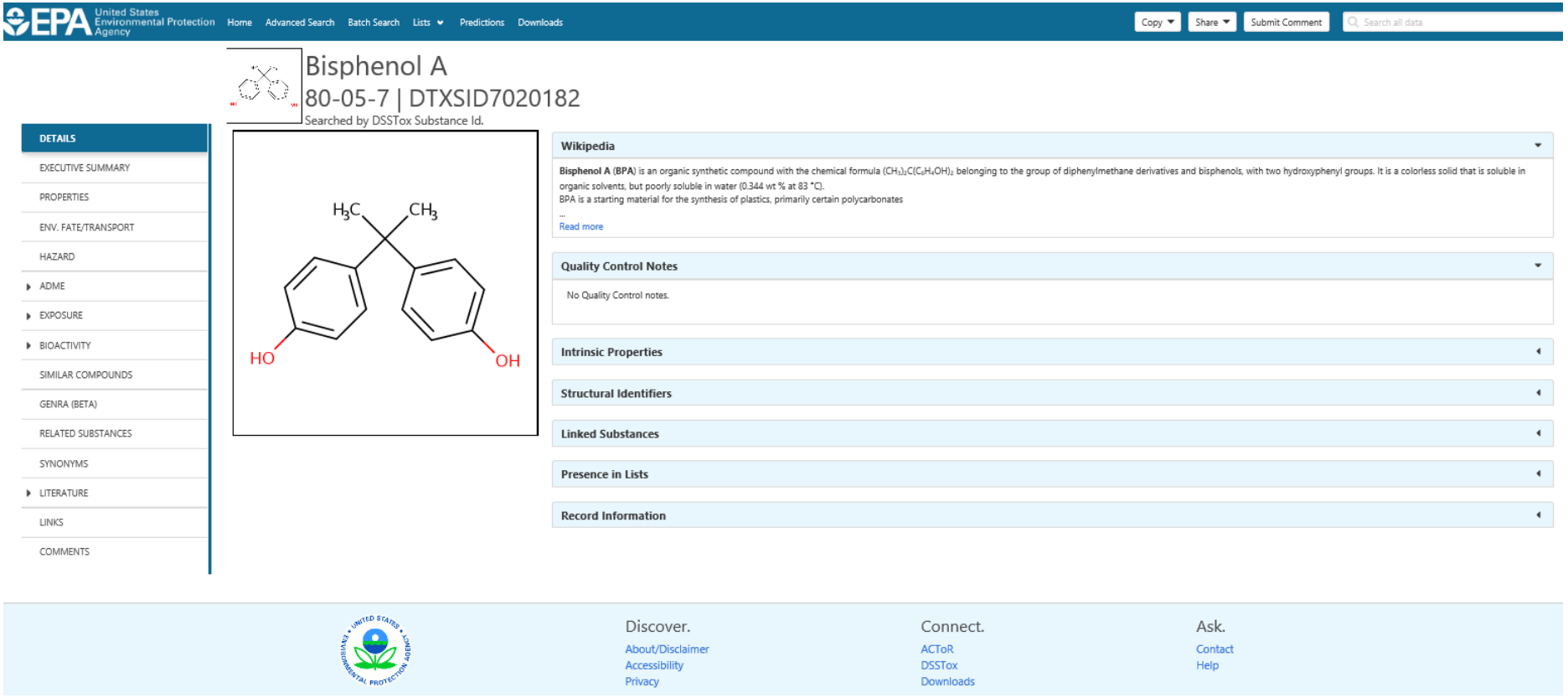
https://www.epa.gov/chemical-research/comptox-chemicals-dashboard

EPA CompTox Chemicals Dashboard

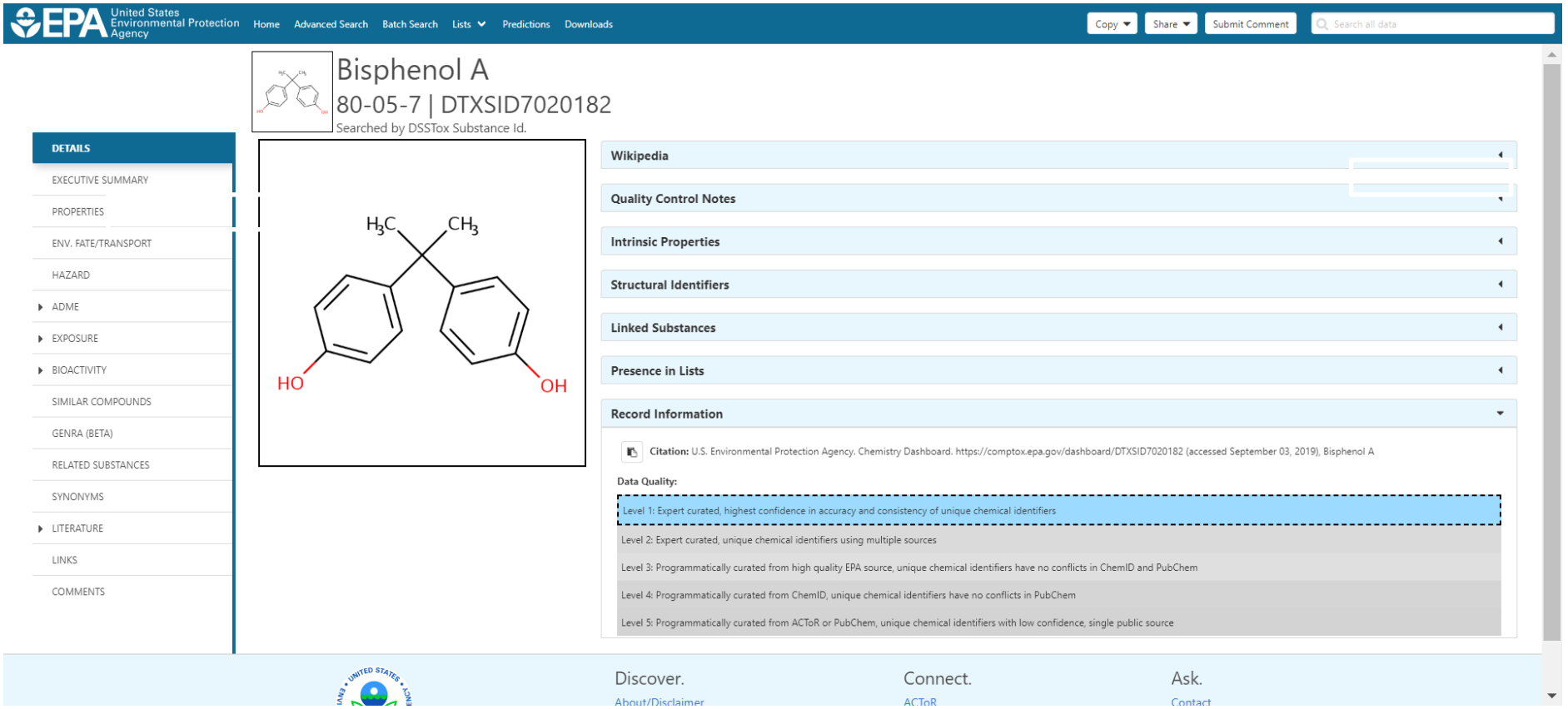


https://comptox.epa.gov/dashboard

Detailed Chemical Pages

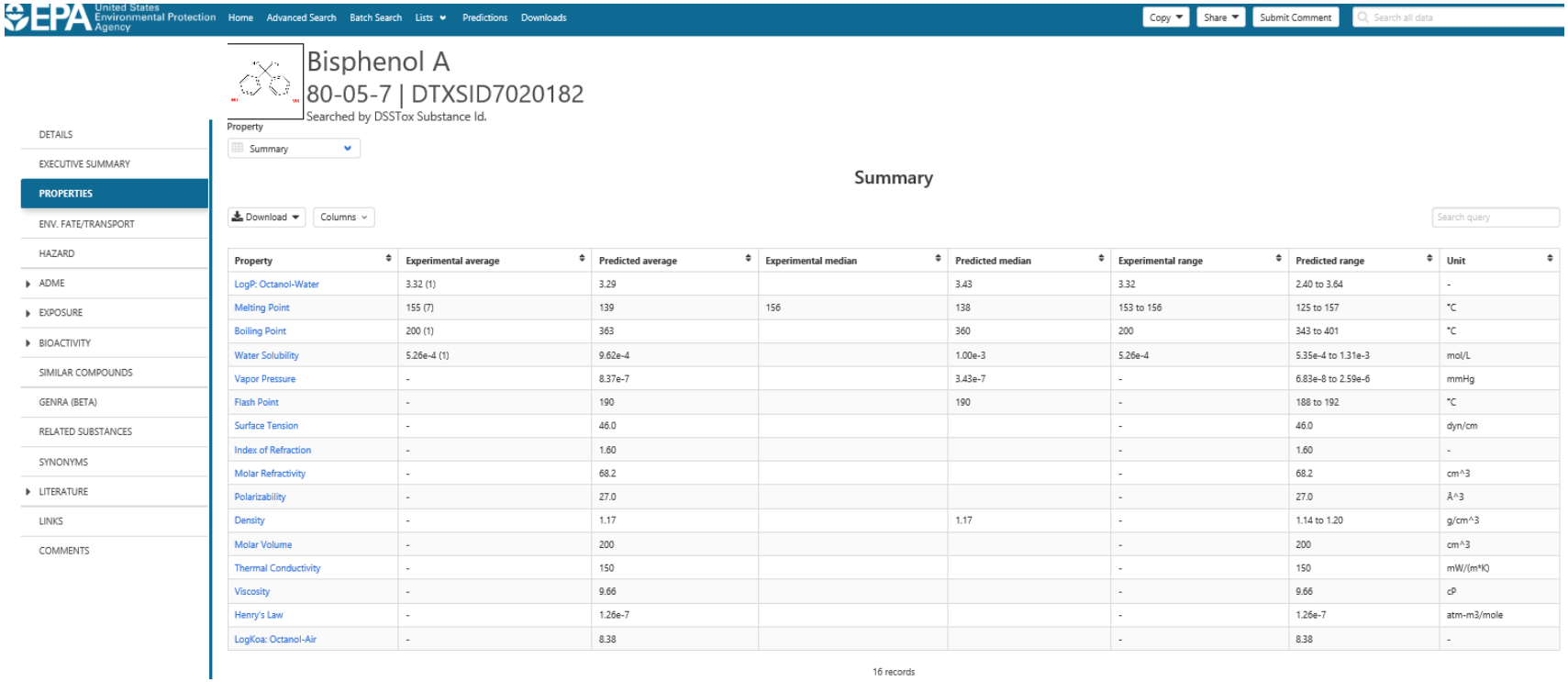


Data Quality



Grulke et al. Computational Toxicology 12 (2019) 100096

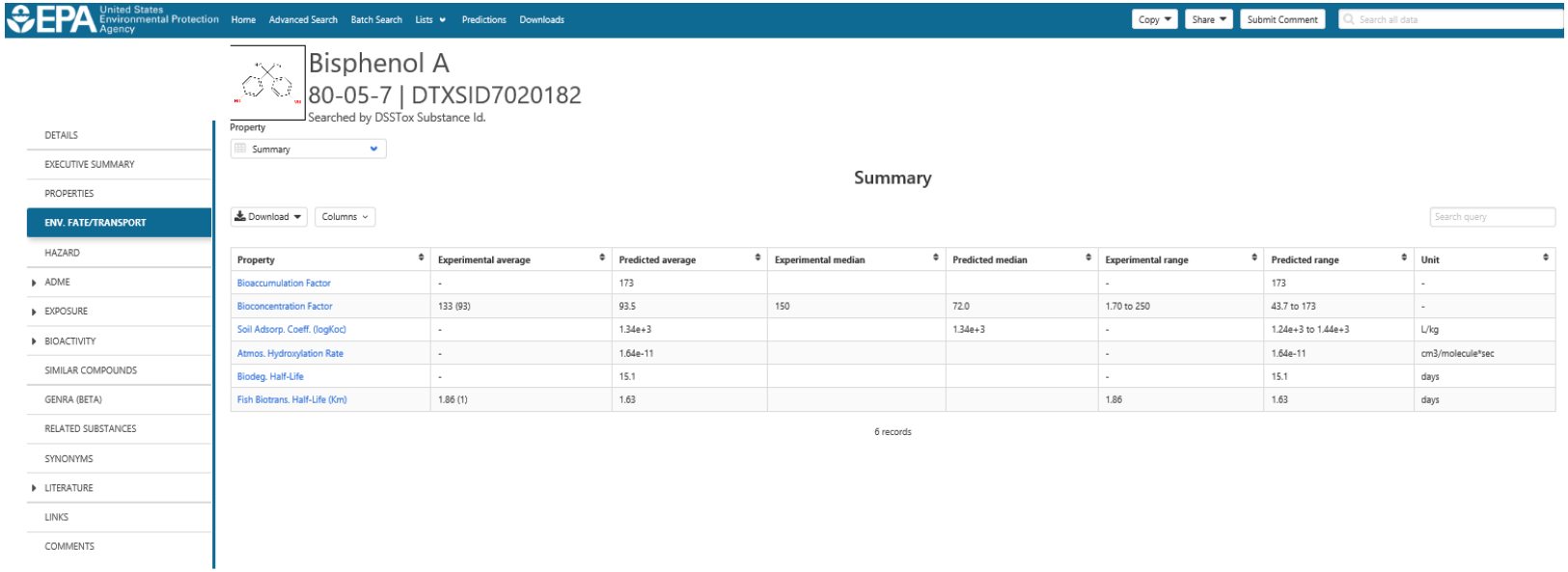
Properties



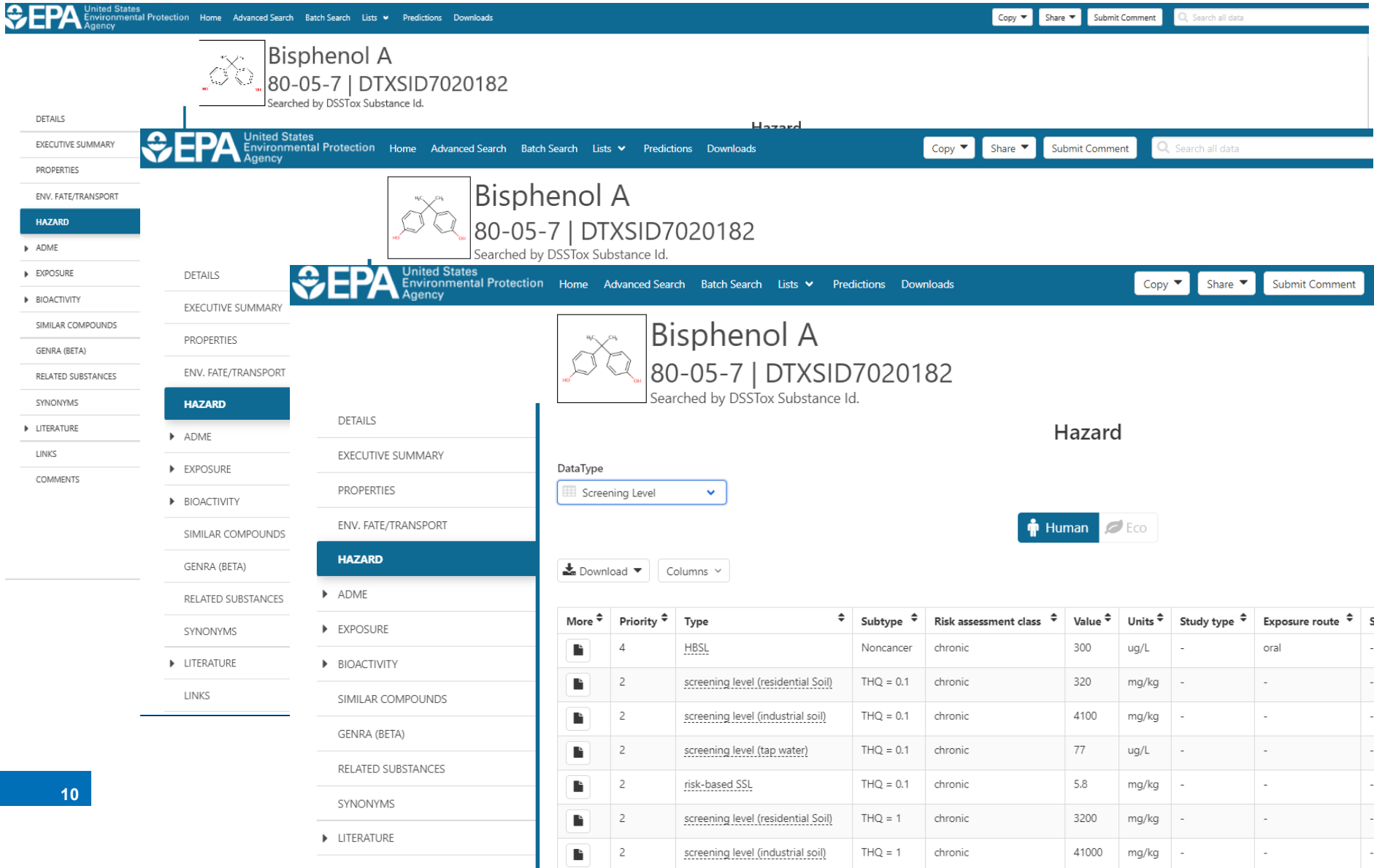
Property	Experimental average	Predicted average	Experimental median	Predicted median	Experimental range	Predicted range	Unit
LogP: Octanol-Water	3.32 (1)	3.29		3.43	3.32	2.40 to 3.64	-
Melting Point	155 (7)	139	156	138	153 to 156	125 to 157	°C
Boiling Point	200 (1)	363		360	200	343 to 401	°C
Water Solubility	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

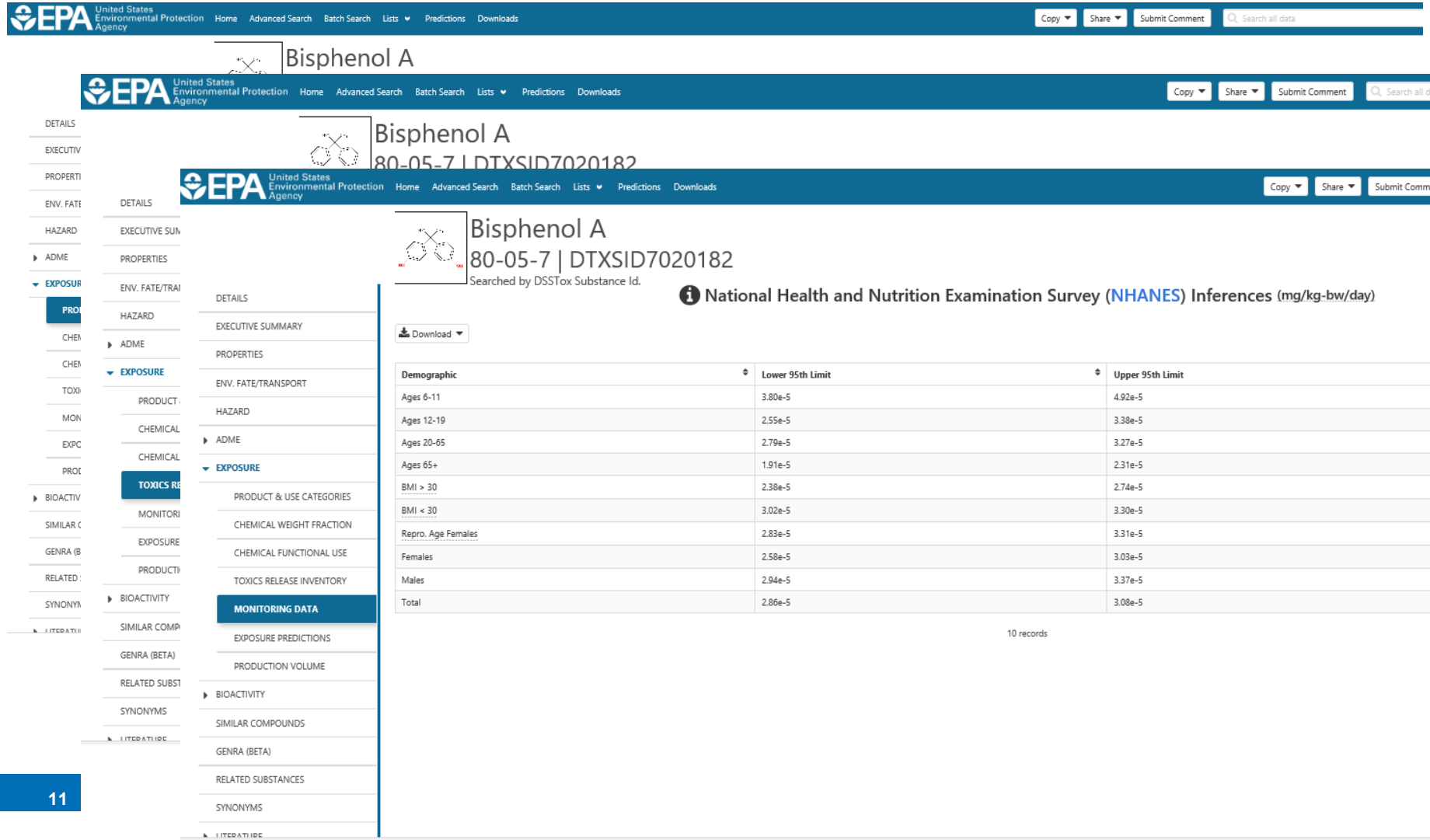
Environmental Fate and Transport



Chemical Hazard Data

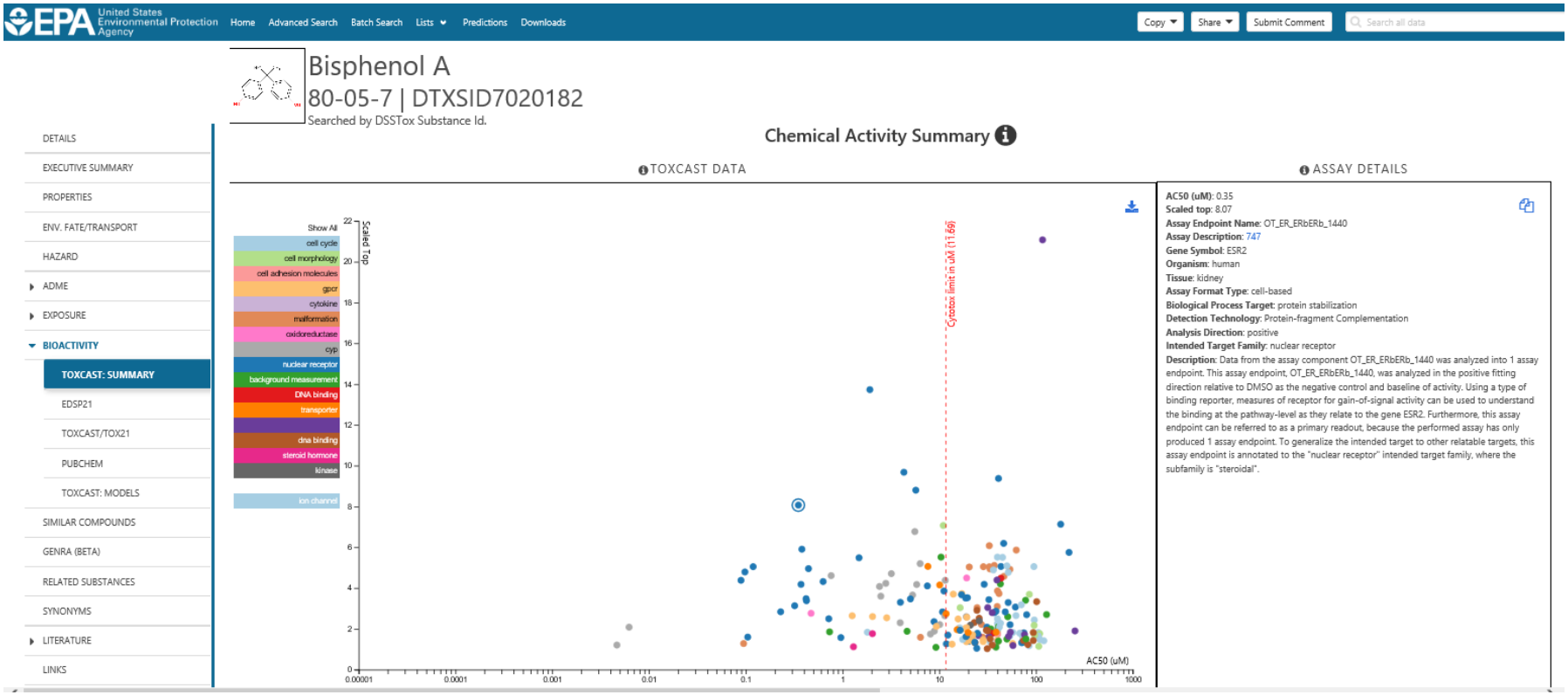


Sources of Exposure to Chemicals

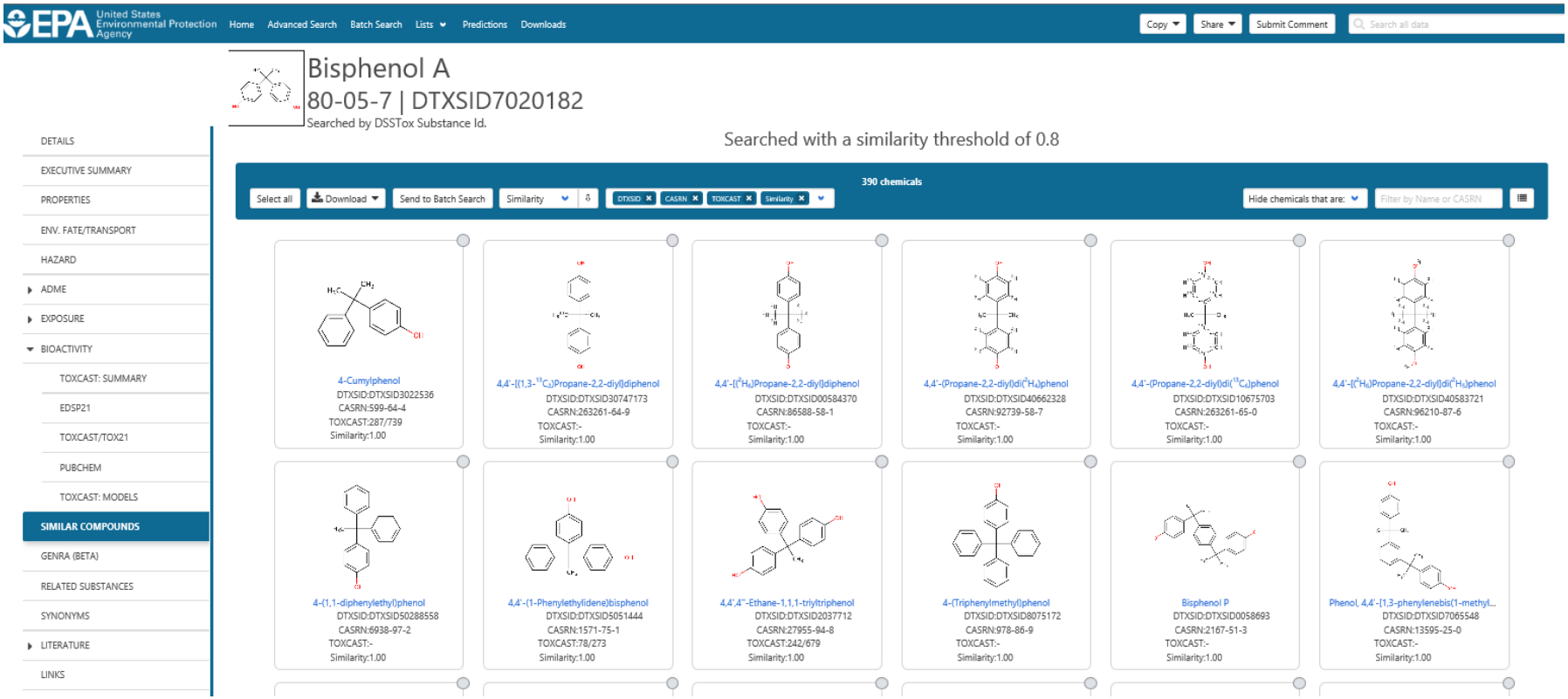


In Vitro Bioassay Screening

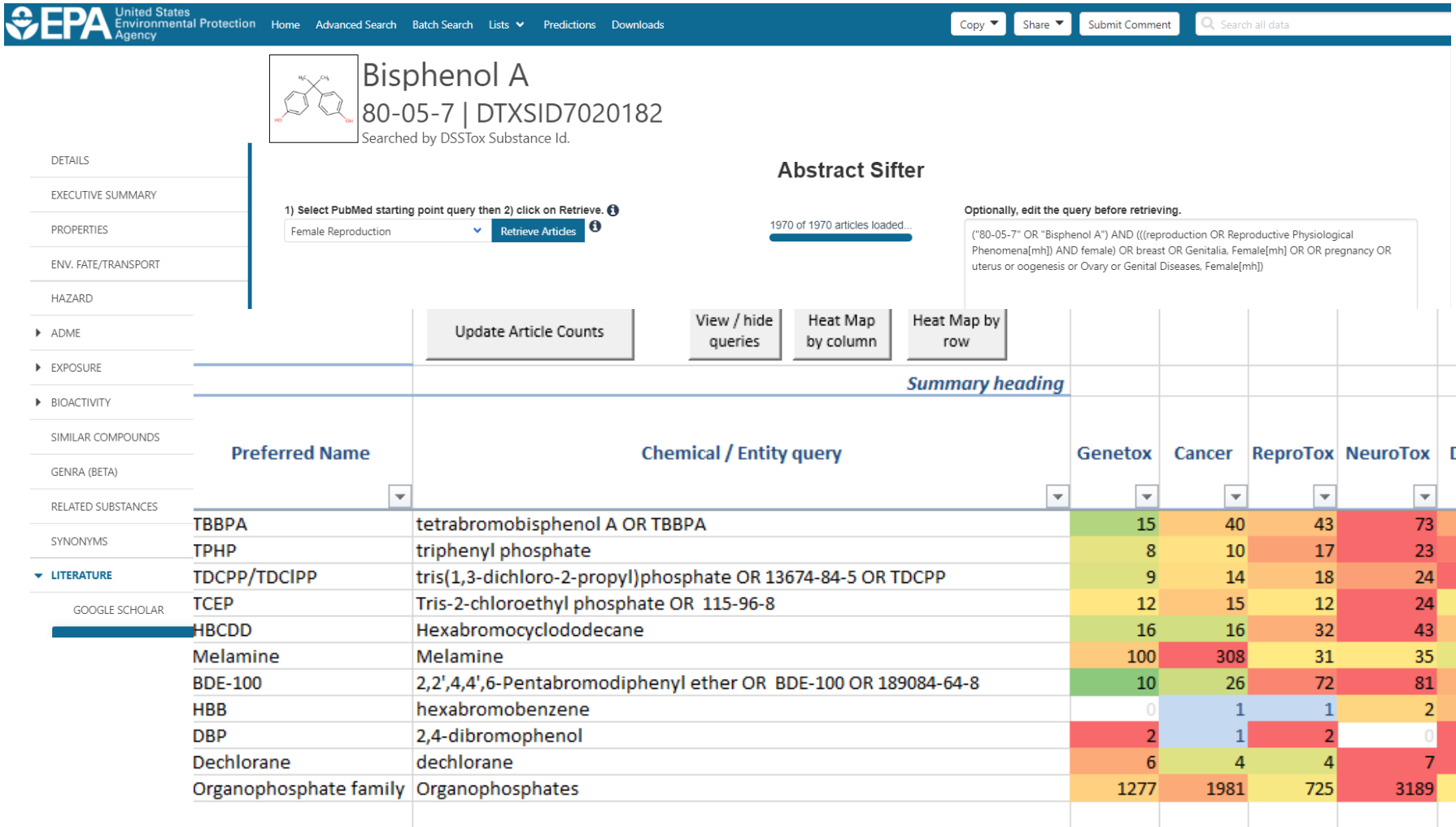
ToxCast Summary



Similar Compounds

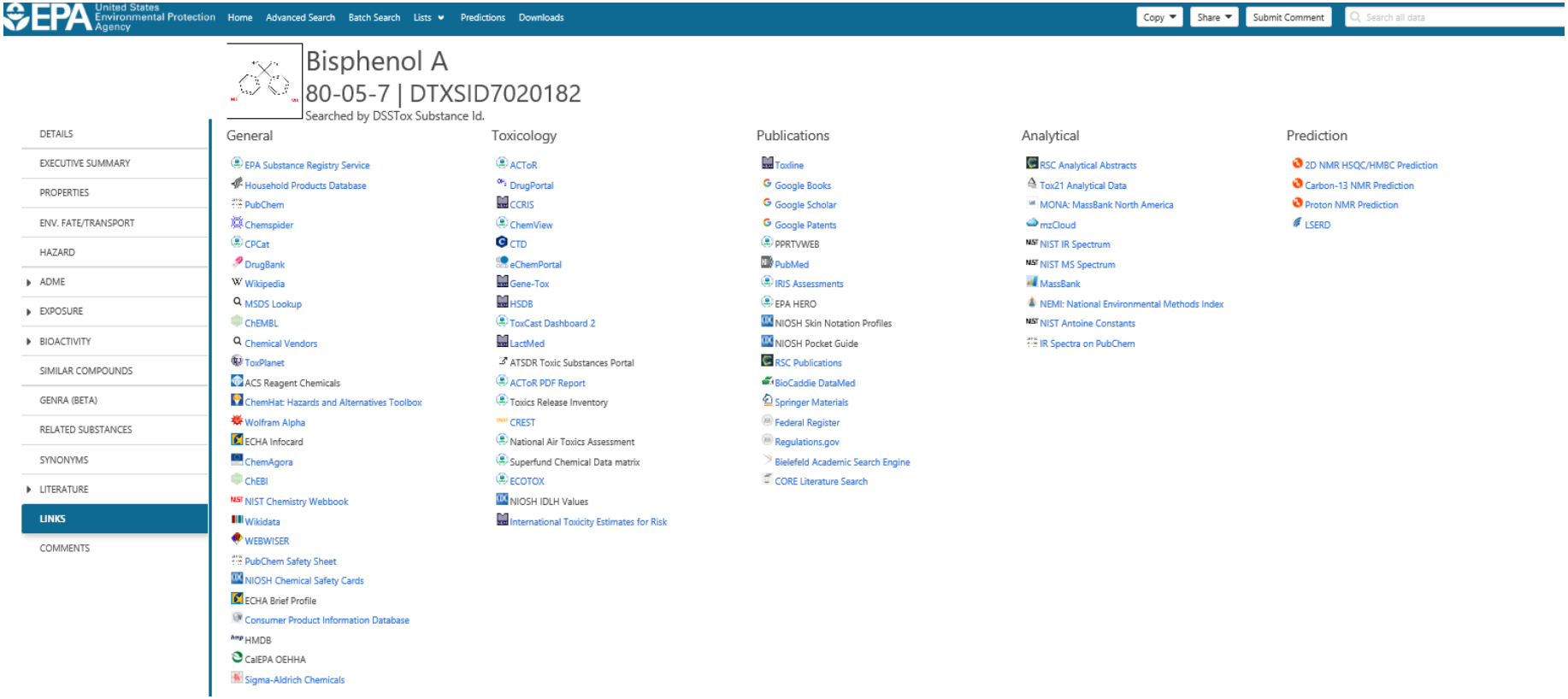


Literature



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


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
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
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International Toxicity Estimates for Risk
Publications
Toxline
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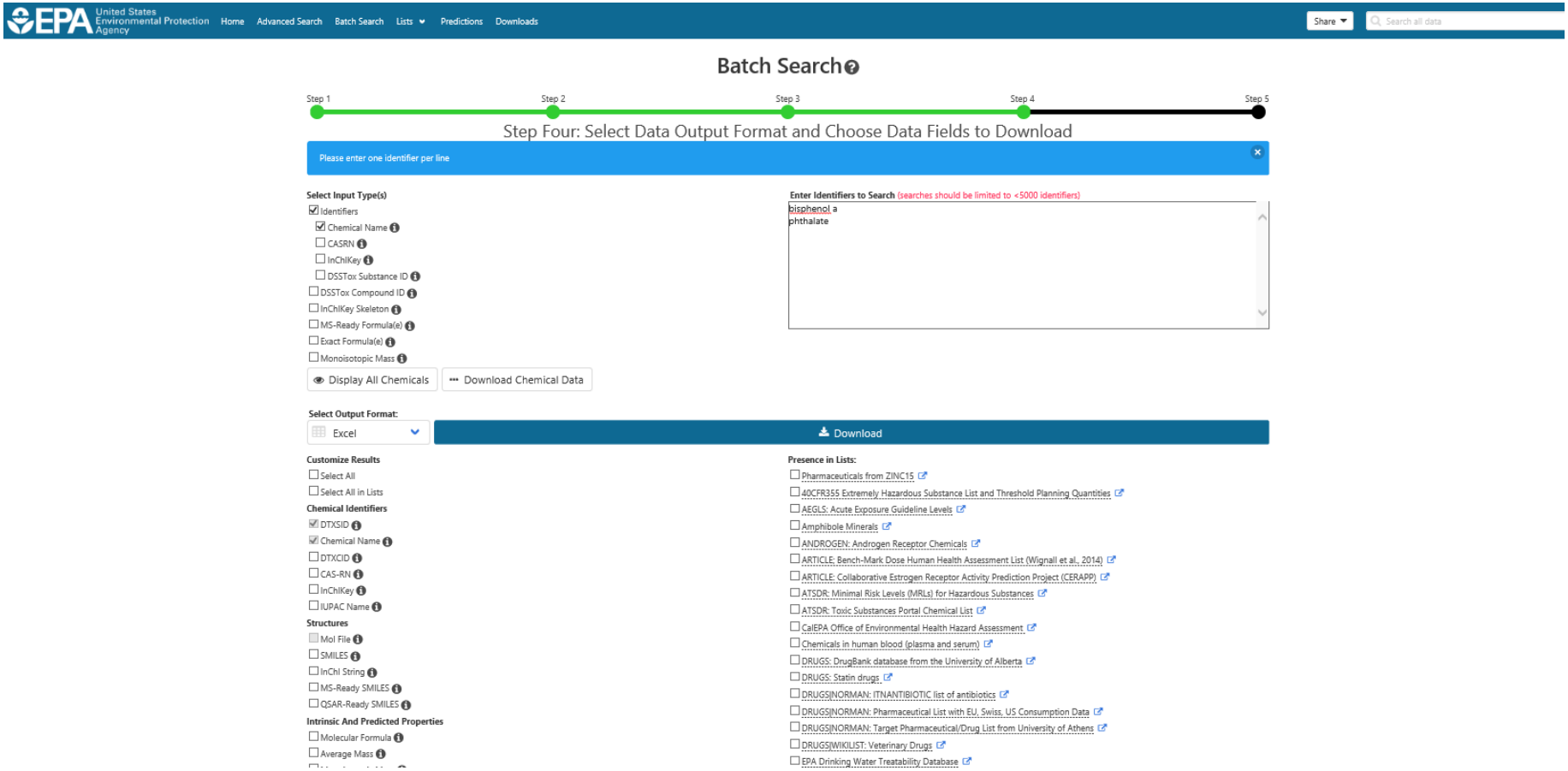
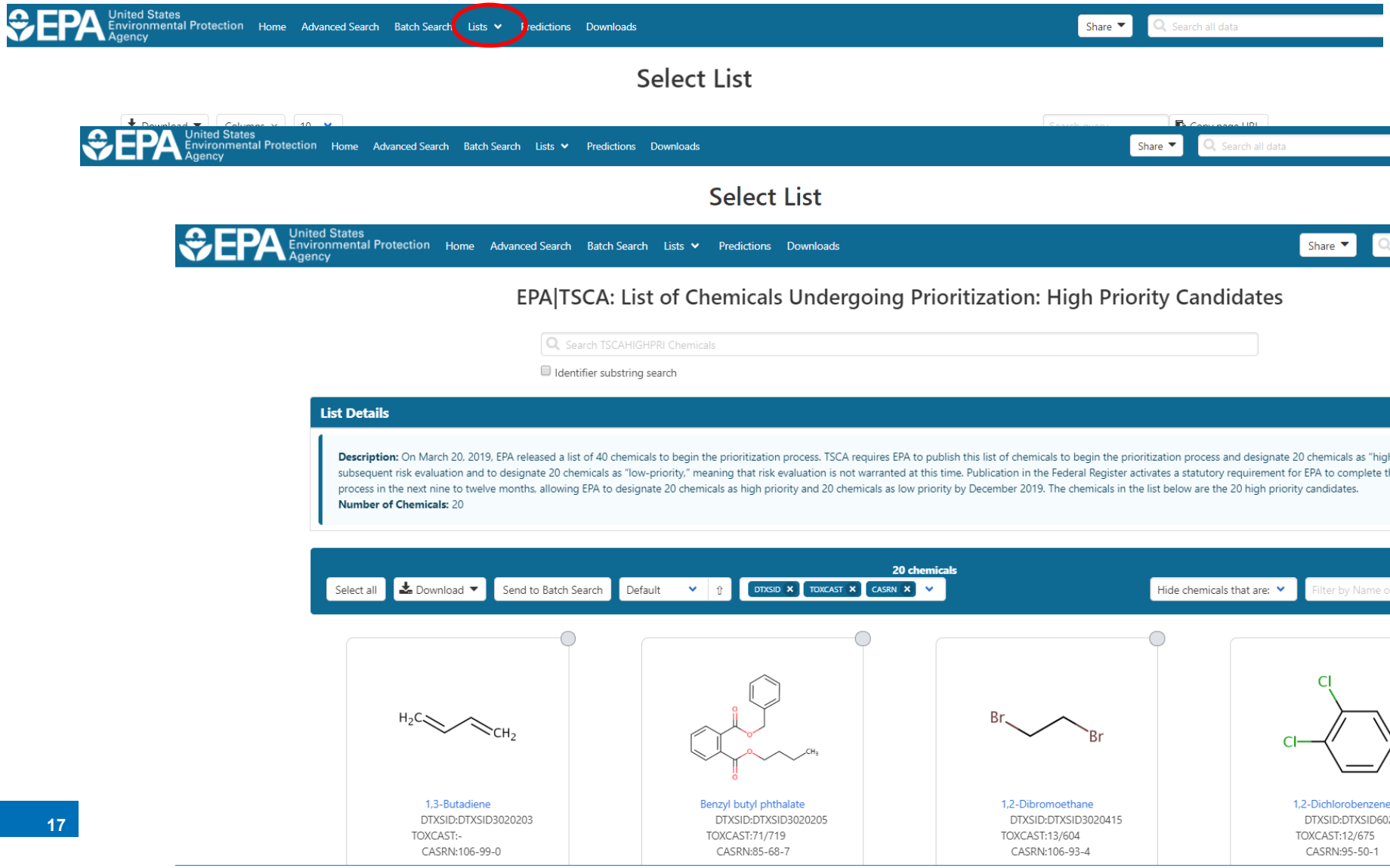
Google Scholar
Google Patents
PPRTVWEB
PubMed
IRIS Assessments
EPA HERO
NIOSH Skin Notation Profiles
NIOSH Pocket Guide
RSC Publications
BioCaddie DataMed
Springer Materials
Federal Register
Regulations.gov
Bielefeld Academic Search Engine
CORE Literature Search
Analytical
RSC Analytical Abstracts
Tox21 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

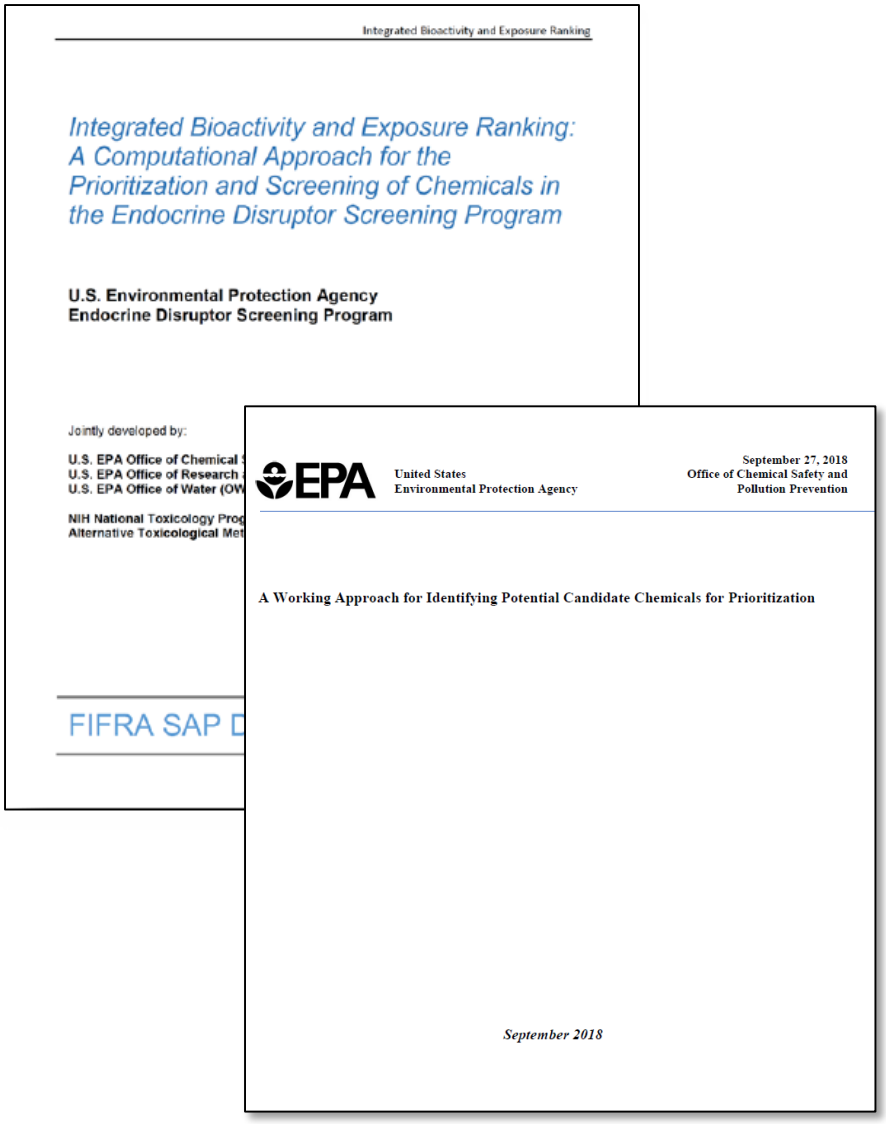


Lists


United States Environmental Protection Agency
Home
Advanced Search
Batch Search
Lists
Predictions
Downloads
Share
Search all data
Select List
Select List
EPA|TSCA: List of Chemicals Undergoing Prioritization: High Priority Candidates
Search TSCAHIGHPRI Chemicals
Identifier substring search
List Details
Description: On March 20, 2019, EPA released a list of 40 chemicals to begin the prioritization process. TSCA requires EPA to publish this list of chemicals to begin the prioritization process and designate 20 chemicals as "high-prior
subsequent risk evaluation and to designate 20 chemicals as "low-priority," meaning that risk evaluation is not warranted at this time. Publication in the Federal Register activates a statutory requirement for EPA to complete the prio
process in the next nine to twelve months, allowing EPA to designate 20 chemicals as high priority and 20 chemicals as low priority by December 2019. The chemicals in the list below are the 20 high priority candidates.
Number of Chemicals: 20
20 chemicals
Select all
Download
Send to Batch Search
Default
DTXSID
TOXCAST
CASRN
Hide chemicals that are:
1,3-Butadiene
DTXSID:DTXSID3020203
TOXCAST:-
CASRN:106-99-0
Benzyl butyl phthalate
DTXSID:DTXSID3020205
TOXCAST:71/719
CASRN:85-68-7
1,2-Dibromoethane
DTXSID:DTXSID3020415
TOXCAST:13/604
CASRN:106-93-4
1,2-Dichlorobenzene
DTXSID:DTXSID6020430
TOXCAST:12/675
CASRN:95-50-1

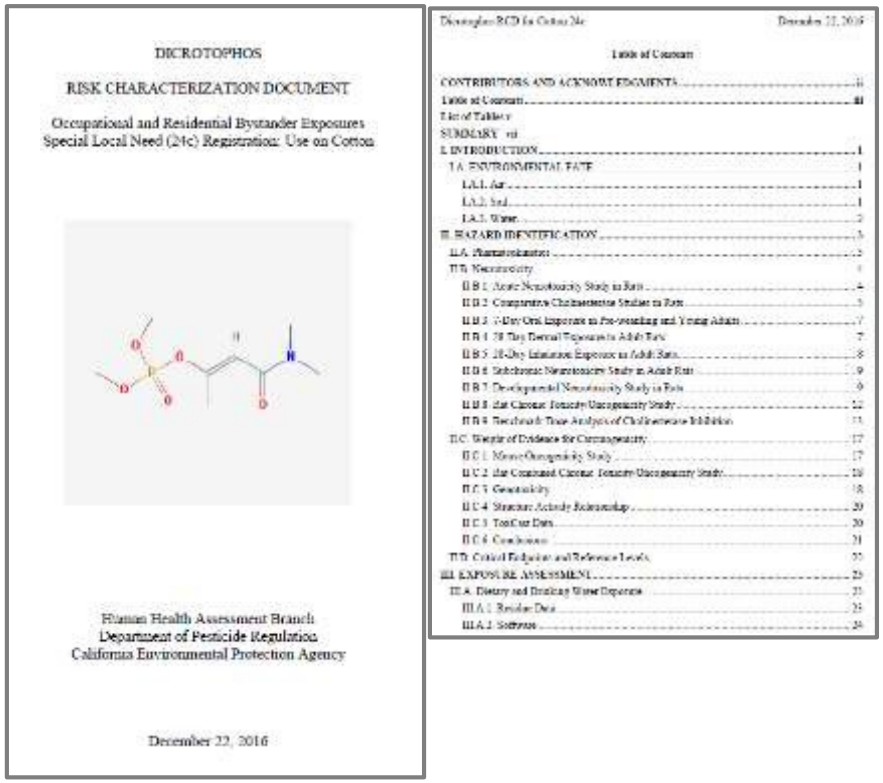
Impact

- CompTox Chemicals Dashboard integrates chemical data
- Used by EPA and others to support chemical assessment
  - Endocrine Disruptor Screening Program in the 21st Century (EDSP21)
  - Screening and Prioritization in support of TSCA



Impact

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

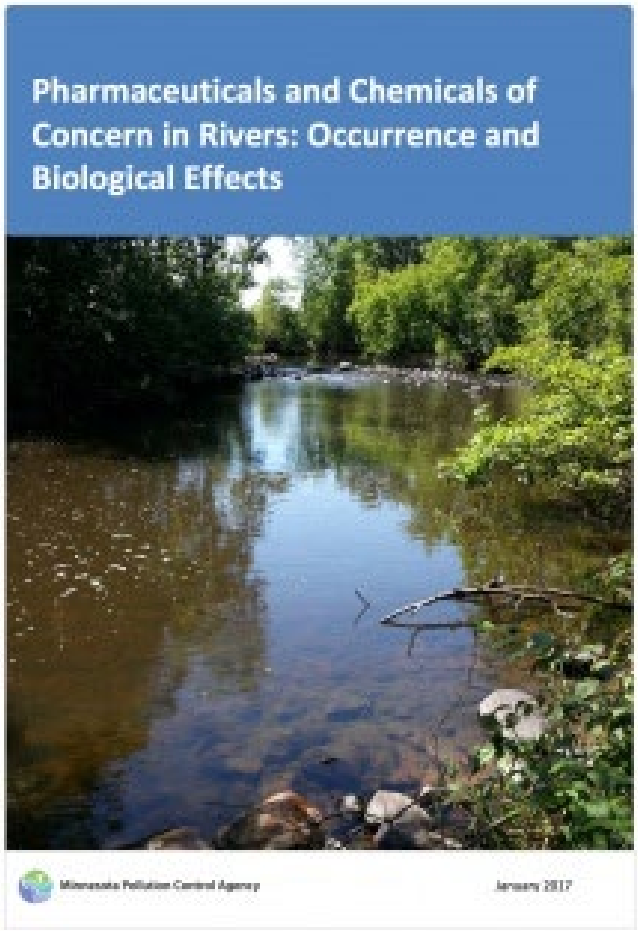
Table of Contents

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

"California benefits significantly from our partnership with EPA ORD. We use ToxCast data to provide valuable insight into how chemicals may cause toxicity, and we use their lifecycle analytic and exposure modeling and monitoring for various state efforts including our work on safer consumer products. EPA ORD resources are helping us to make more informed decisions about the potential health effects of chemicals."

– CalEPA Secretary Matthew Rodriquez

Impact



"EPA's variety of tools have been critical in developing aquatic toxicity profiles (ATPs) for contaminants detected across Minnesota. The MPCA uses EPA's estimation tools and databases to quickly obtain relevant information about contaminants that have only recently been detected in an aquatic environment. Prior to the development of these tools, information about contaminants has been limited or time-consuming to find. The profiles combine contaminant information such as fate in the environment, aquatic life toxicity, and endocrine activity to screen contaminants detected in Minnesota. The MPCA uses this information to communicate potential effects of the contaminants found in Minnesota and to identify pollution prevention opportunities for contaminants of highest concern."

– MPCA Commissioner John Linc Stine

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

Contacts

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