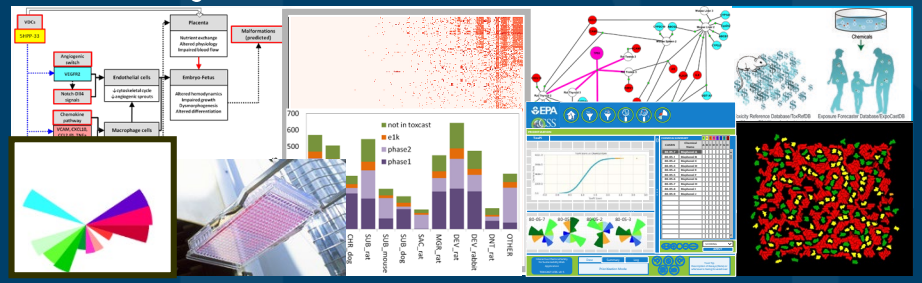
Perspectives on the Development, Evaluation, and Application of *in Silico* Approaches for Predicting Toxicity



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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 U.S. EPA

Conflict of Interest Statement

- No conflict of interest declared.

- Disclaimer:
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Outline

- Regulatory Drivers
- Computational (*in silico*) Toxicology [scope for today's talk]
- Integrated Approaches to Testing and Assessment (IATA) – definitions and Adverse Outcome Pathway (AOP) informed
- Decision contexts and their impact on the approaches applied
- Risk-based prioritisation
- Read-across approaches
  - Generalised Read-across (GenRA)
- Summary remarks
- Acknowledgements

Regulatory and Non-Regulatory drivers

- Societal demands for safer and sustainable chemical products are stimulating changes in toxicity testing and assessment frameworks
- Chemical safety assessments are expected to be conducted faster and with fewer animals, yet the number of chemicals that require assessment is also rising with the number of different regulatory programmes worldwide.
- In the EU, the use of alternatives to animal testing is promoted.
- Animal testing is prohibited in some sectors e.g. EU Cosmetics regulation
- The European Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) legislation lays out specific information requirements, based on tonnage level triggers. However, the regulation explicitly expresses the need to use non-testing approaches to reduce the extent of experimental testing in animals.

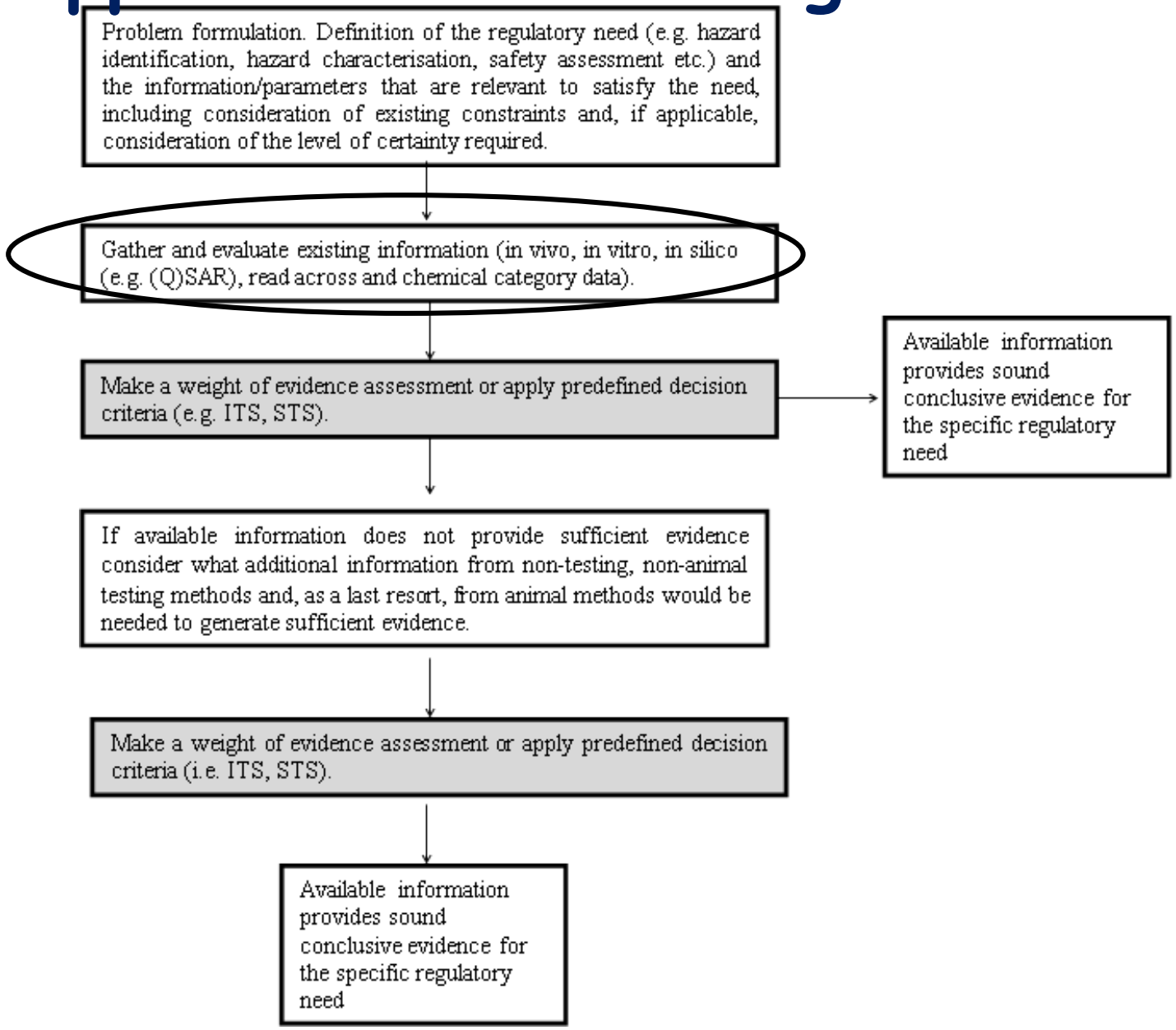
Regulatory and Non-Regulatory drivers

- REACH-like schemes also have been established in China, South Korea, and Turkey.
- In the US, the new Frank Lautenberg Chemical Safety for the 21st Century Act (LCSA) requires that a risk based prioritisation is conducted for all substances in commerce, ~40,000, many of which are lacking sufficient publicly available toxicity information.
- EPA Administrator signed memo 10/9/19 to "direct the agency to aggressively reduce animal testing, including reducing mammal study requests and funding 30% by 2025 and completely eliminating them by 2035"
- Risk based prioritisation is also an important aspect of regulatory frameworks in Canada (the Domestics Substance List), Australia and the EU.
- Non-testing approaches offer a means of facilitating the regulatory challenges in chemical safety assessment

Computational (*In Silico*) Toxicology

- Databases/Dashboards of existing information
- Structure-Activity Relationships (SAR)
- Quantitative Structure-Activity Relationships (QSAR)
- Expert Systems
- Category formation (grouping) read-across
- Bioinformatics
- Chemoinformatics
- Biokinetics (PBPK)

Integrated Approaches to Testing and Assessment (IATA)



From OECD

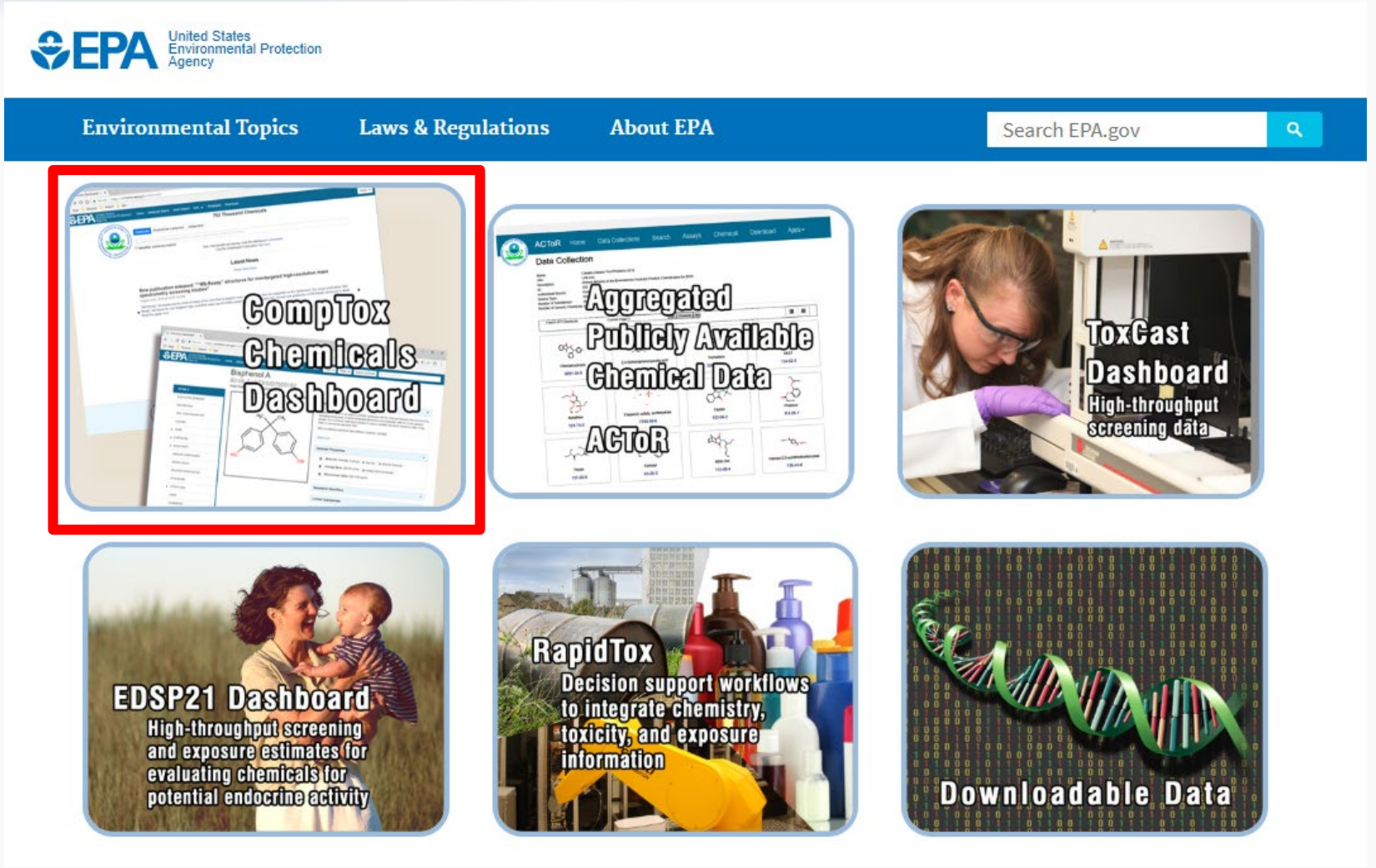
Typical Information within an IATA: IATA elements

- Historical information on the chemical of interest
- Non-standard *in vivo* tests
- Information from "similar" chemicals
- Predictions from other 'non-testing' approaches such as (Q)SAR
- *In chemico* tests
- *In vitro* tests
- Molecular biology, -omics
- Exposure, (bio-)kinetics

The EPA CompTox Chemicals Dashboard: An Integration Hub for Data Supporting Computational Toxicology

Project Lead: Antony Williams

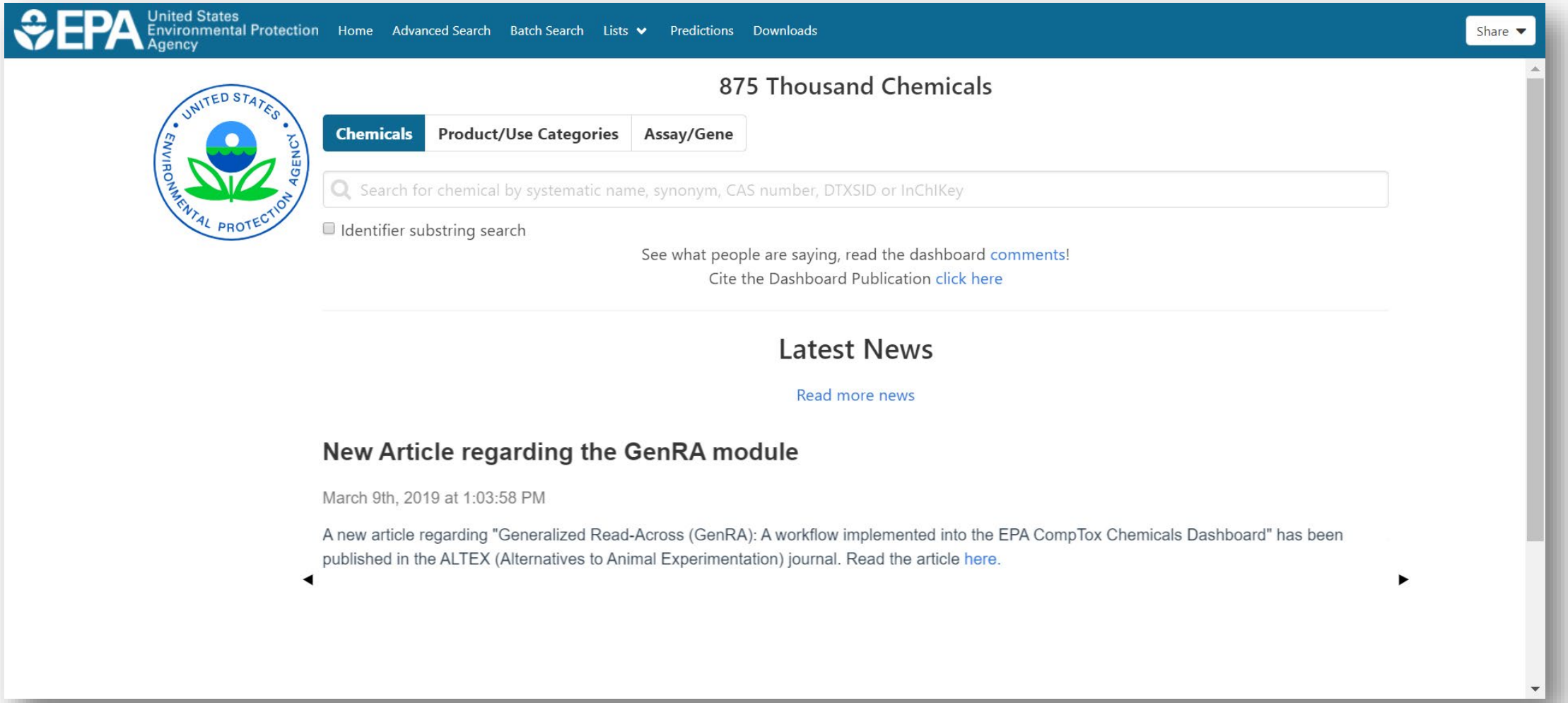
The CompTox Portal
https://comptox.epa.gov/



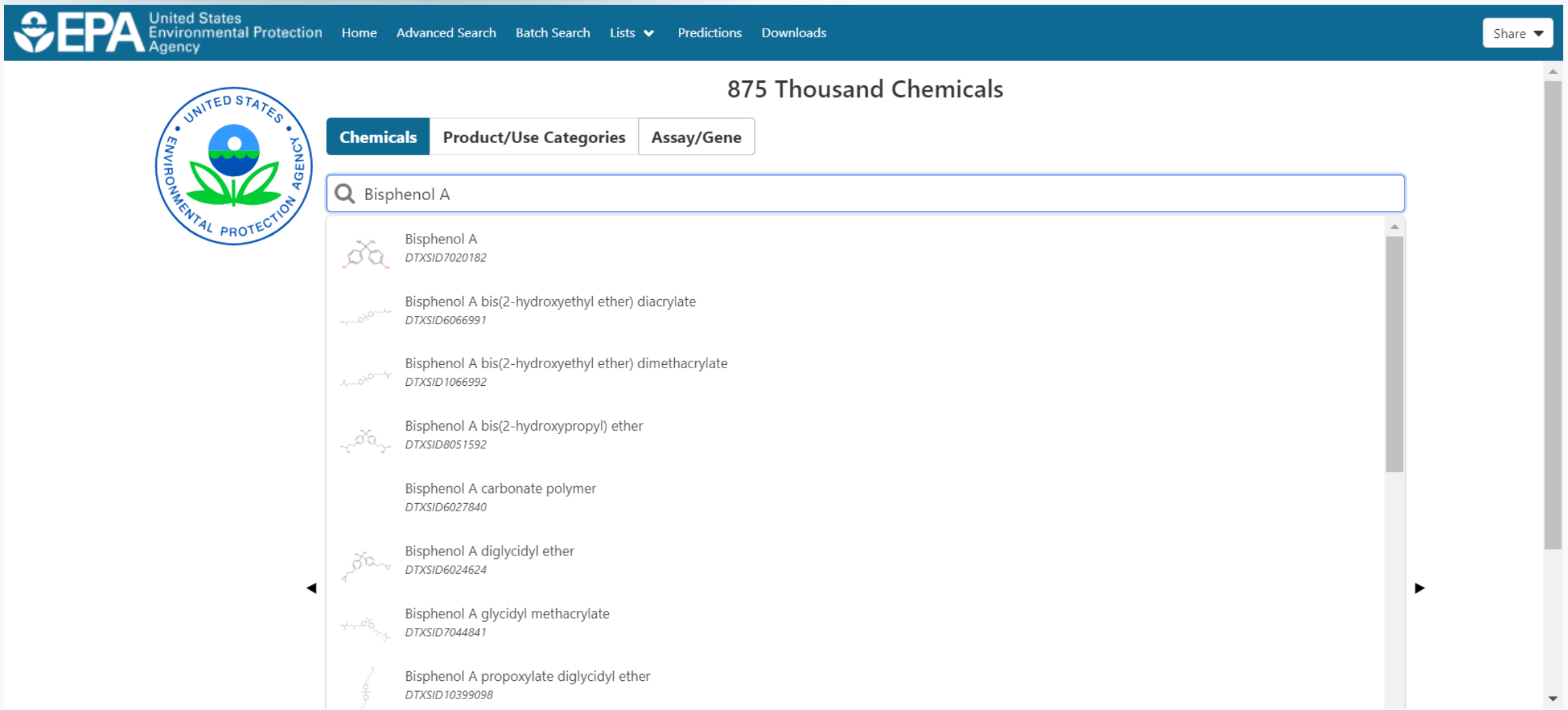
CompTox Chemicals Dashboard

- A **publicly accessible website** delivering access:
  - ~875,000 chemicals with related property data
  - Experimental and predicted physicochemical property data
  - Integration to "biological assay data" for 1000s 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

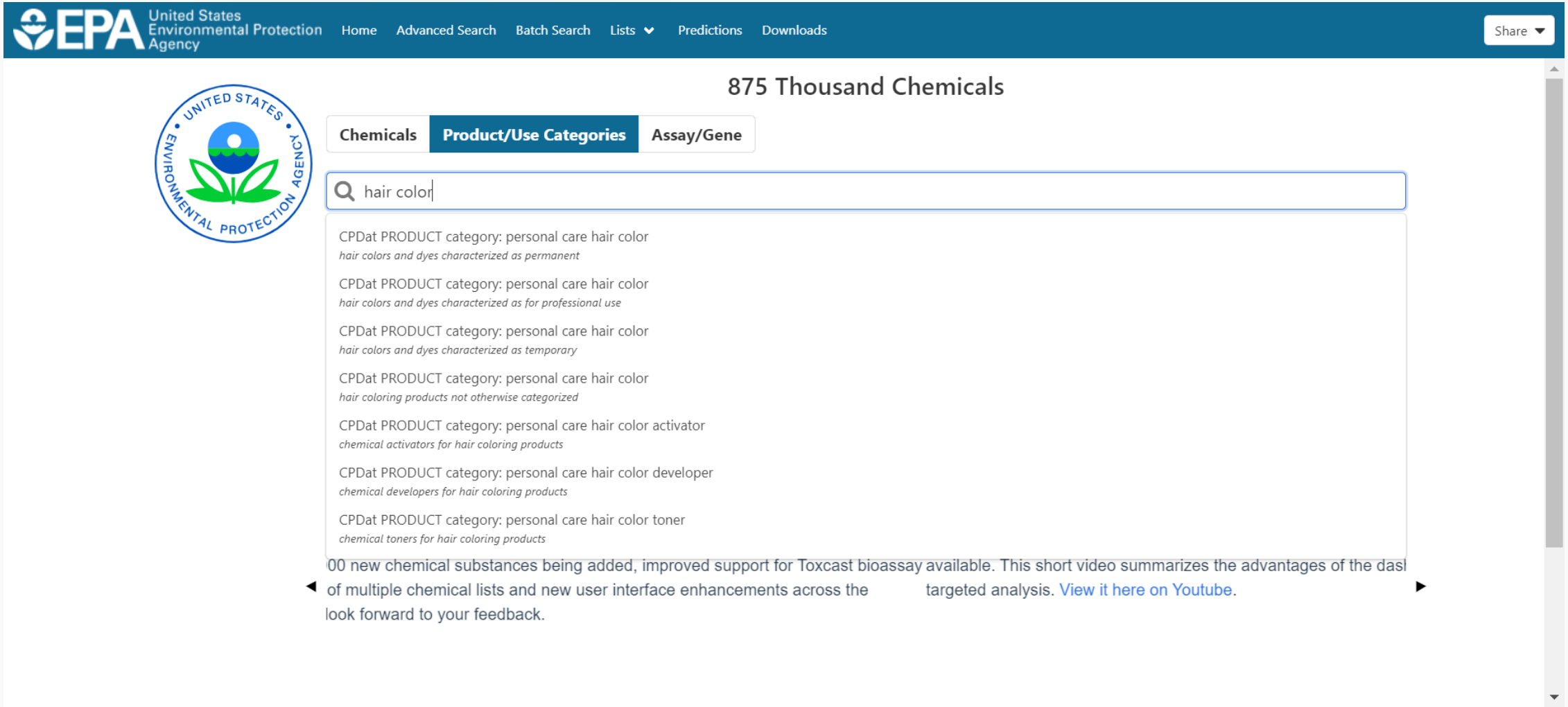
CompTox Chemicals Dashboard



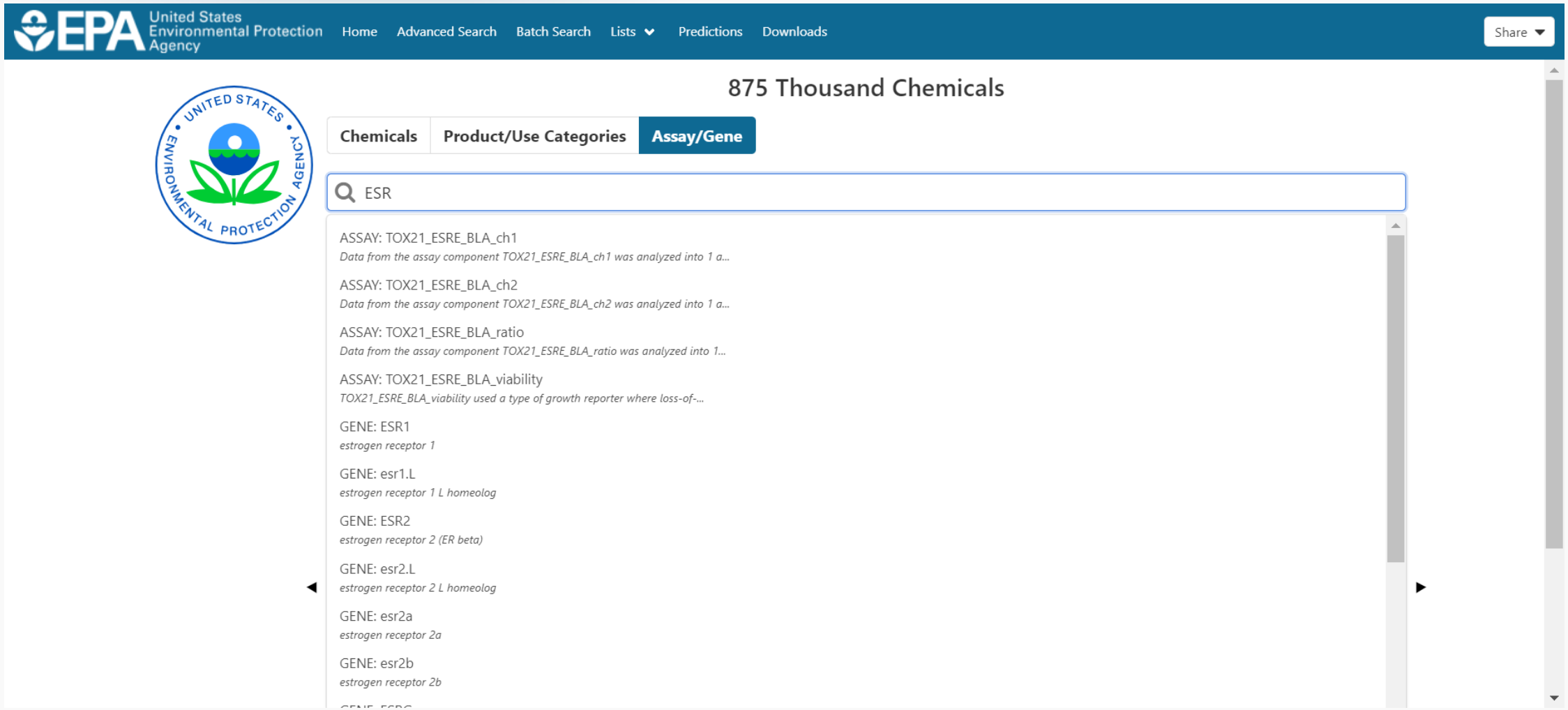
CompTox Chemicals Dashboard
Chemicals



CompTox Chemicals Dashboard
Products and Use Categories



CompTox Chemicals Dashboard
Assays and Genes



Detailed Chemical Pages: Landing page

EPA United States Environmental Protection Agency

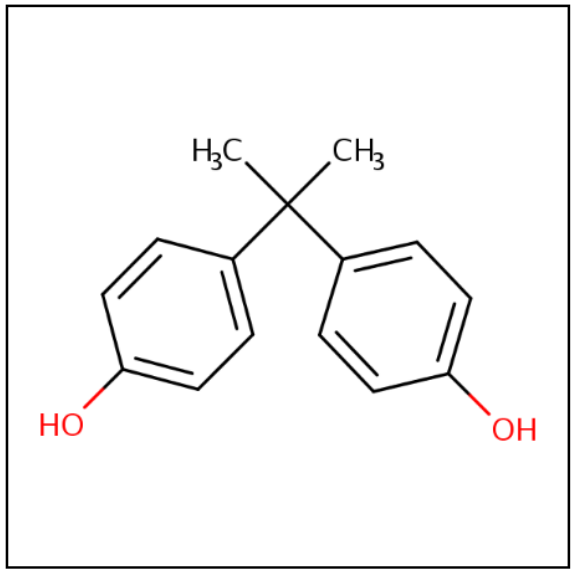
Home | Advanced Search | Batch Search | Lists | Predictions | Downloads | Copy | Share | Submit Comment | Search all data

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



Wikipedia

Bisphenol A (**BPA**) is an organic synthetic compound with the chemical formula $(CH_3)_2C(C_6H_4OH)_2$ belonging to the group of diphenylmethane derivatives and bisphenols, with two hydroxyphenyl groups. It is a colorless solid that is soluble in organic solvents, but poorly soluble in water. It has been in commercial use since 1957.

BPA is a starting material for the synthesis of plastics, primarily

...

Read more

Intrinsic Properties

Structural Identifiers

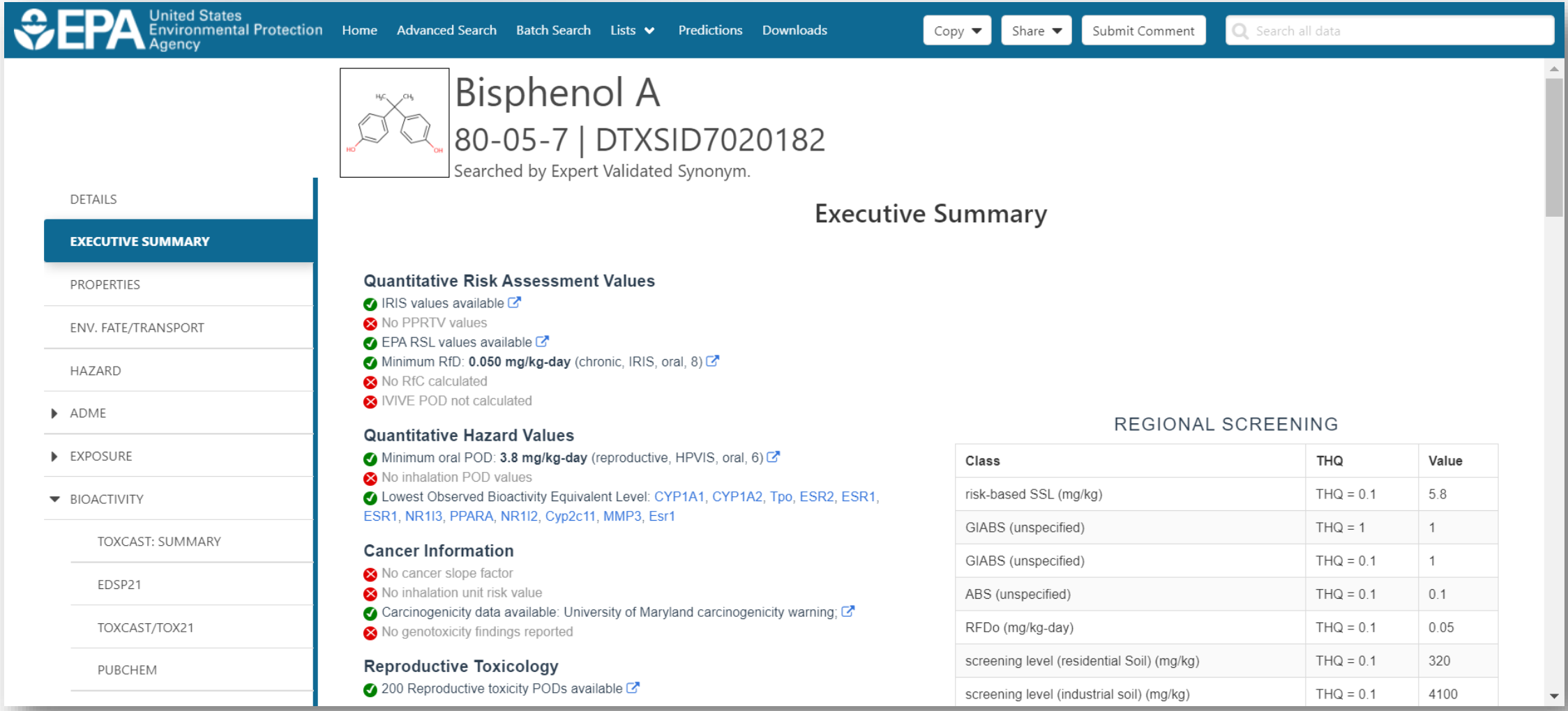
Linked Substances

Presence in Lists

Record Information

Quality Control Notes

An "Executive Summary"



An "Executive Summary" Quick Look Tox Info

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.

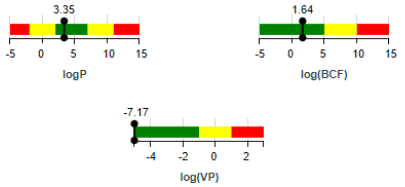
POINT-OF-DEPARTURE PLOTS

ASSAY PLOTS

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



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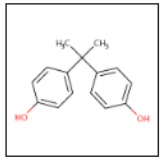
Physicochemical properties

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 Expert Validated Synonym.

- DETAILS
- EXECUTIVE SUMMARY
- **PROPERTIES**
- ENV. FATE/TRANSPORT
- HAZARD
- ADME
- EXPOSURE
- BIOACTIVITY
  - TOXCAST: SUMMARY
  - EDSP21
  - TOXCAST/TOX21
  - PUBCHEM
  - TOXCAST: MODELS
- SIMILAR COMPOUNDS

Property

Summary

Summary

Download | Columns | Search query

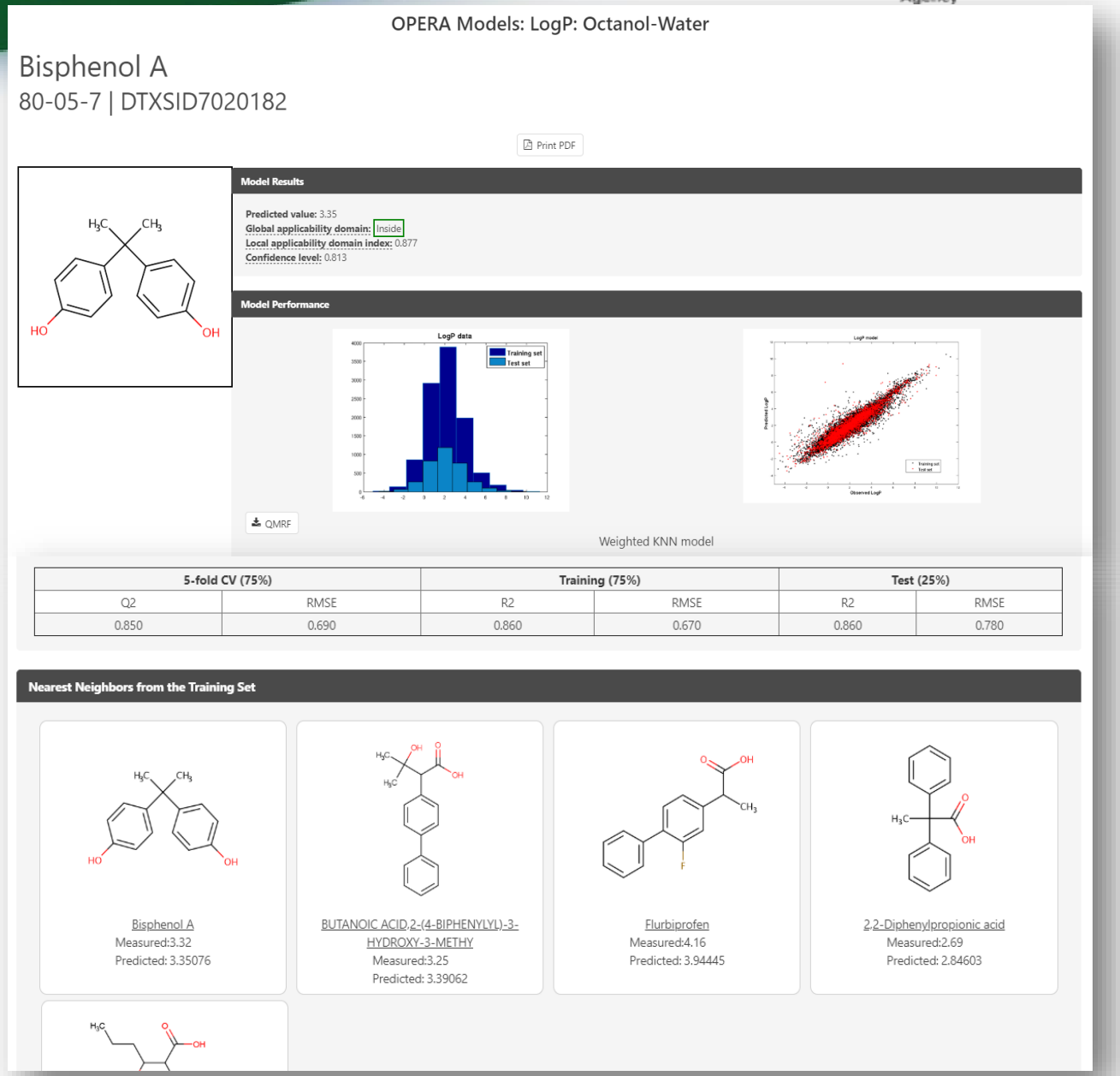
Property	Experimental average	Predicted average	Experimental median	Predicted median	Experimental range	Predicted range	Unit
LogP: Octanol-Water	3.32 (1)	3.29		3.43	3.32	2.40 to 3.64	
Melting Point	155 (7)	139	156	138	153 to 156	125 to 157	°C
Boiling Point	200 (1)	363		360	200	343 to 401	°C
Water Solubility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

Detailed QSAR Prediction Reports from OPERA

QSAR Prediction Reporting Format (QPRF):
Standardised template to document a prediction from a given QSAR model

QSAR Model Reporting Format (QMRF)
Template to document a QSAR model itself

Underpinned by the OECD QSAR Validation Principles (2004)



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

LogP data

QMRF

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.850	0.690	0.860	0.670	0.860	0.780

Nearest Neighbors from the Training Set

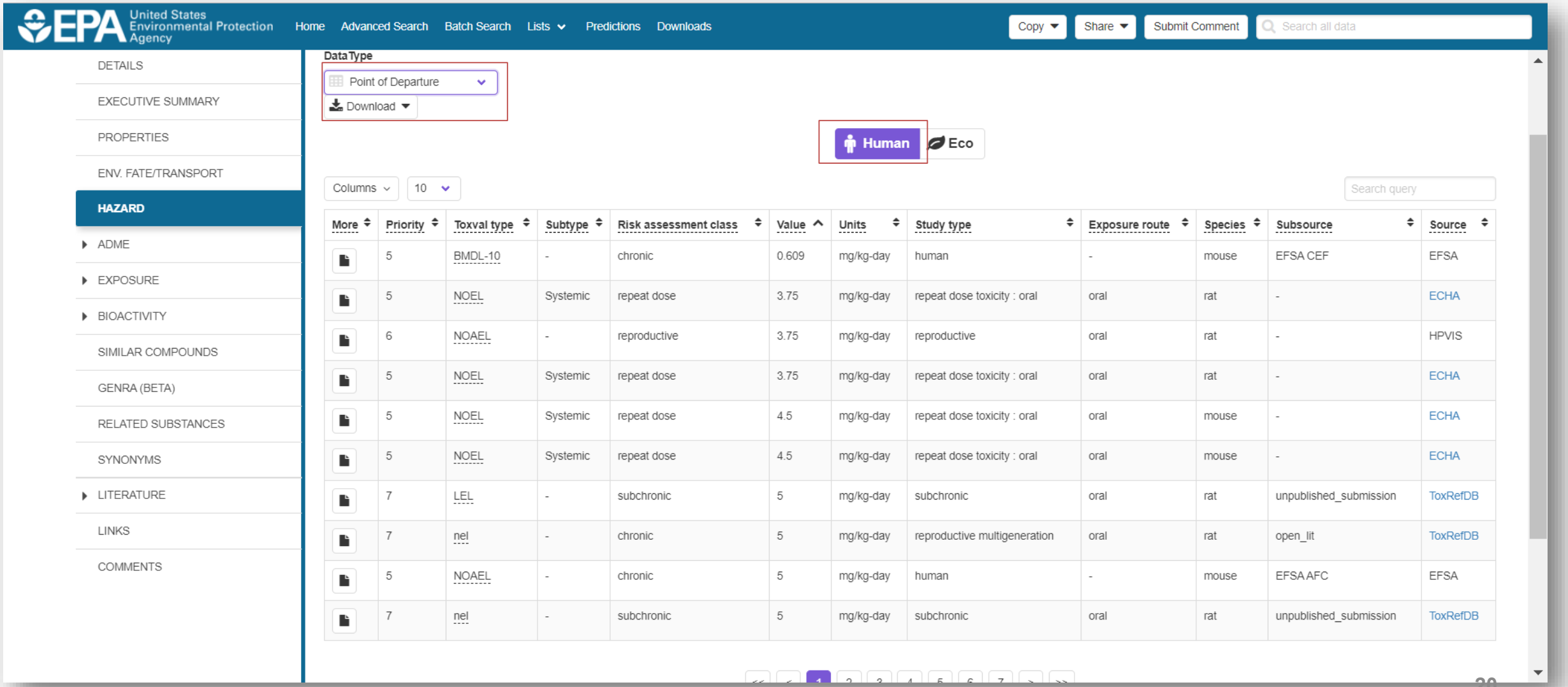
Bisphenol A
Measured:3.32
Predicted: 3.35076

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

Other Data: Human and Ecological Chemical Hazard Data

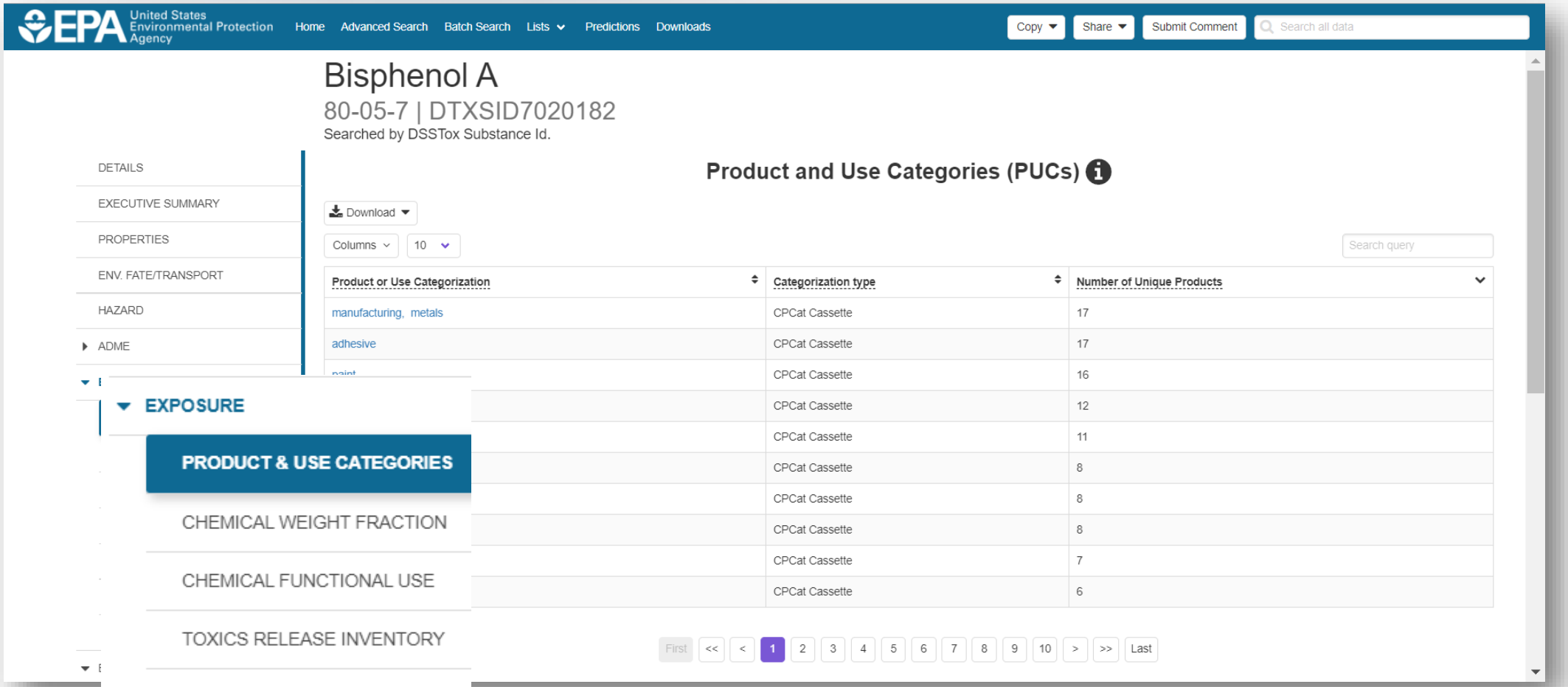


More	Priority	Toxval type	Subtype	Risk assessment class	Value	Units	Study type	Exposure route	Species	Subsource	Source
	5	BMDL-10	-	chronic	0.609	mg/kg-day	human	-	mouse	EFSA CEF	EFSA
	5	NOEL	Systemic	repeat dose	3.75	mg/kg-day	repeat dose toxicity : oral	oral	rat	-	ECHA
	6	NOAEL	-	reproductive	3.75	mg/kg-day	reproductive	oral	rat	-	HPVIS
	5	NOEL	Systemic	repeat dose	3.75	mg/kg-day	repeat dose toxicity : oral	oral	rat	-	ECHA
	5	NOEL	Systemic	repeat dose	4.5	mg/kg-day	repeat dose toxicity : oral	oral	mouse	-	ECHA
	5	NOEL	Systemic	repeat dose	4.5	mg/kg-day	repeat dose toxicity : oral	oral	mouse	-	ECHA
	7	LEL	-	subchronic	5	mg/kg-day	subchronic	oral	rat	unpublished_submission	ToxRefDB
	7	nel	-	chronic	5	mg/kg-day	reproductive multigeneration	oral	rat	open_lit	ToxRefDB
	5	NOAEL	-	chronic	5	mg/kg-day	human	-	mouse	EFSA AFC	EFSA
	7	nel	-	subchronic	5	mg/kg-day	subchronic	oral	rat	unpublished_submission	ToxRefDB

Hazard Data from "ToxVal_DB"

- ToxVal Database contains following structured data:
  - ~30,000 chemicals
  - ~750,000 toxicity values
  - ~30 sources of data
  - ~4500 journals cited
  - ~70,000 literature citations

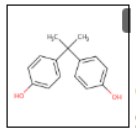
Sources of Exposure to Chemicals



ADME-IVIVE

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



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- ADME
  - IVIVE
- EXPOSURE
- BIOACTIVITY
- SIMILAR COMPOUNDS
- GENRA (BETA)
- RELATED SUBSTANCES

IVIVE

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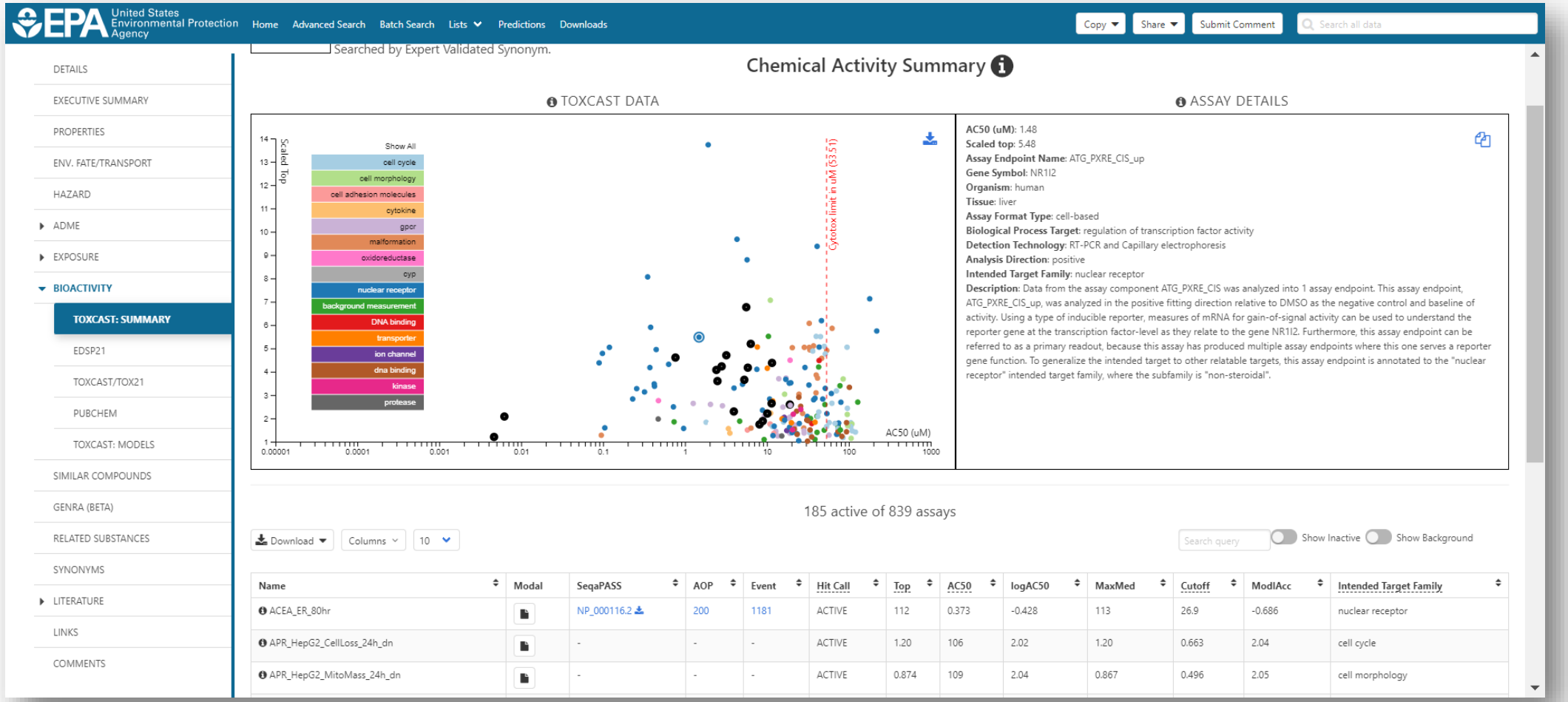
Label	Measured	Predicted	Computed	Unit
In Vitro Intrinsic Hepatic Clearance	19.29	-	-	uL/min/million hepatocytes
Fraction Unbound in Human Plasma	0.07	-	-	
Volume of Distribution	-	-	6.69	L/kg
Days to Steady State	-	-	8	Days
PK Half Life	-	-	29.83	hours
Human Steady-State Plasma Concentration	-	-	1.98	mg/L

6 records

In Vitro Bioassay Screening

ToxCast and Tox21



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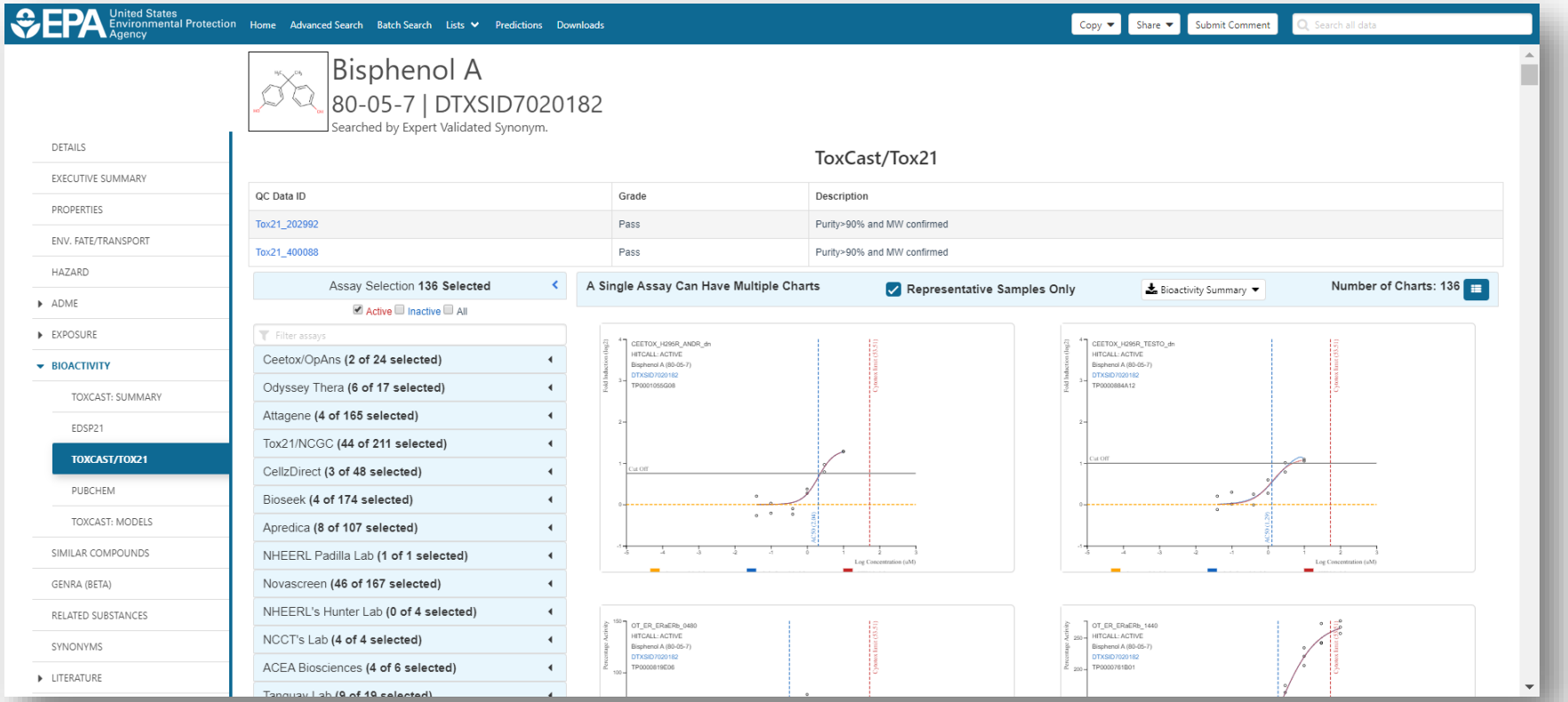

Bioactivity: Downloadable Data

https://www.epa.gov/chemical-research/exploring-toxcast-data-downloadable-data

Exploring ToxCast Data: Downloadable Data

The results after processing through the Pipeline are available on the ToxCast Dashboard, and for most users EPA recommends accessing the data there.

- ToxCast Chemicals
- ToxCast Assays

Resources

- Toxicity Forecaster (ToxCast) Fact Sheet
- ToxCast Publications
- ToxCast Citation
- About ToxCast

ToxCast Data and Information

- **ToxCast & Tox21 Summary Files.** Data for a single chemical endpoint pair for thousands of chemicals and assay endpoints for 20 variables such as the activity or hit call, activity concentrations, whether the chemical was tested in a specific assay, etc.
  - Download ToxCast Summary Information
  - Download ReadMe
- **ToxCast & Tox21 Data Spreadsheet.** A spreadsheet of EPA's analysis of the chemicals screened through ToxCast and the Tox21 collaboration which includes EPA's activity calls from the screening of over 1,800 chemicals.
  - Download Data
  - Download ReadMe
- **ToxCast Data Pipeline R Package.** The R computer programming package used to process and model all EPA ToxCast and Tox21 chemical screening data. The files include the R programming package as well as documents that provide overviews of the data analysis pipeline used and the R package. Users will need experience with R to use these files.
  - Download Package
  - TCPL Overview

BUILT-IN "MODULES"

Landing page

EPA United States Environmental Protection Agency

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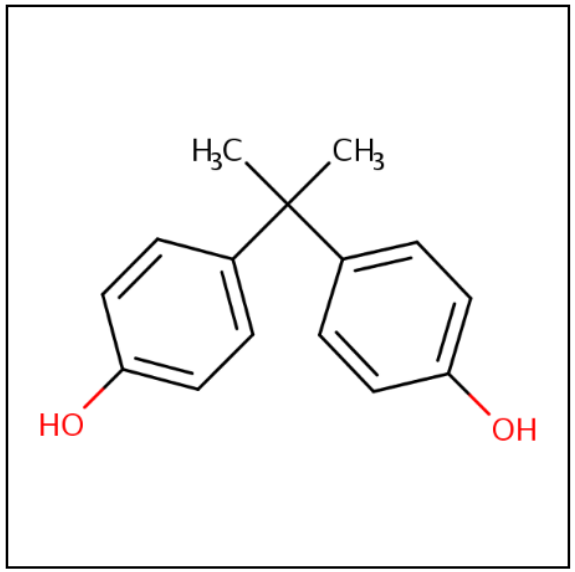

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...

Read more

Intrinsic Properties

Structural Identifiers

Linked Substances

Presence in Lists

Record Information

Quality Control Notes

Related Publications

Regulatory Toxicology and Pharmacology
Volume 79, August 2016, Pages 12-24

Systematically evaluating read-across prediction and performance using a local validity approach characterized by chemical structure and bioactivity information

Contents lists available at ScienceDirect
Computational Toxicology
journal homepage: www.elsevier.com

Navigating through the minefield of read-across frameworks: A commentary perspective

Grace Patlewicz[a,*], Mark T.D. Cronin[b], George Helman[a,c], Jason C. Lambert[d], Lucina E. Lizarraga[d], Imran Shah[a]

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[b] School of Pharmacy and Biomolecular Sciences, Liverpool John Moores University, Byrom Street, Liverpool L3 3AF, UK
[c] Oak Ridge Institute for Science and Education (ORISE), 1299 Bethel Valley Road, Oak Ridge, TN 37830, USA
[d] National Center for Evaluation Assessment (NCEA), US Environmental Protection Agency (US EPA), 26 West Martin Luther King Dr, Cincinnati, OH 45268, USA

Available online 23 July 2018
In Press, Corrected Proof

Extending the Generalised Read-Across approach (GenRA): A systematic analysis of the impact of physicochemical property information on read-across performance

George Helman [a, b], Imran Shah [b], Grace Patlewicz [b]

Short Communication

Generalized Read-Across (GenRA): A Workflow Implemented into the EPA CompTox Chemicals Dashboard

George Helman[1,2], Imran Shah[2], Antony J. Williams[2], Jeff Edwards[2], Jeremy Dunne[2] and Grace Patlewicz[2]

[1]Oak Ridge Institute for Science and Education (ORISE), Oak Ridge, TN, USA; [2]National Center for Computational Toxicology (NCCT), Office of

Contents lists available at ScienceDirect
Computational Toxicology
journal homepage: http://ees.elsevier.com

Transitioning the generalised read-across approach (GenRA) to quantitative predictions: A case study using acute oral toxicity data

George Helman[a,b], Imran Shah[b], Grace Patlewicz[b,*]

[a] Oak Ridge Institute for Science and Education (ORISE), Oak Ridge,
[b] National Center for Computational Toxicology (NCCT), Office of R
27711, USA

ARTICLE INFO

Keywords:
Generalized read-across (GenRA)
Acute oral toxicity
Quantitative predictions

Regulatory Toxicology and Pharmacology 109 (2019) 104480
Contents lists available at ScienceDirect
Regulatory Toxicology and Pharmacology
journal homepage: www.elsevier.com/locate/yrtph

Quantitative prediction of repeat dose toxicity values using GenRA

G. Helman[a,b], G. Patlewicz[b], I. Shah[b,*]

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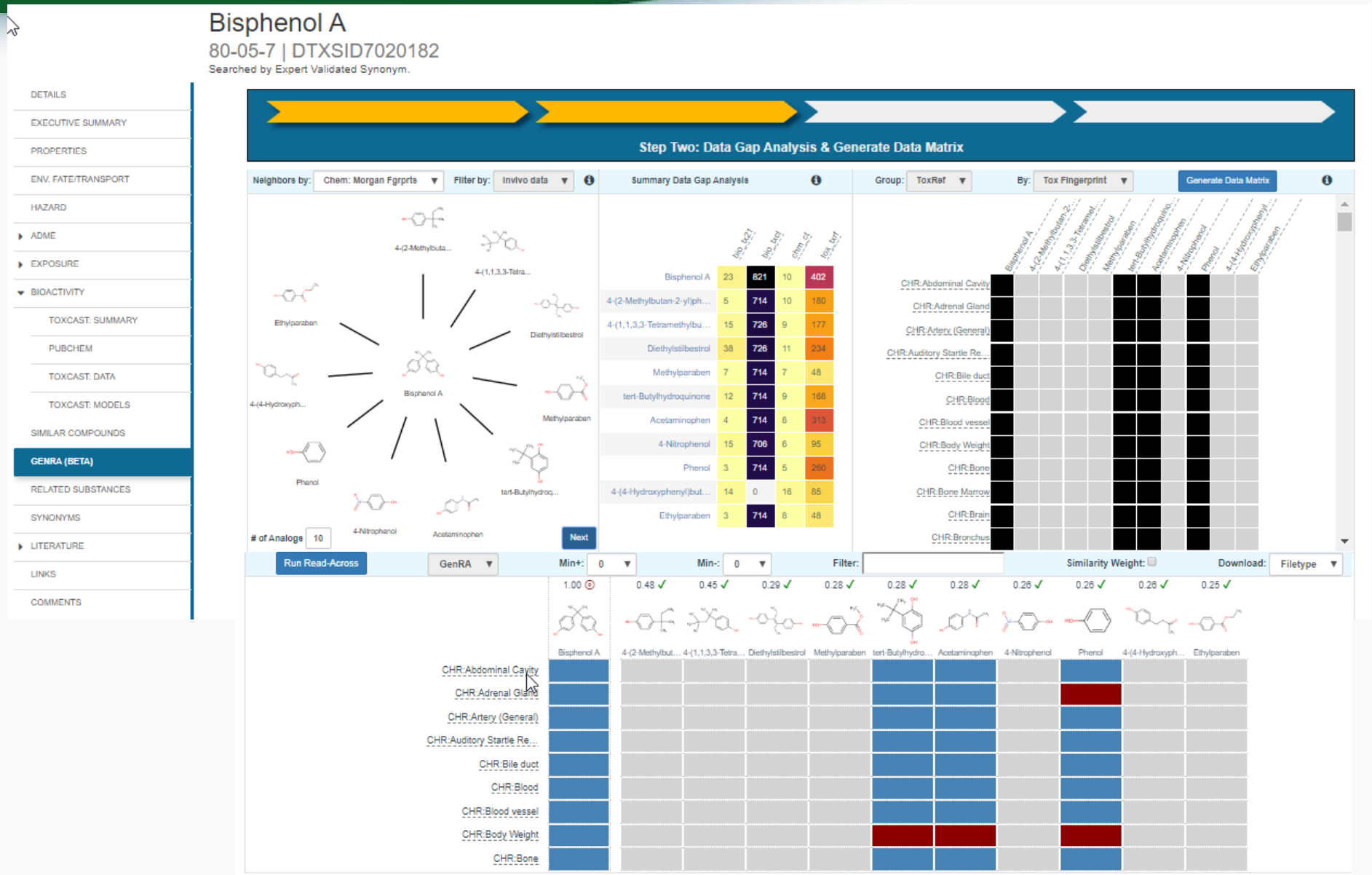
have recently gained popularity in the field of read-across to automatically fill data-
. Previously, we developed the generalized read-across (GenRA) tool, which utilizes
onjunction with chemical descriptor information to derive local validity domains to
in vivo toxicity studies. Here, we modified GenRA to quantitatively predict point of
tained from US EPA's Toxicity Reference Database (ToxRefDB) version 2.0. To
evaluate GenRA predictions, we first aggregated oral Lowest Observed Adverse Effect Levels (LOAEL) for 1,014
chemicals by systemic, developmental, reproductive, and cholinesterase effects. The mean LOAEL values for
each chemical were converted to log molar equivalents. Applying GenRA to all chemicals with a minimum

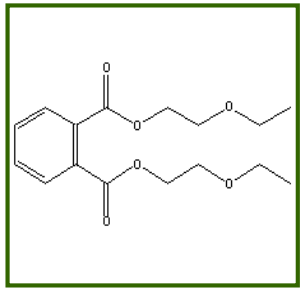
Point of contact:
Grace Patlewicz & Imran Shah

Generalised Read-Across (GenRA)



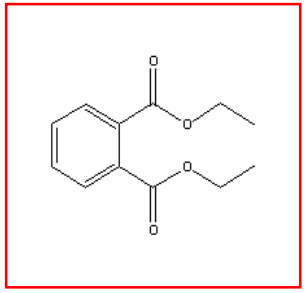
Read-across

- Read-across describes the method of filling a data gap whereby a chemical with existing data values is used to make a prediction for a 'similar' chemical.
- A target chemical is a chemical which has a data gap that needs to be filled i.e. the subject of the read-across.
- A source analogue is a chemical that has been identified as an appropriate chemical for use in a read-across based on similarity to the target chemical and existence of relevant data.



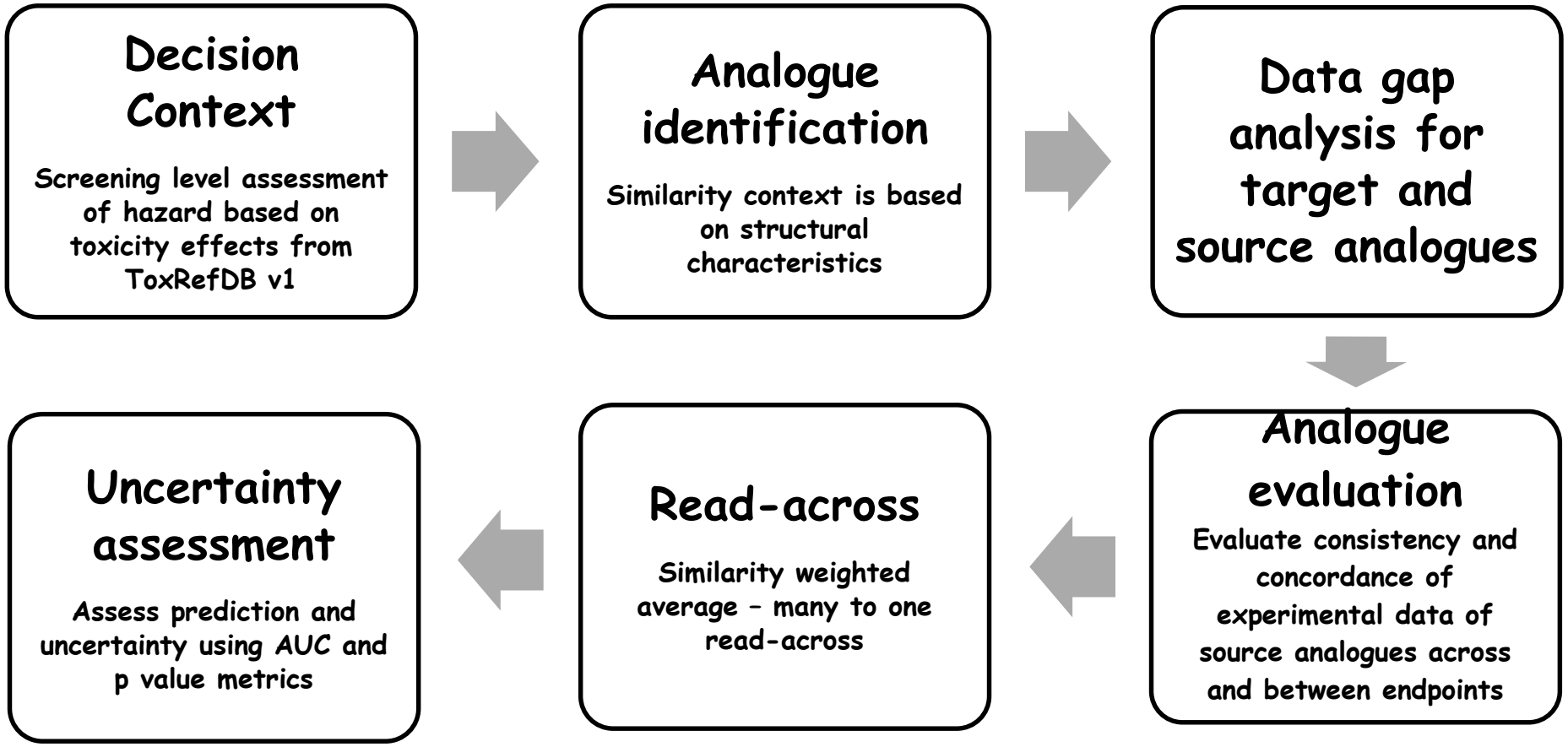
Known to be harmful

Acute toxicity?



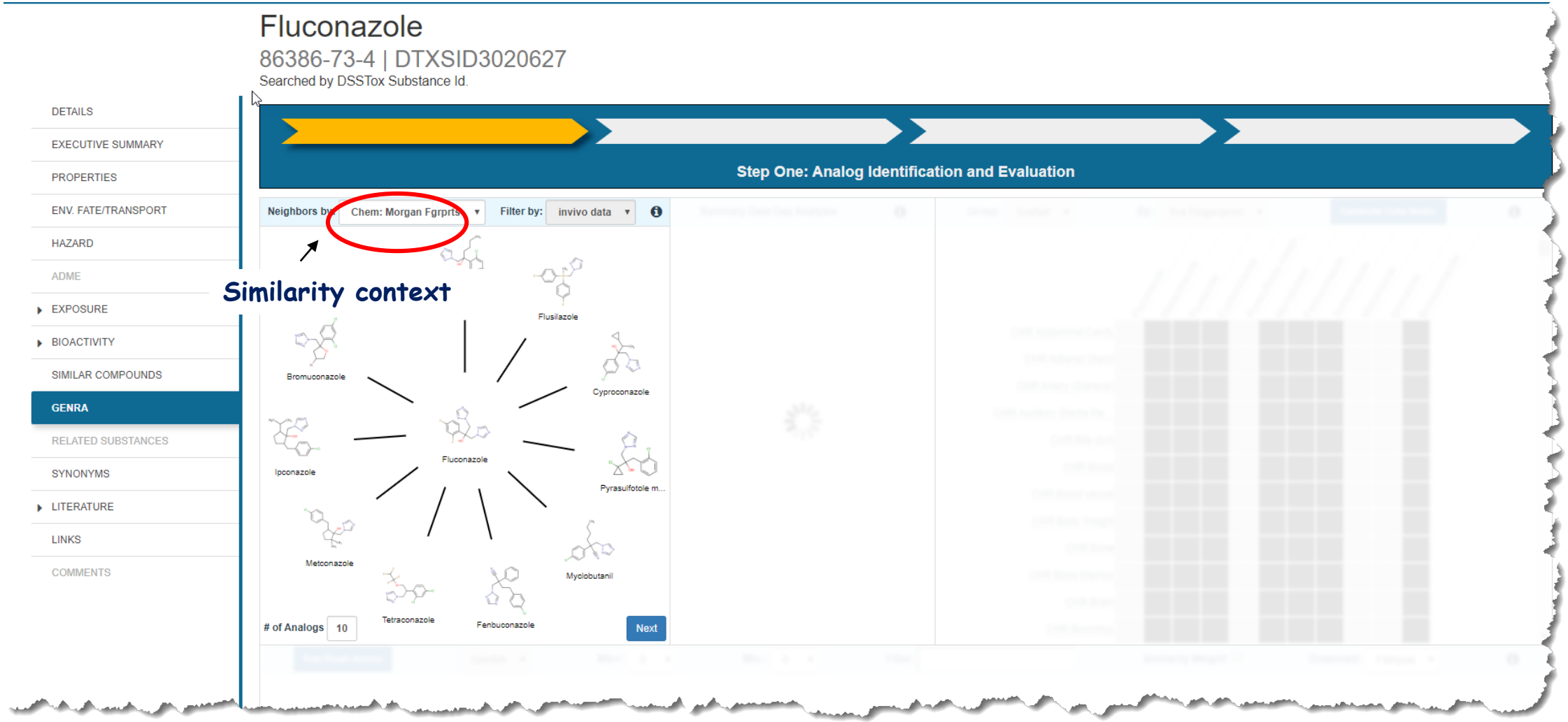
Predicted to be harmful

Read-across workflow in GenRA v1.0

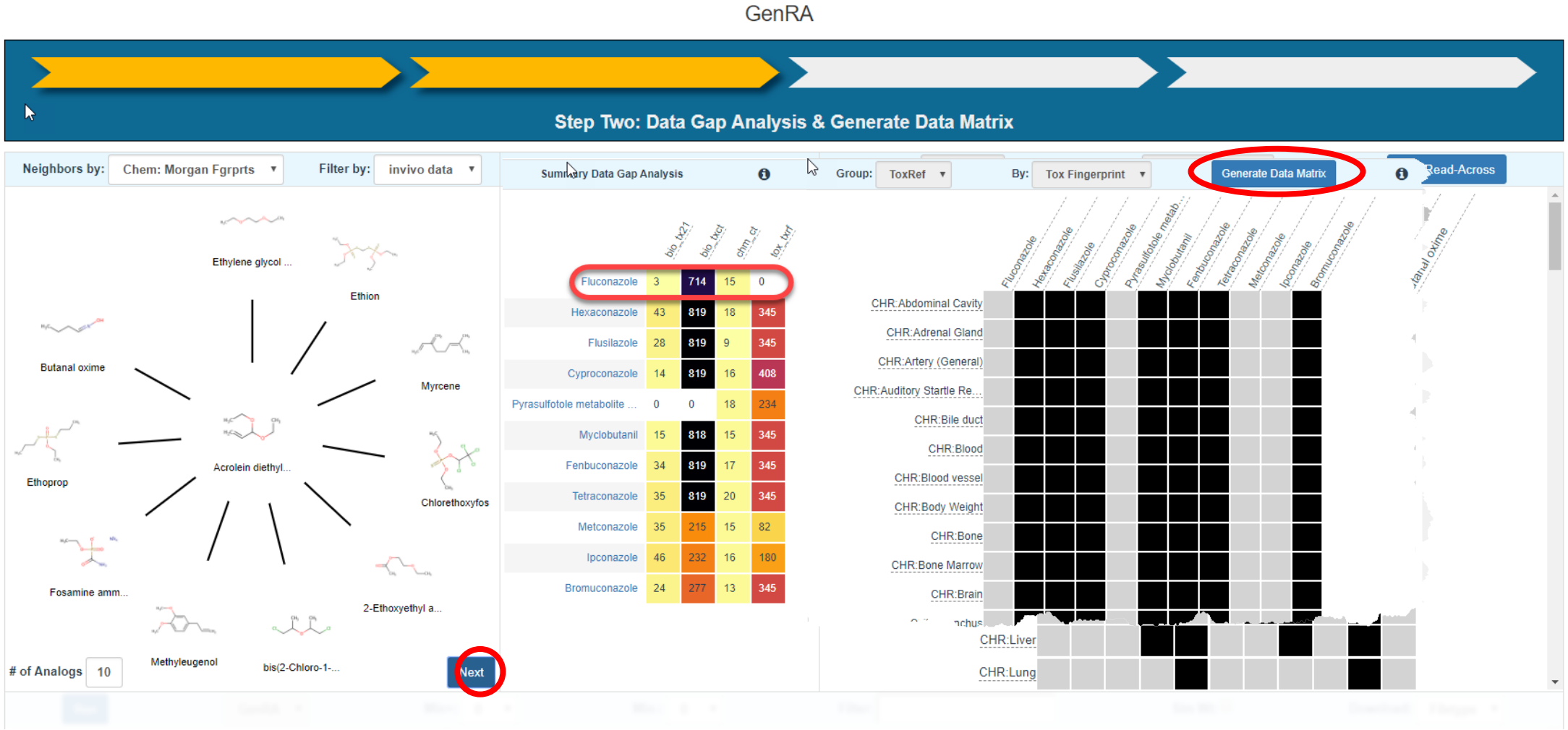


GenRA tool in practice

- Structured as a workflow

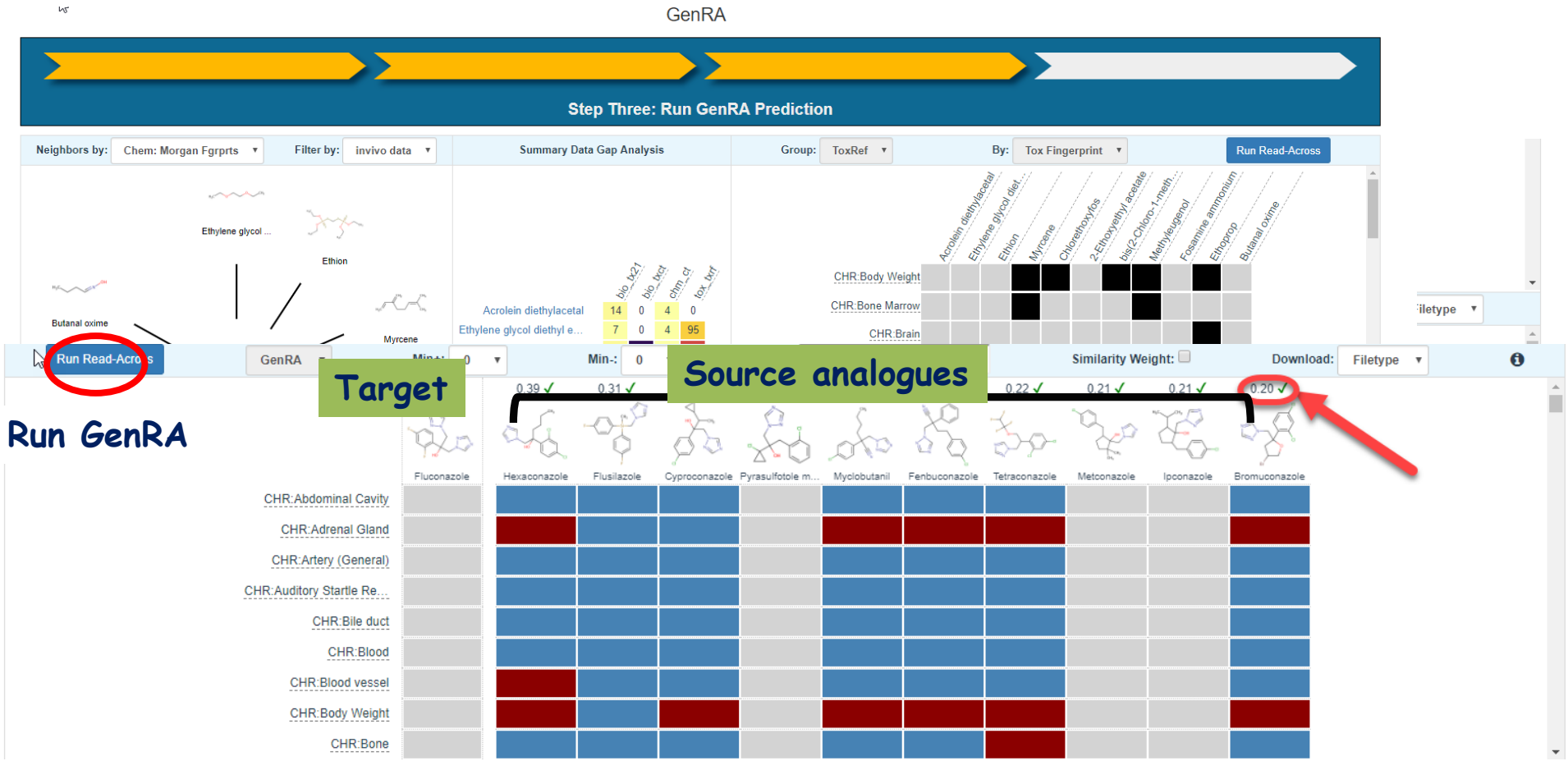


GenRA tool in practice

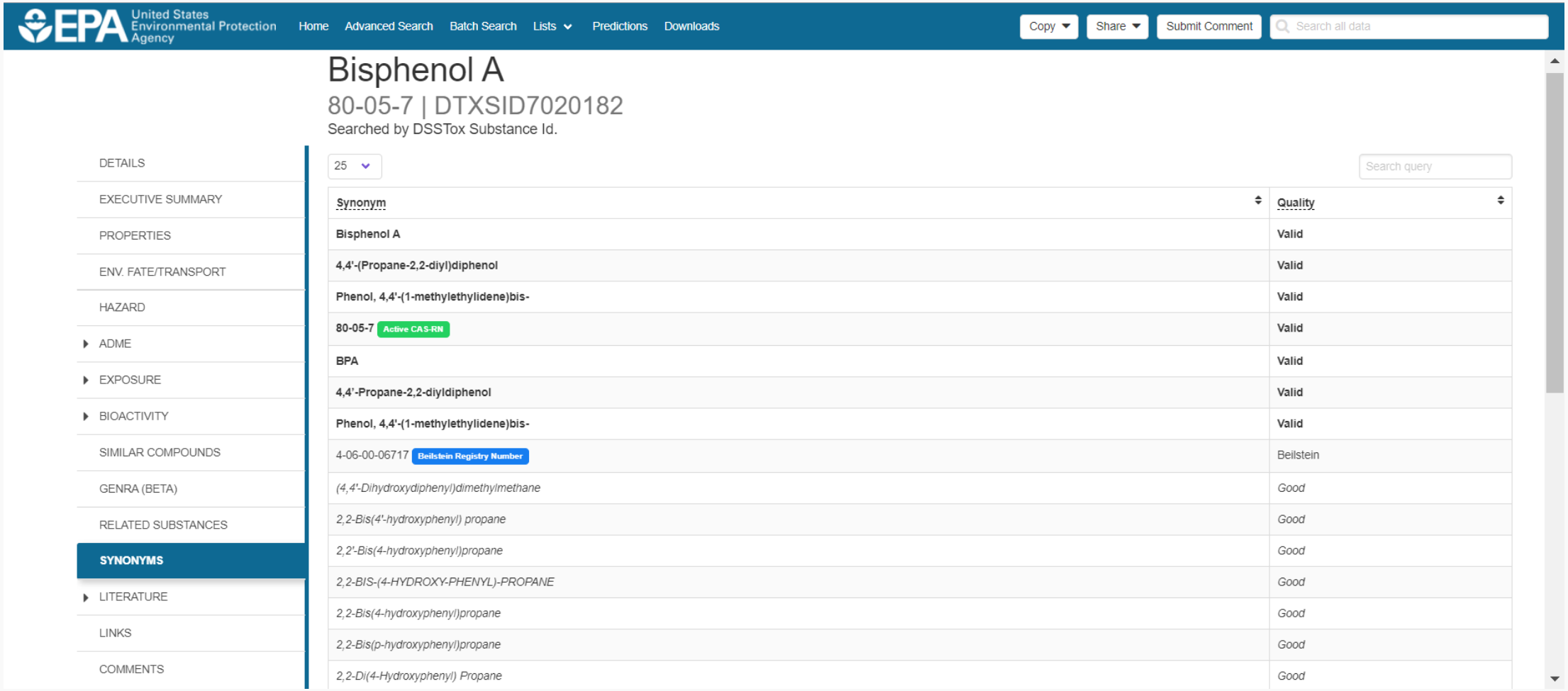


Data gap analysis

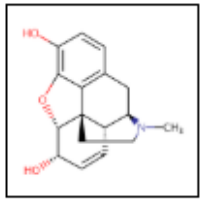
GenRA tool in practice



Names and CASRNs to Support Searches



Literature Searching



Morphine

57-27-2 | DTXSID9023336

Searched by Approved Name.

Abstract Sifter

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

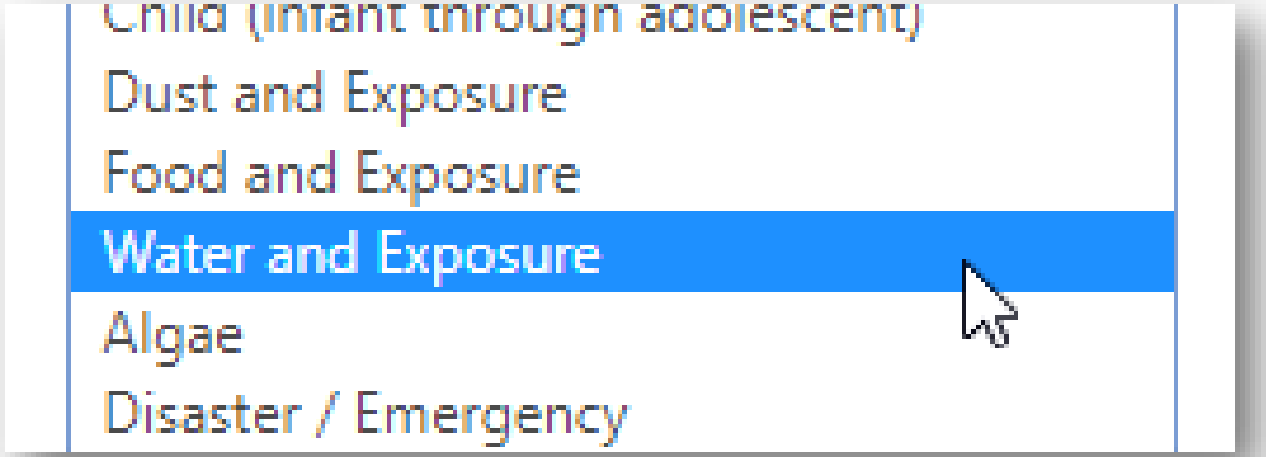
Select a Query Term | Retrieve Articles

- 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

37 of 37 articles loaded...

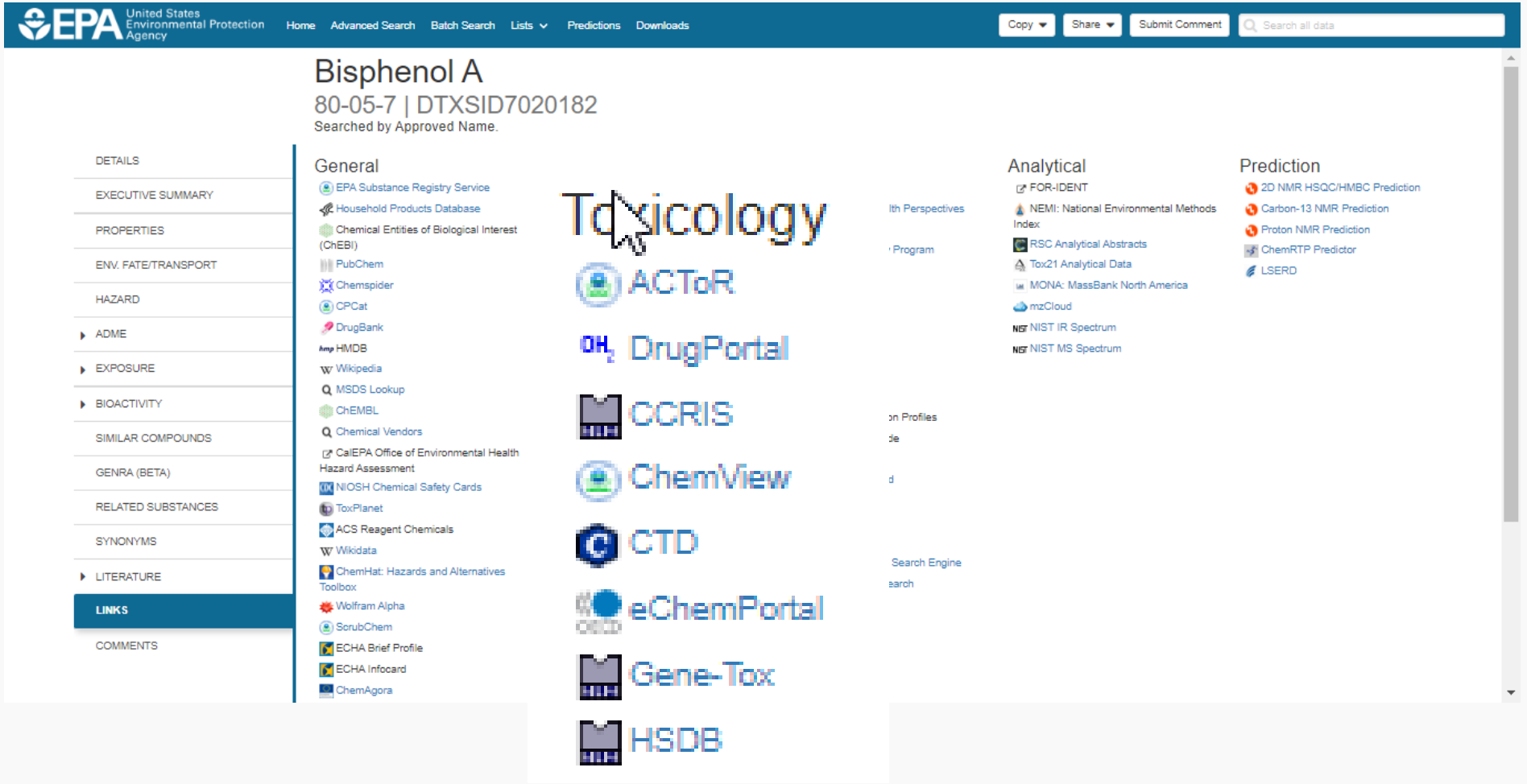
To find articles quickly, enter terms to sift abstracts.

wastewater | Spectrometry | EPA | Clear Terms

Download / Send to... | Download Sifter for Excel

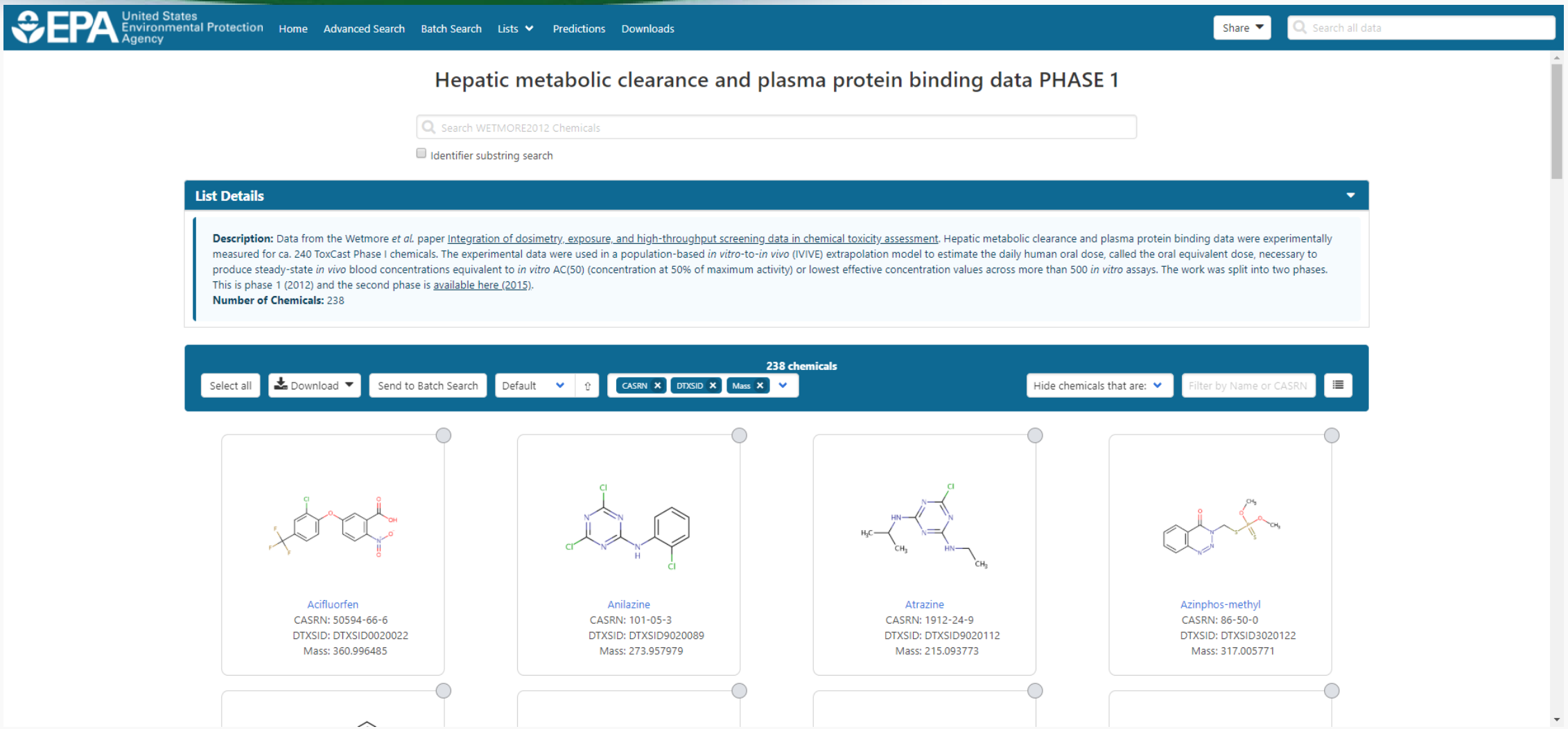
wastewater	Spectrometry	EPA	Total	PMID	Year	Title	Authors	Journal	Rev
4	2	0	6	29274731	2017	Simultaneous analysis of opioid analgesics and thei...	Krizman-Matasic; Kostanjevecki; Ahel; Terzic	Journal of chromatography. A	
0	1	0	1	25768972	2015	Evaluating external contamination of polybrominate...	Poon; 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	

External Links to ~80 websites



CHEMICAL LISTS AND CATEGORIES

An Example List



BATCH SEARCHING

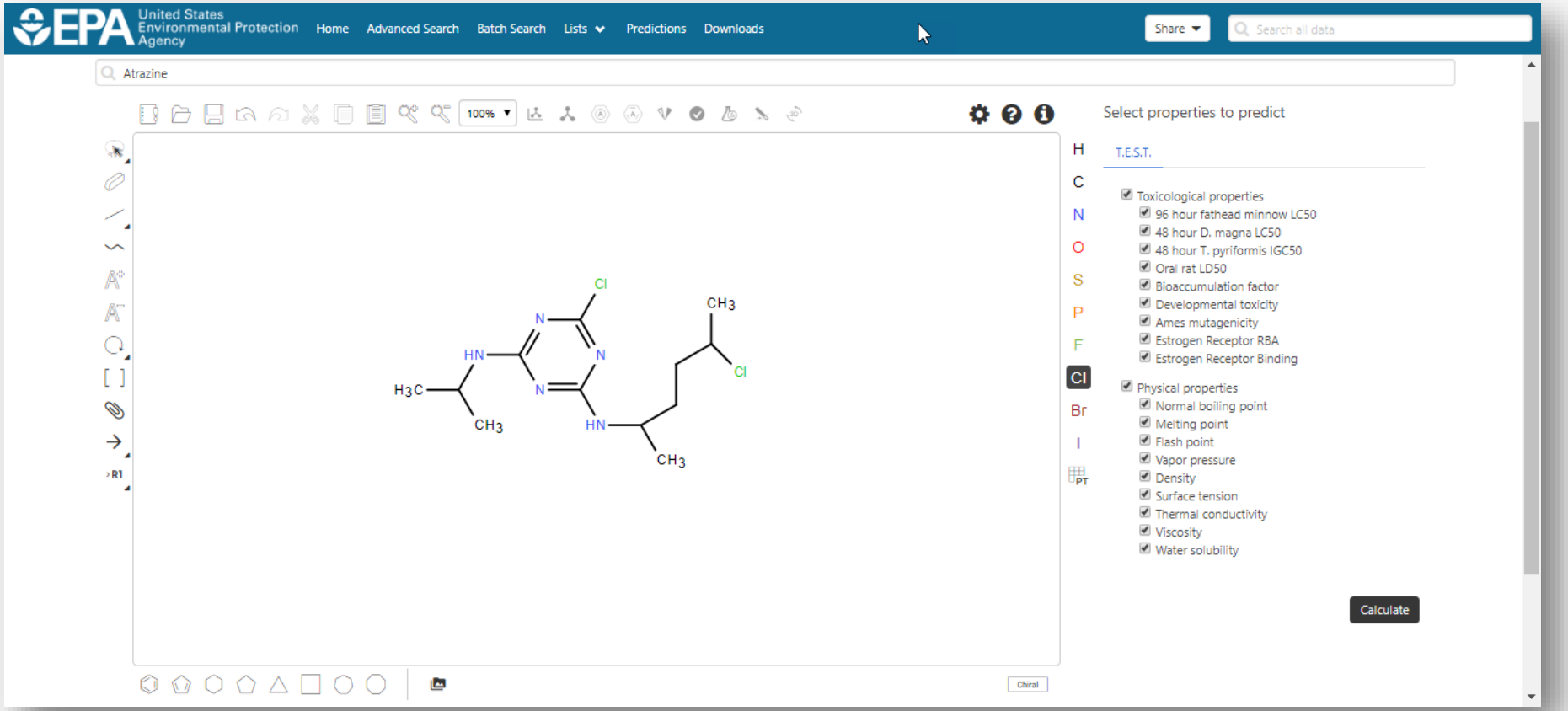
Batch Searching

- Singleton searches are useful but what if you need data on LOTS of chemicals at the same time…

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

REAL-TIME PREDICTIONS

Real-Time Predictions



Conclusions

- Computational toxicology encompasses many types of data streams that are integrated together to address different decision contexts both regulatory and non regulatory

- The EPA CompTox Chemicals Dashboard provides access to data for ~875,000 chemicals that addresses many of these data streams

Acknowledgements

EPA-RTP

- *An enormous team of contributors from CCTE, especially the IT software development team*
- *Our curation team for their care and focus on data quality*
- *Multiple centers and laboratories across the EPA*
- *Many public domain databases and open data contributors*

Contact for the CompTox Chemicals Dashboard

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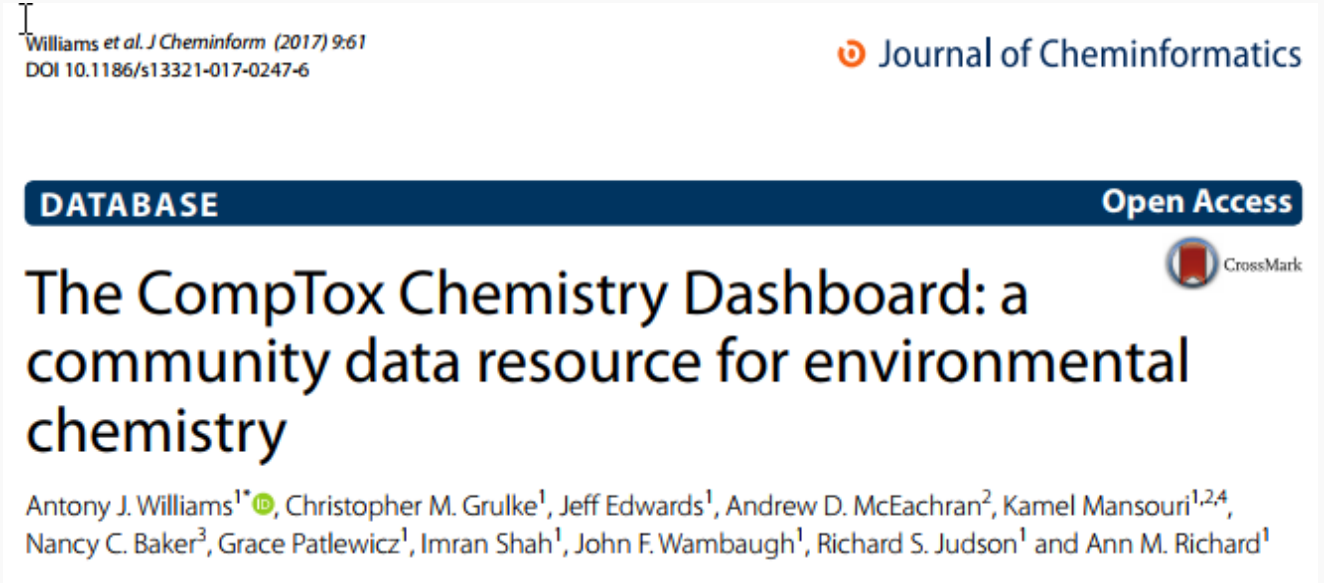

https://doi.org/10.1186/s13321-017-0247-6