New Computational Tools from EPA: The CompTox Chemicals Dashboard and Generalized Read Across

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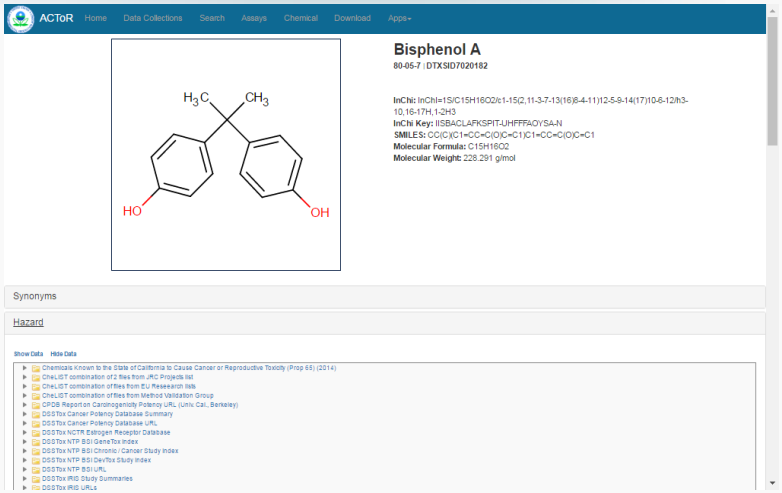
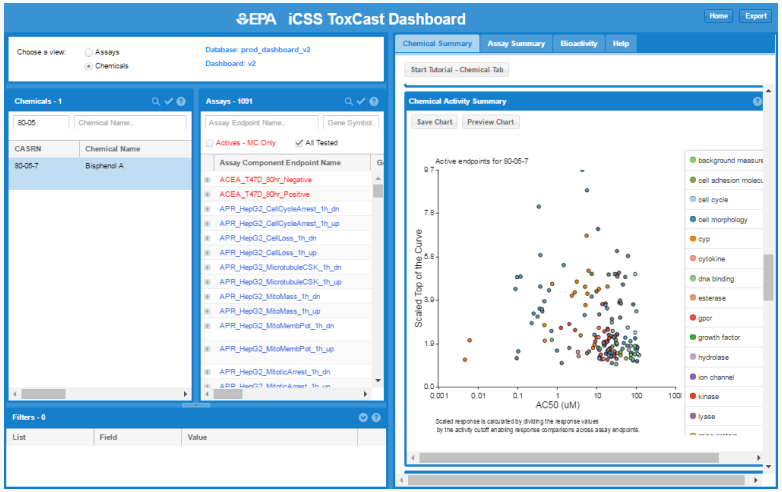
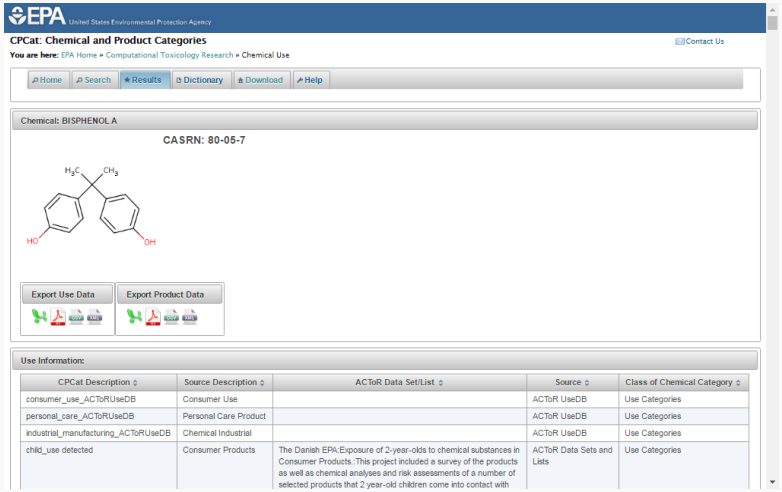
U.S. Environmental Protection Agency, RTP, NC

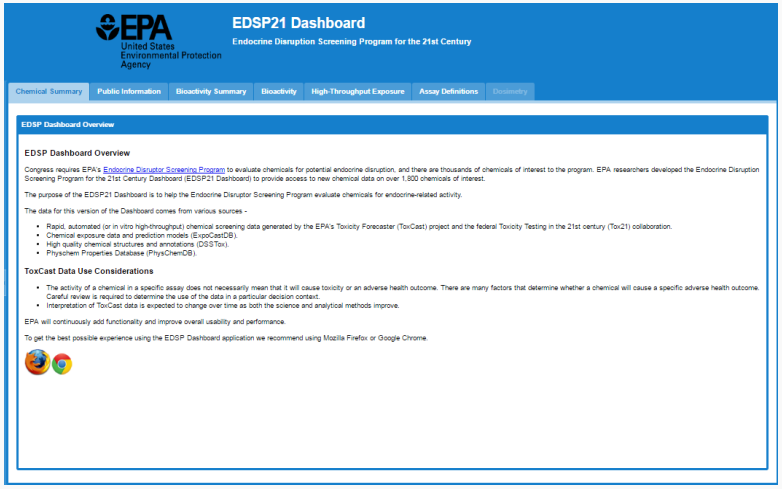
May 9th 2019

Earlier Dashboard Applications: Single architecture in development

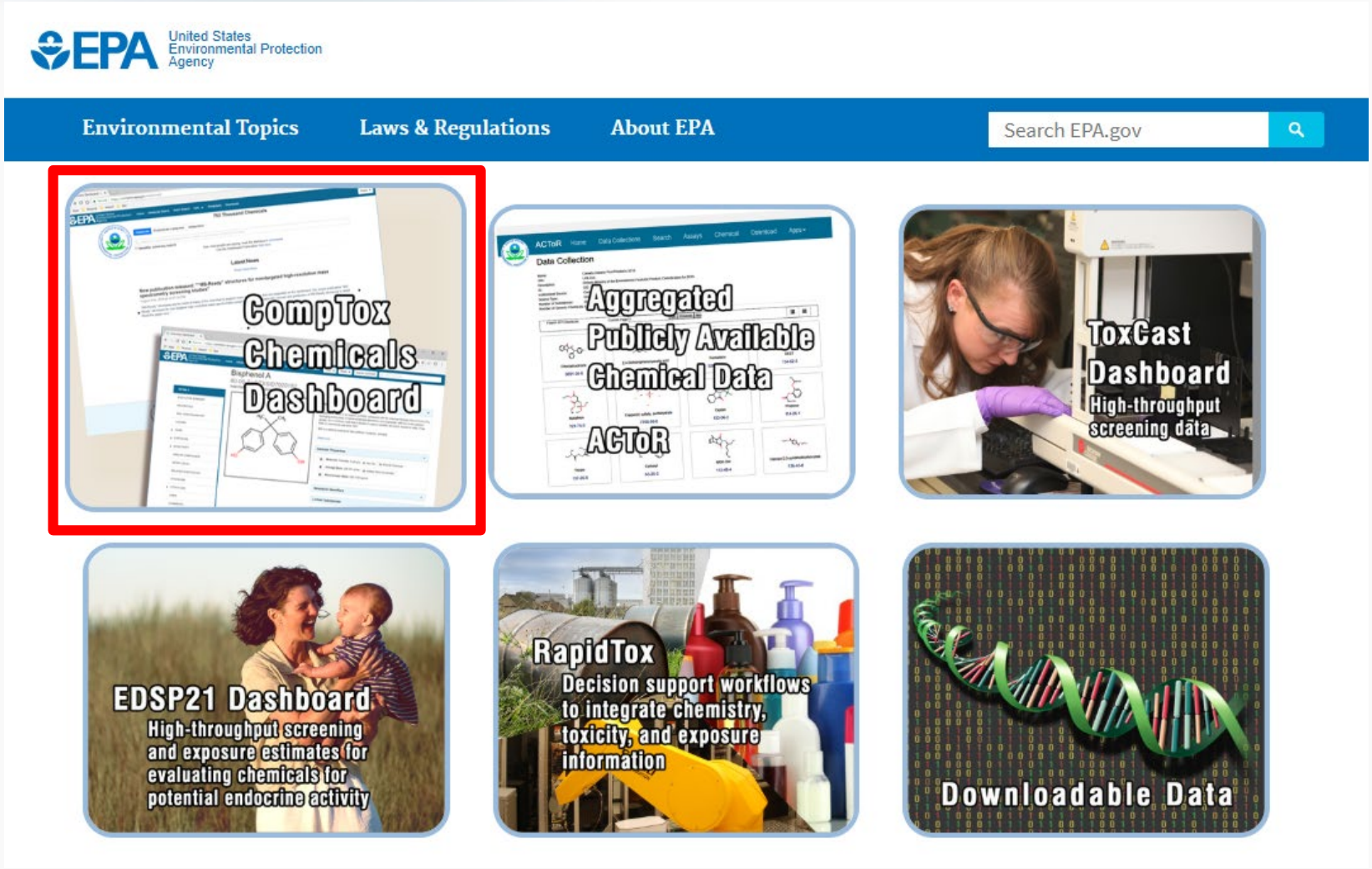








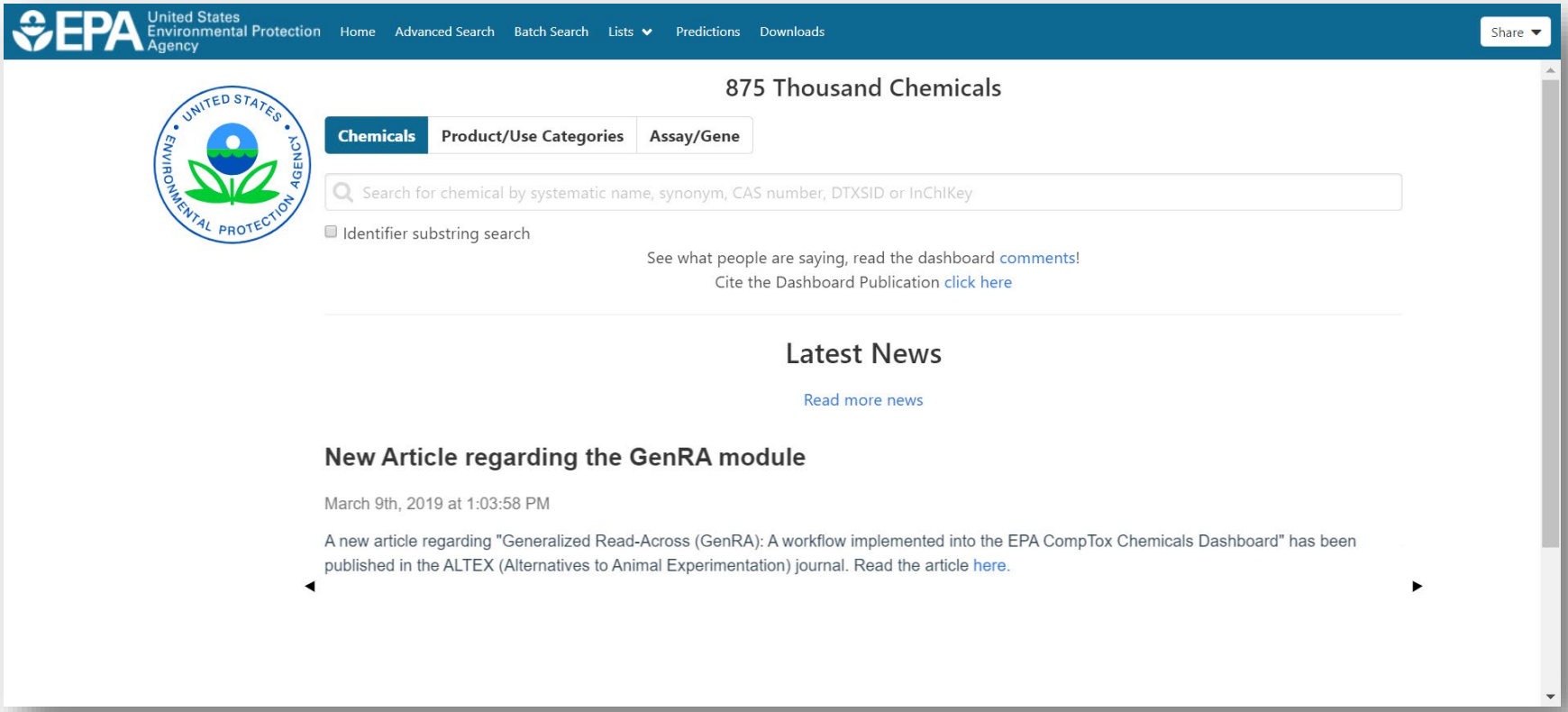
The CompTox Portal
https://comptox.epa.gov/



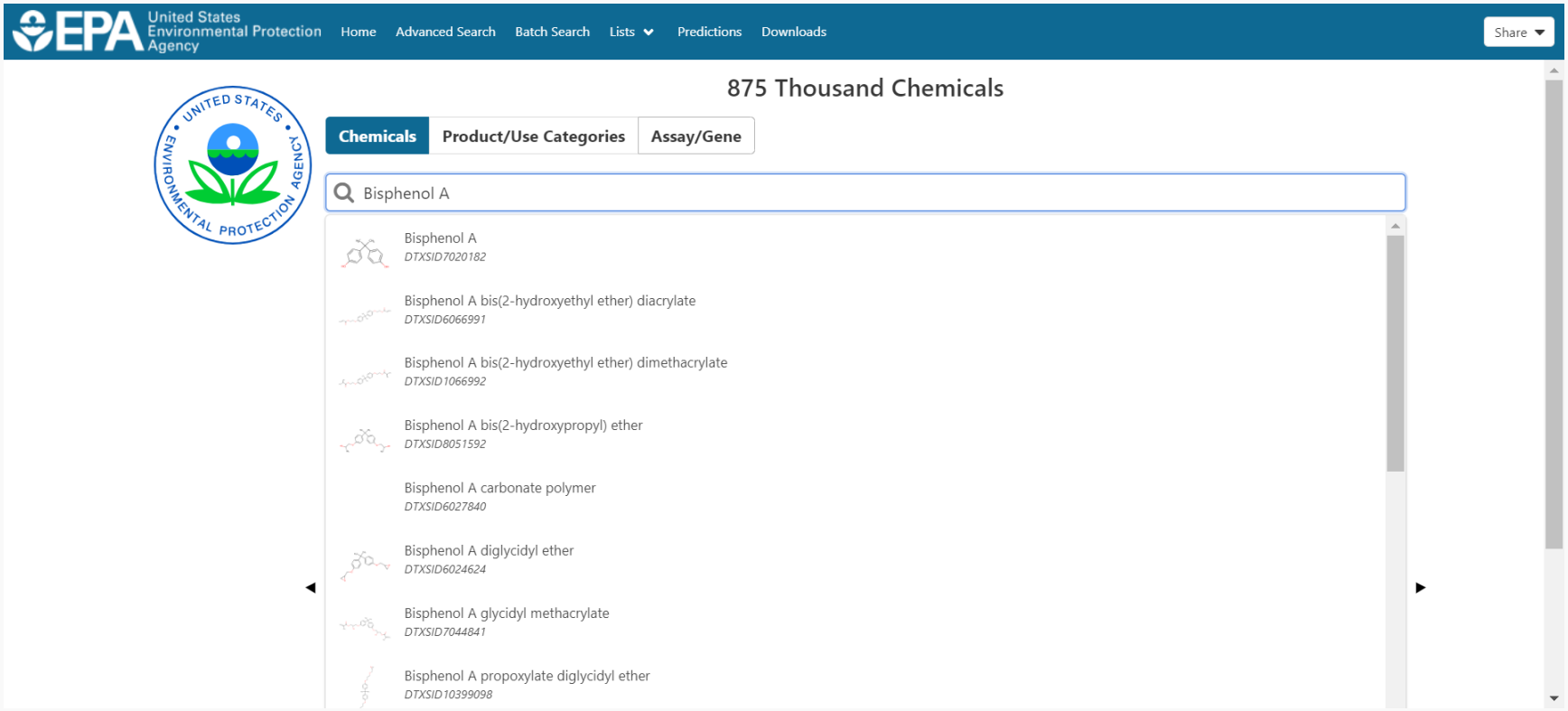
CompTox Chemicals Dashboard

- 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

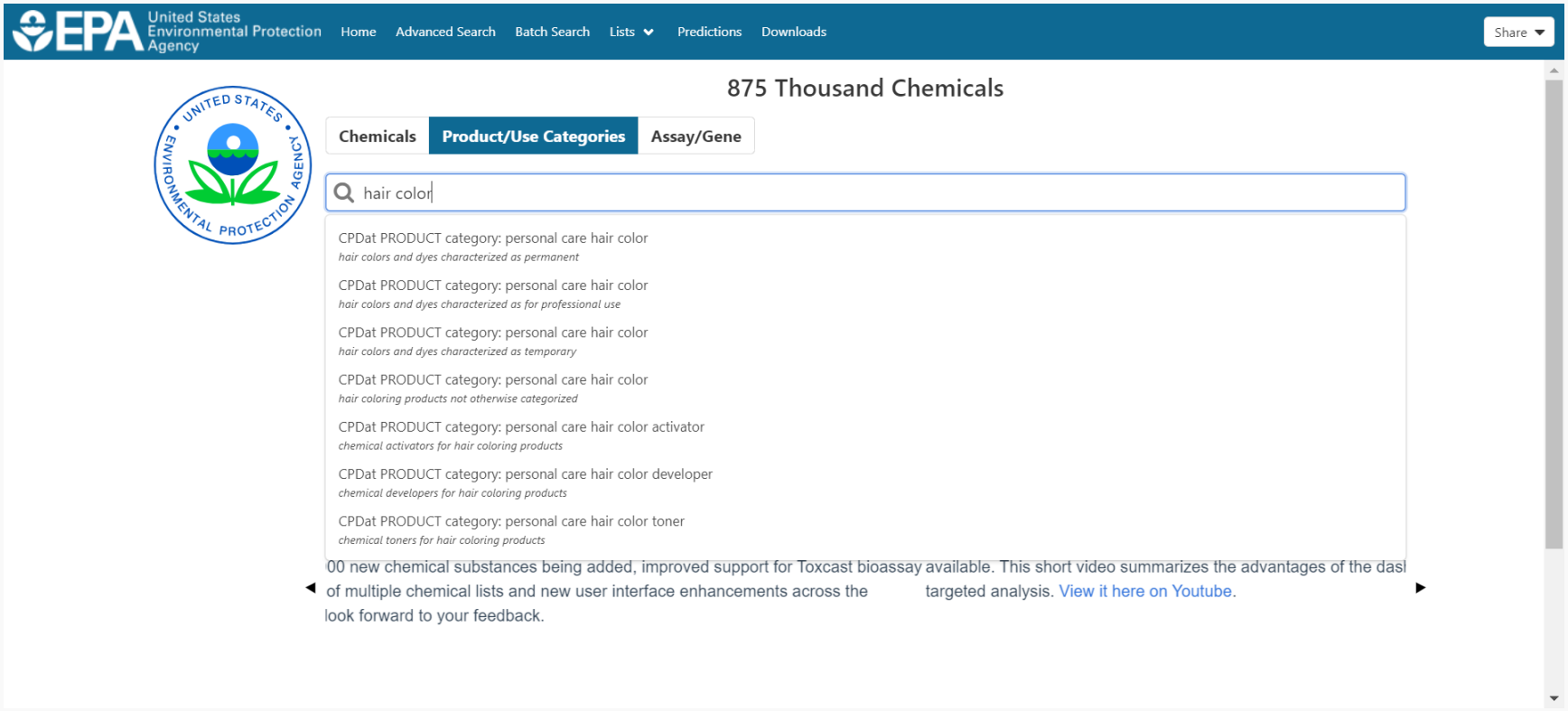
CompTox Chemicals Dashboard



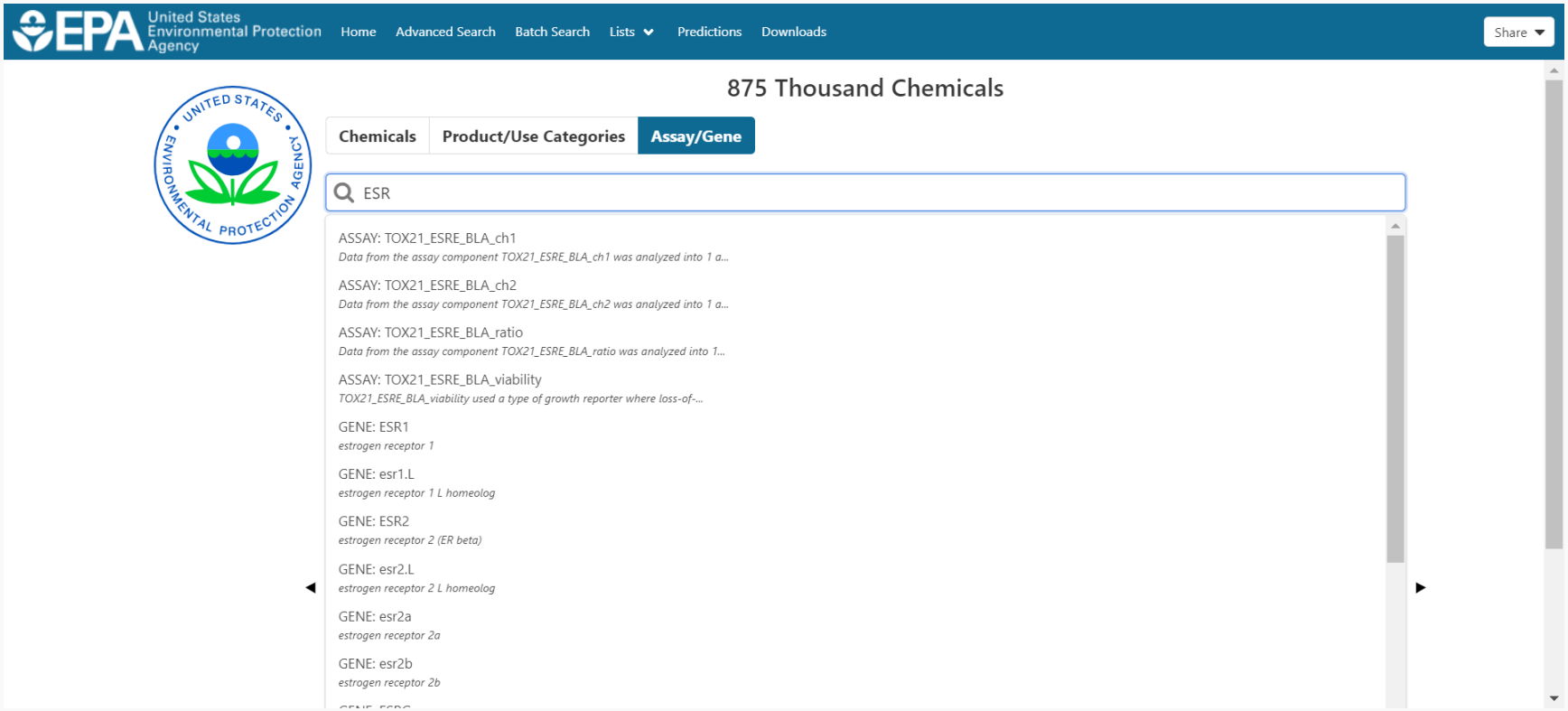
CompTox Chemicals Dashboard
Chemicals



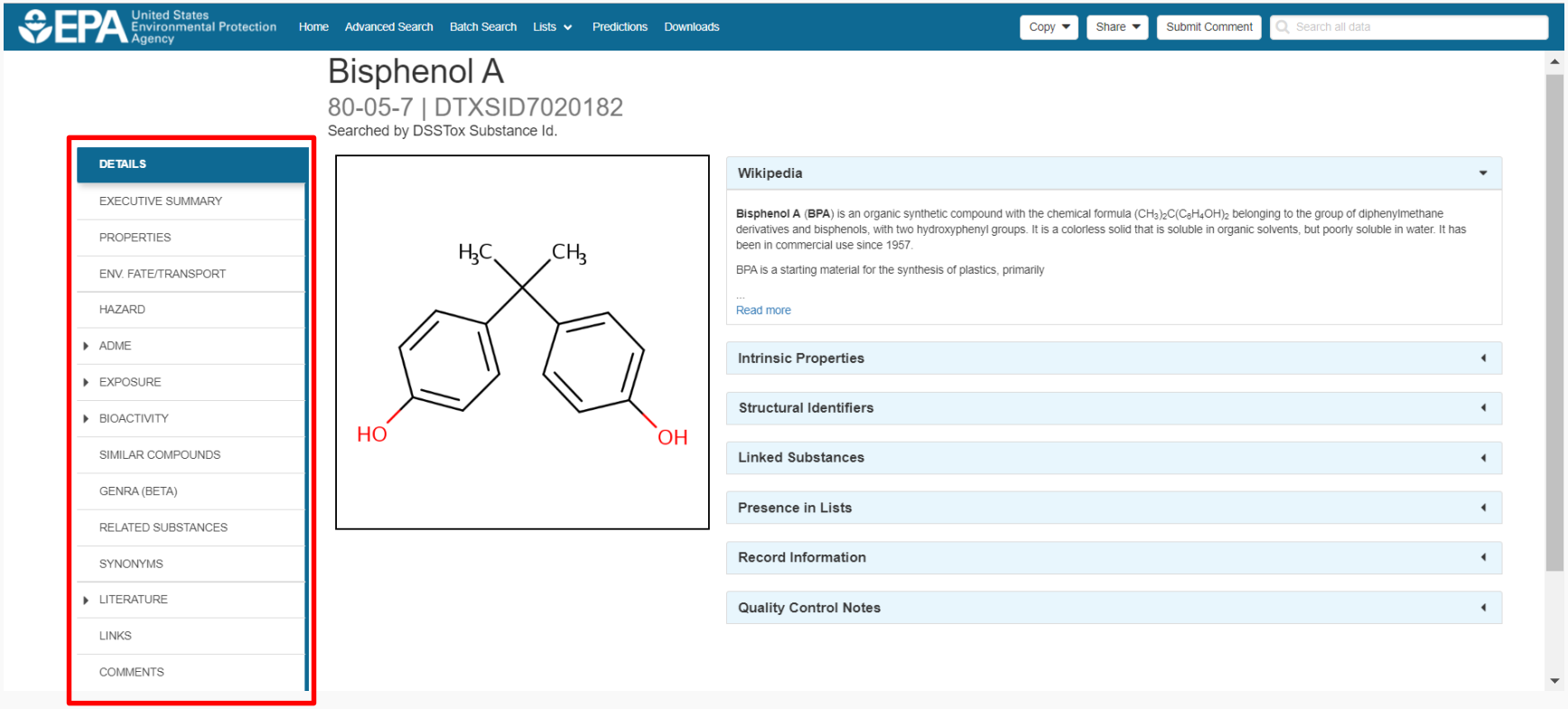
CompTox Chemicals Dashboard
Products and Use Categories



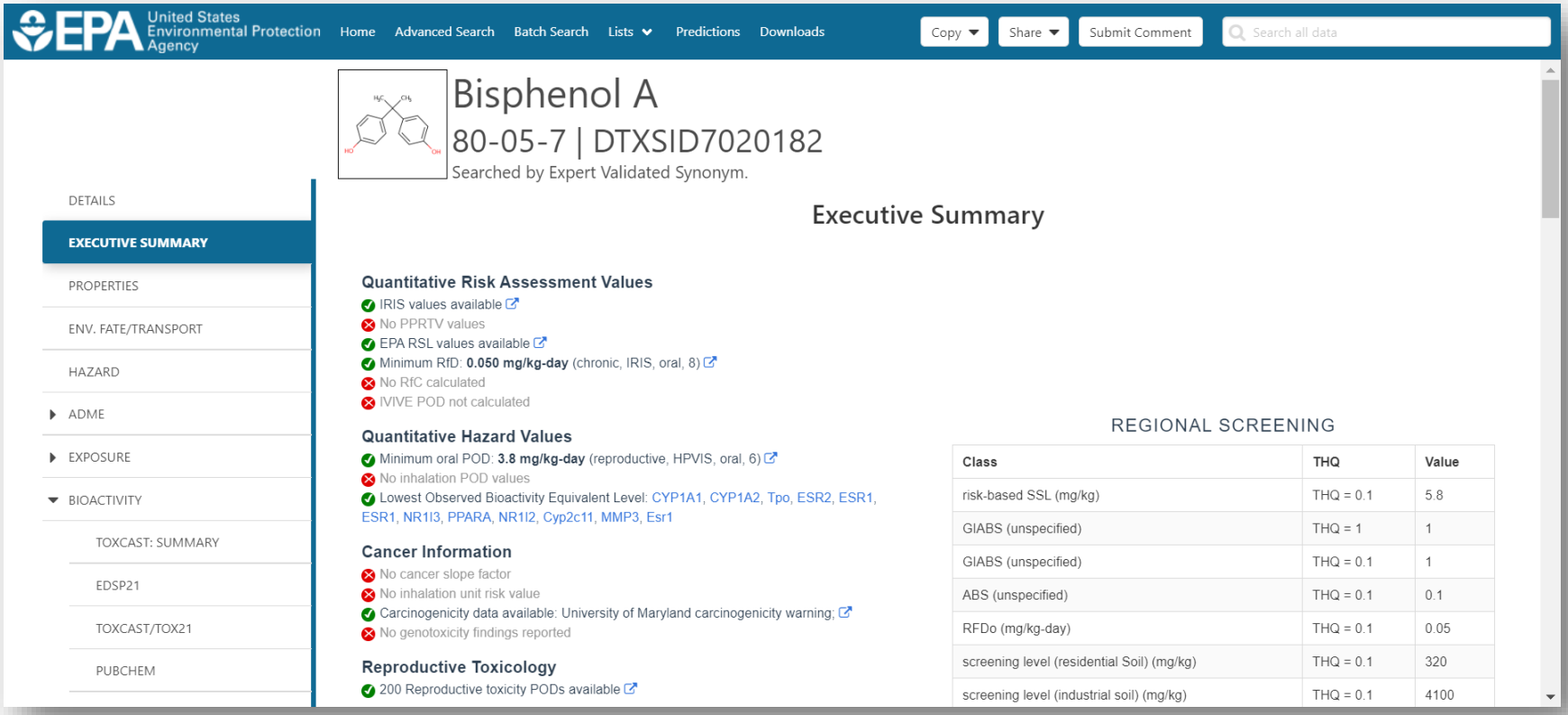
CompTox Chemicals Dashboard
Assays and Genes



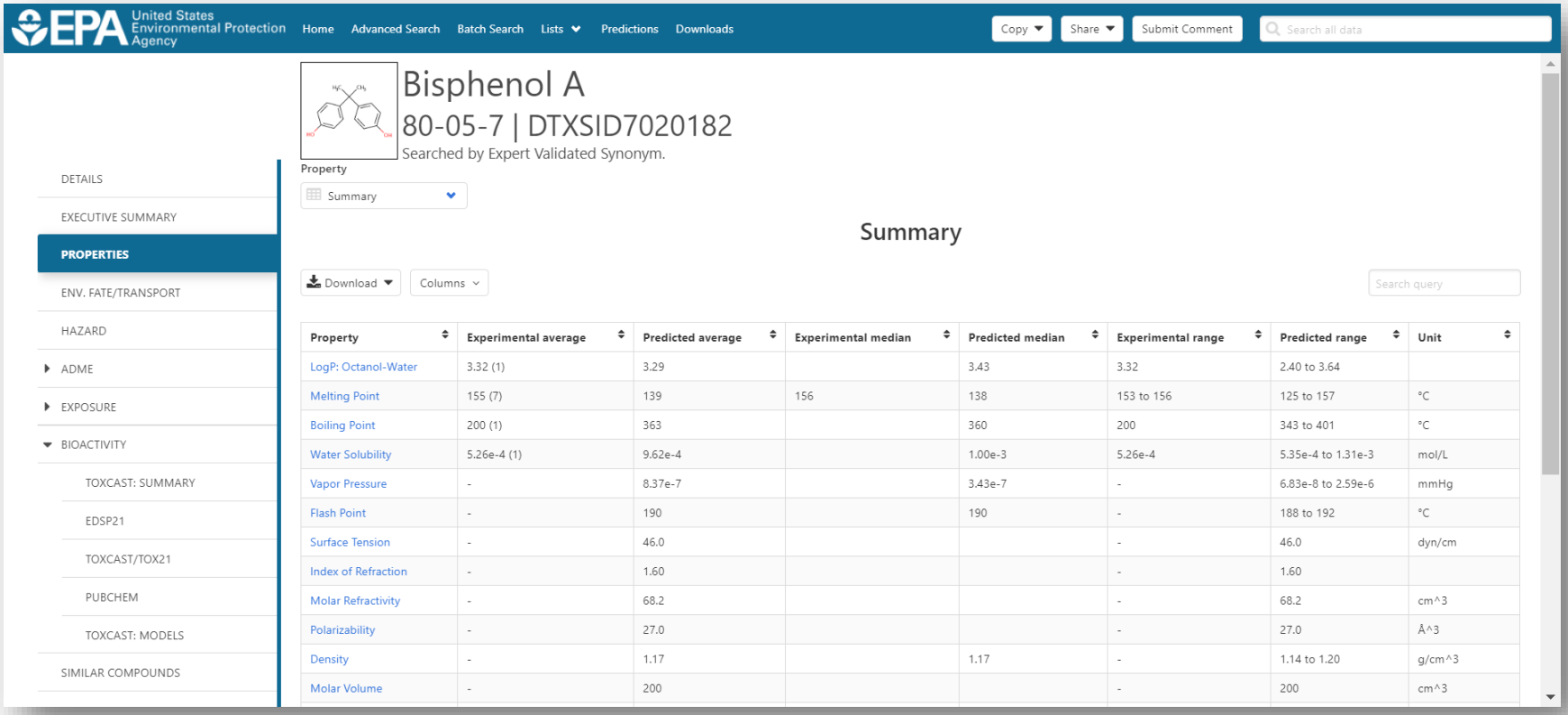
Detailed Chemical Pages



An “Executive Summary”



Physicochemical 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

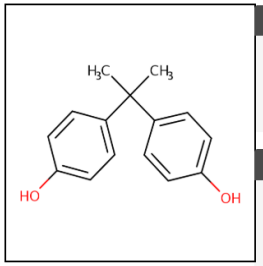
Detailed OPERA Prediction Reports

OPERA Models: LogP: Octanol-Water

Bisphenol A

80-05-7 | DTXSID7020182

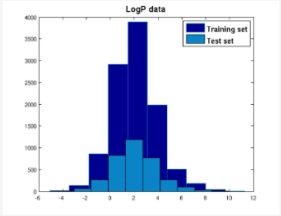
Print PDF

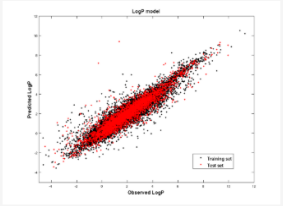


Model Results

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

Model Performance



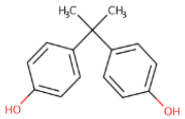


QMRF

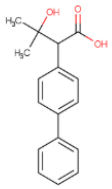
Weighted KNN model

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

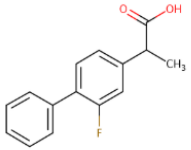
Nearest Neighbors from the Training Set



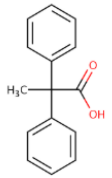
Bisphenol A
Measured:3.32
Predicted: 3.35076



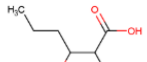
BUTANOIC ACID,2-(4-BIPHENYLYL)-3-HYDROXY-3-METHY
Measured:3.25
Predicted: 3.39062



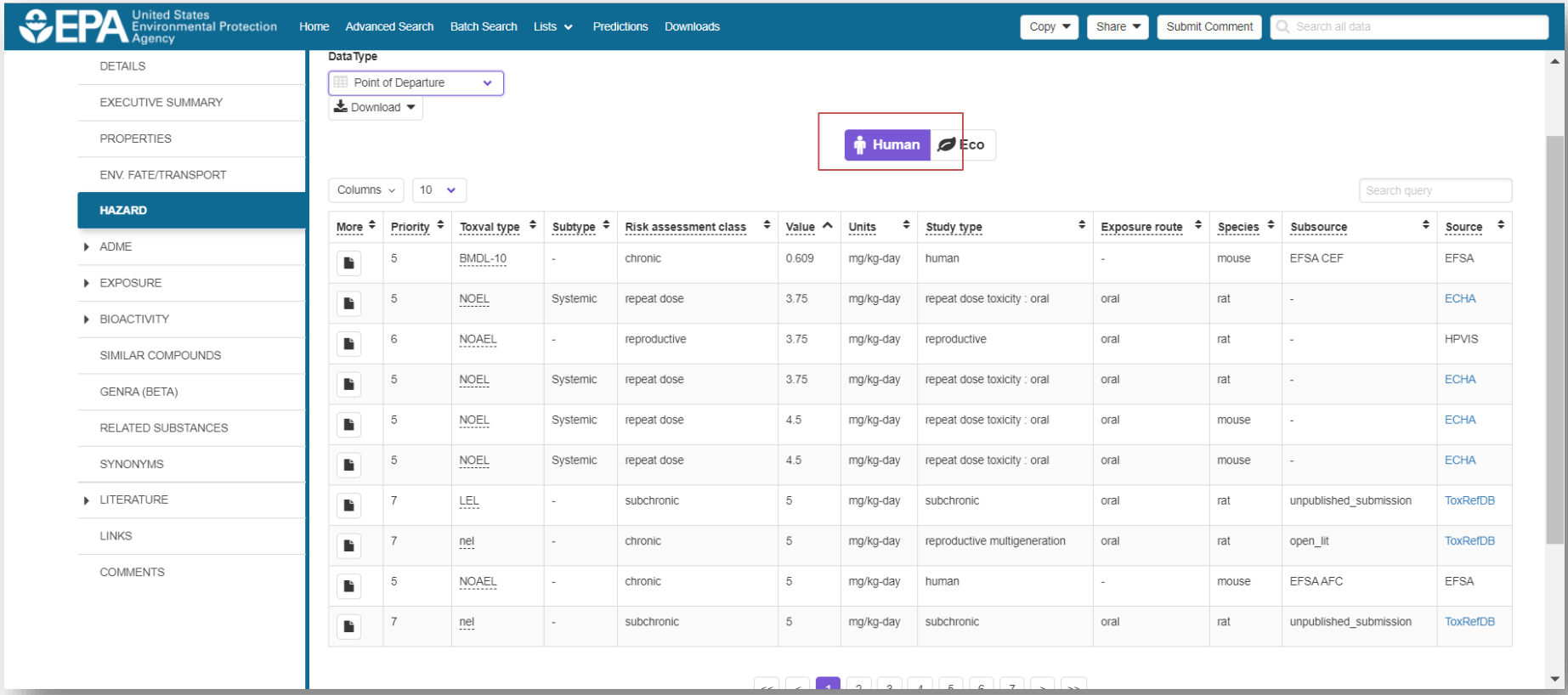
Flurbiprofen
Measured:4.16
Predicted: 3.94445



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



Other Data: Human and Ecological Chemical Hazard Data

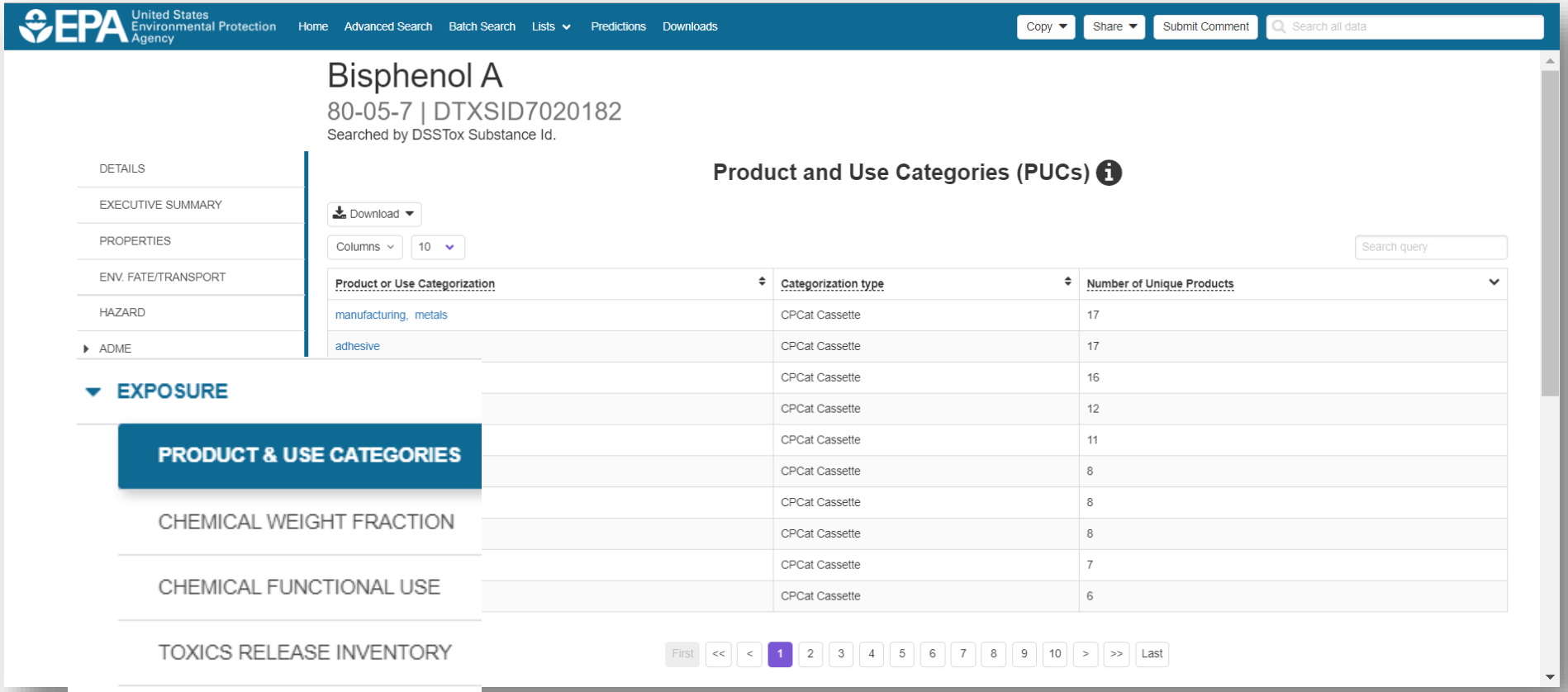


More	Priority	Toxval type	Subtype	Risk assessment class	Value	Units	Study type	Exposure route	Species	Subsource	Source
	5	BMDL-10	-	chronic	0.609	mg/kg-day	human	-	mouse	EFSA CEF	EFSA
	5	NOEL	Systemic	repeat dose	3.75	mg/kg-day	repeat dose toxicity : oral	oral	rat	-	ECHA
	6	NOAEL	-	reproductive	3.75	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

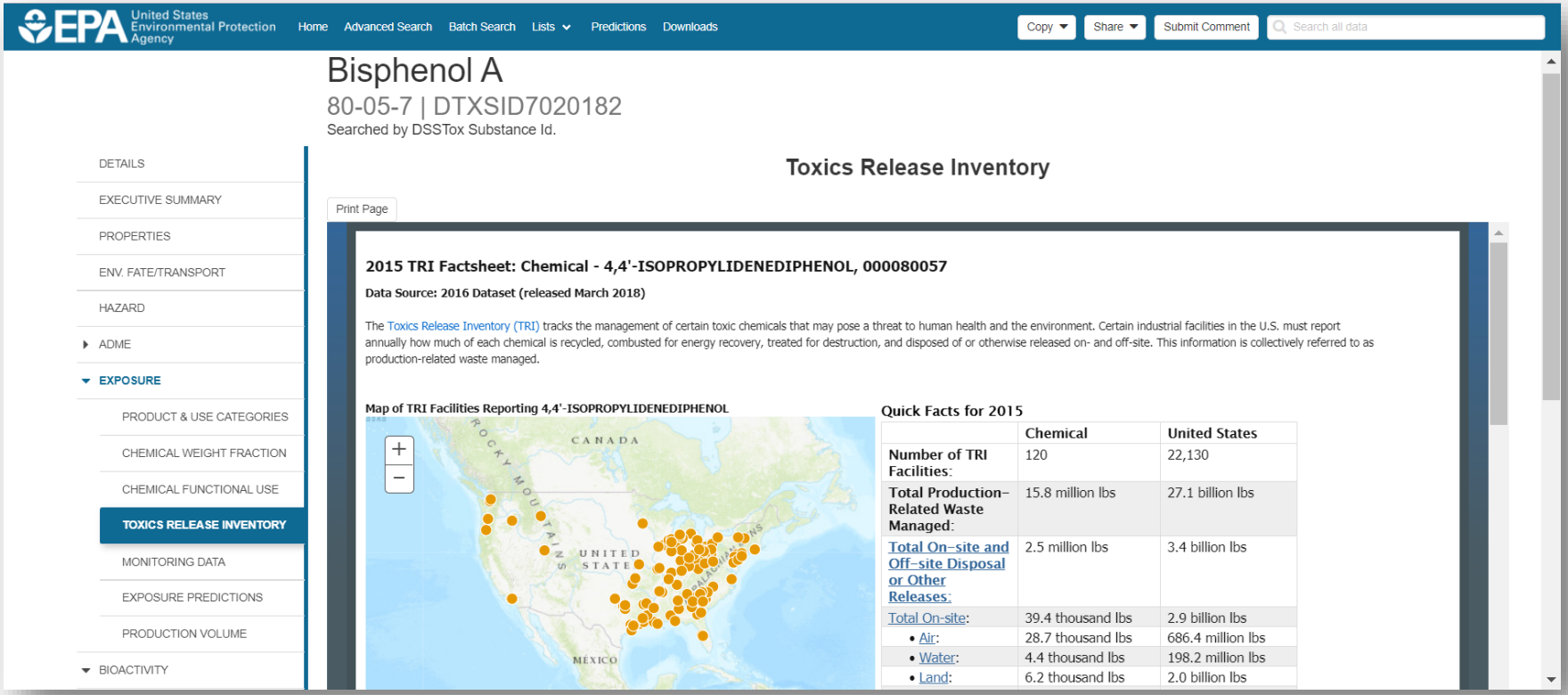
Hazard Data from “ToxVal_DB”

- ToxVal Database contains following data:
  - 30,050 chemicals
  - 772,721 toxicity values
  - 29 sources of data
  - 21,507 sub-sources
  - 4585 journals cited
  - 69,833 literature citations

Sources of Exposure to Chemicals

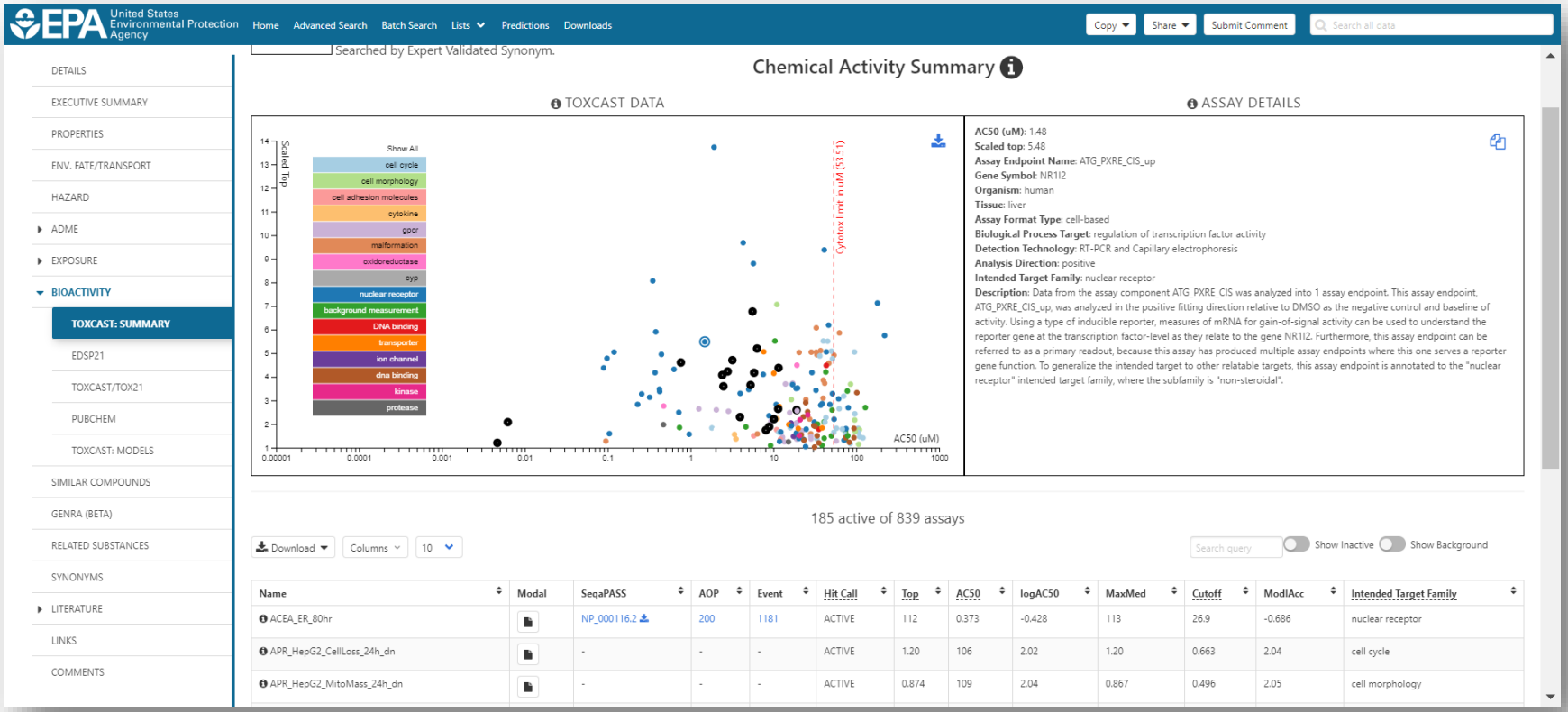


Sources of Exposure to Chemicals



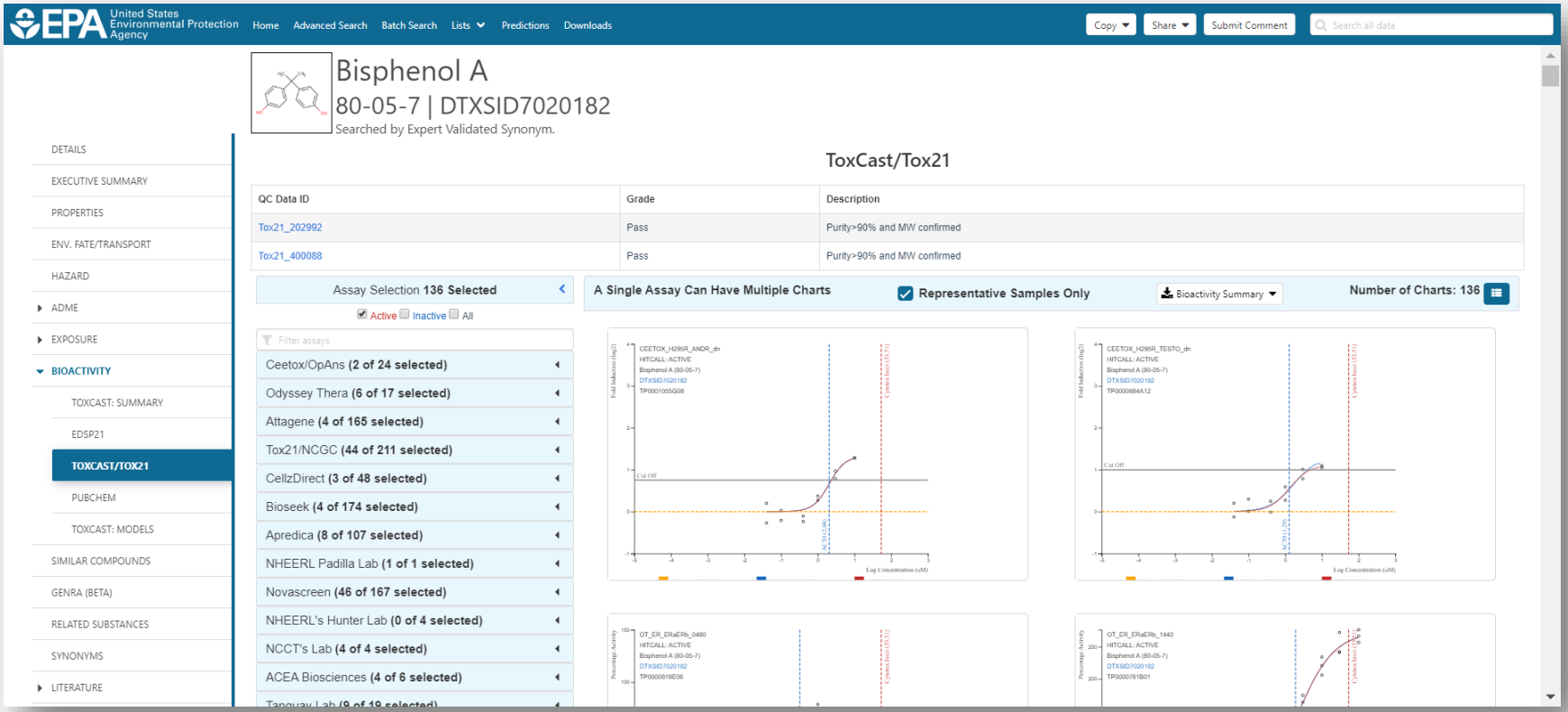
In Vitro Bioassay Screening

ToxCast and Tox21



In Vitro Bioassay Screening

ToxCast and Tox21



Bioactivity: Downloadable Data

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

EPA United States Environmental Protection Agency

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

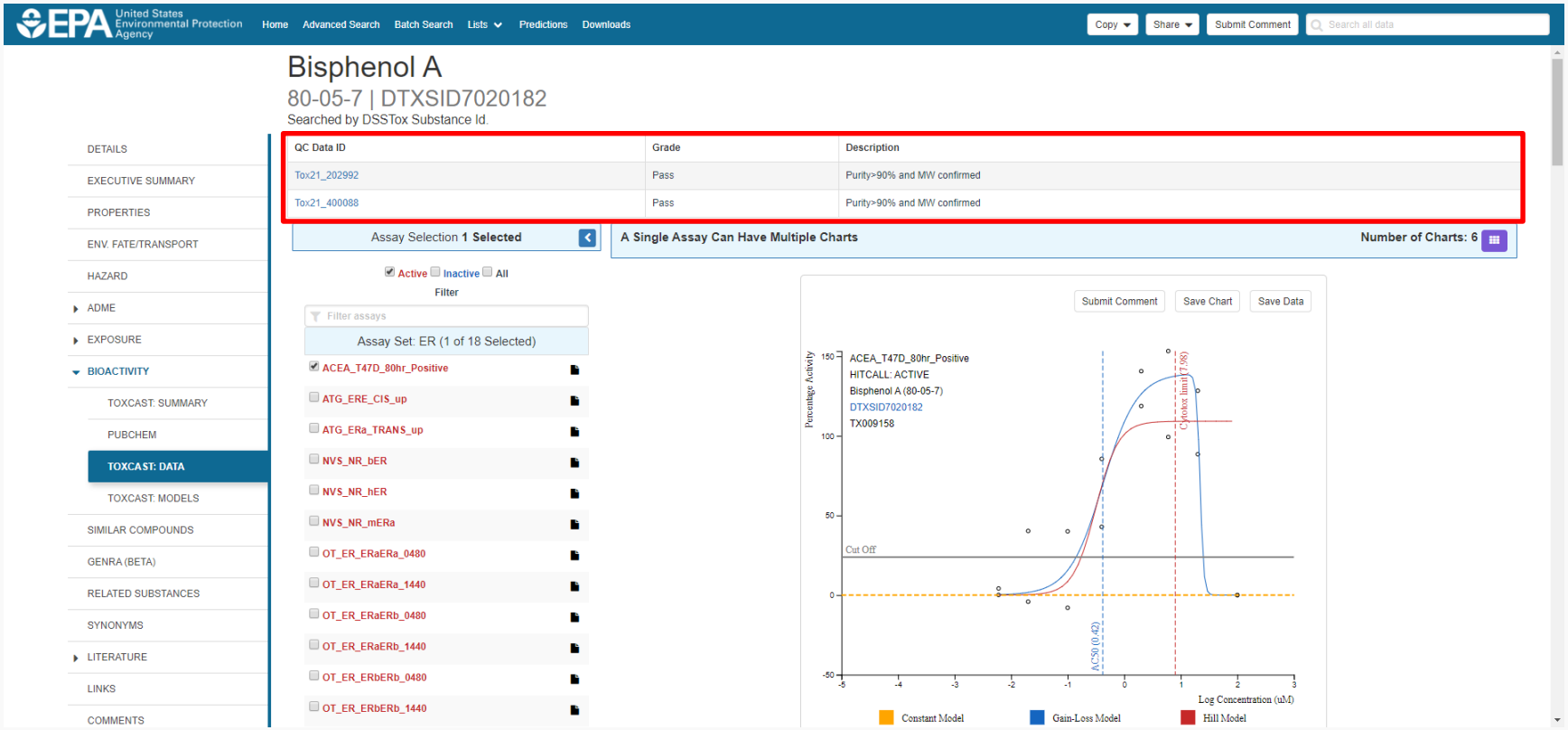
Resources

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

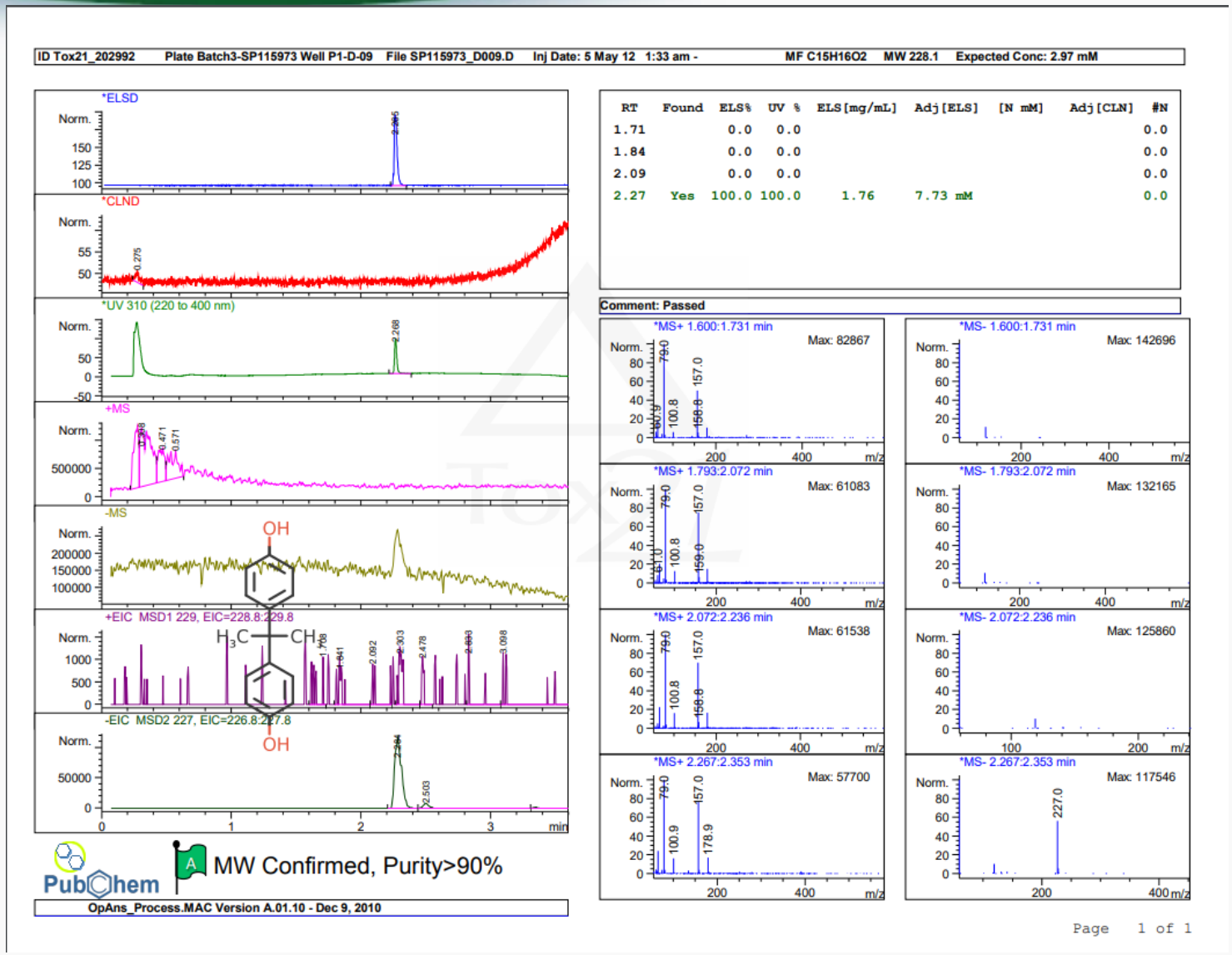
ToxCast Data and Information

- **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

ToxCast/Tox21 Data
Analytical QC of the chemicals

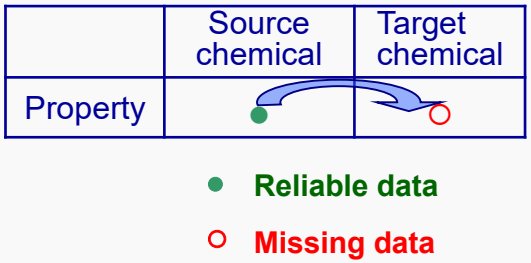


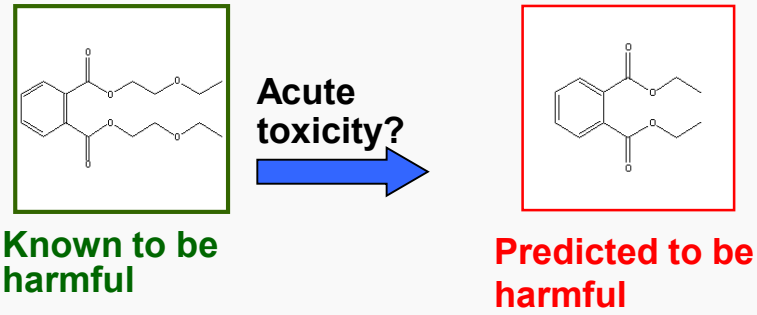
Access to Analytical QC Data



GenRA (Generalised Read-Across)

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



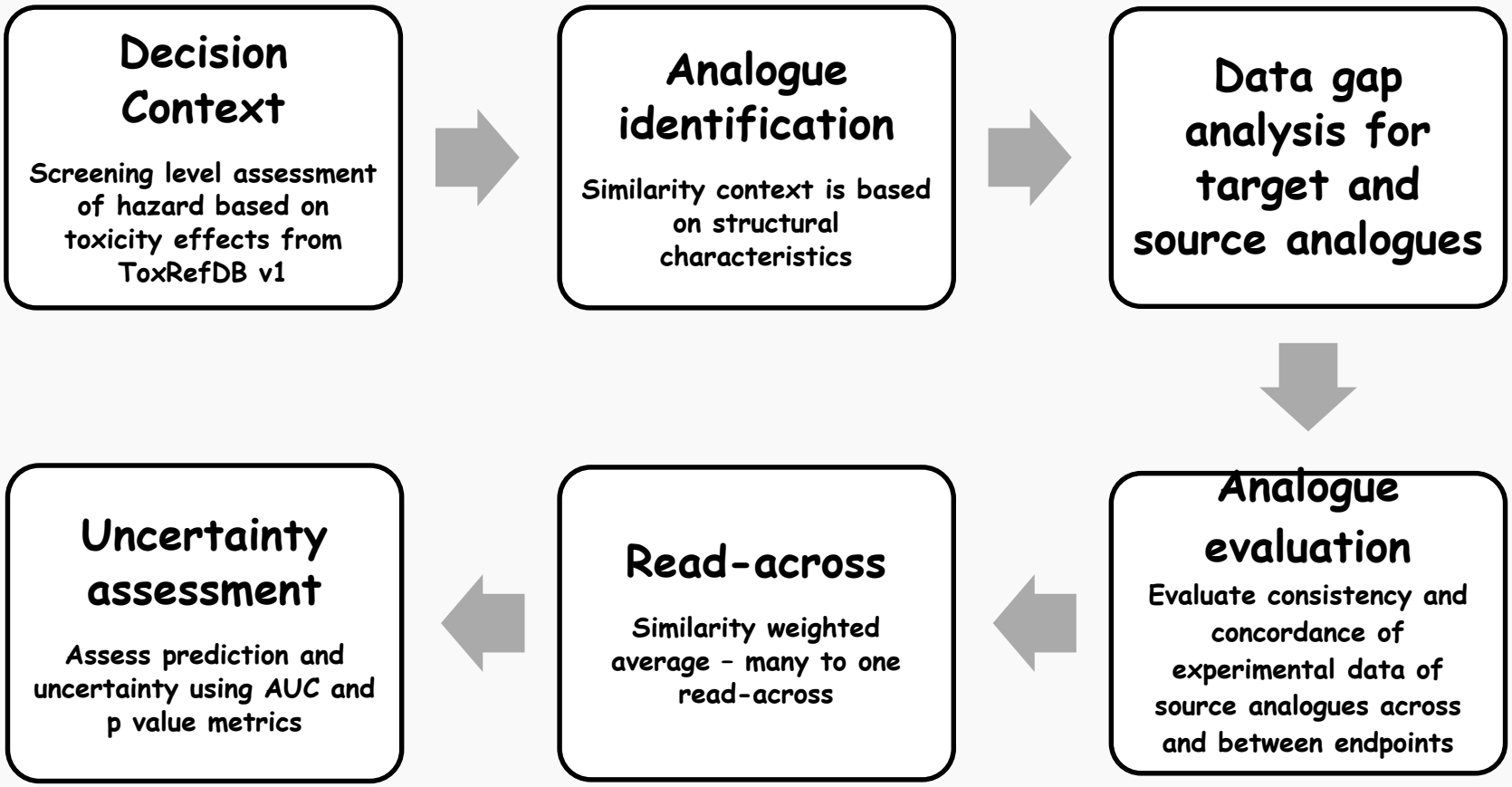


GenRA (Generalised Read-Across)

- Predicting toxicity as a similarity-weighted activity of nearest neighbors based on chemistry and/or bioactivity descriptors
- Systematically evaluates read-across performance and uncertainty using available data

Jaccard similarity:

Implementing GenRA within the workflow



GenRA tool in practice

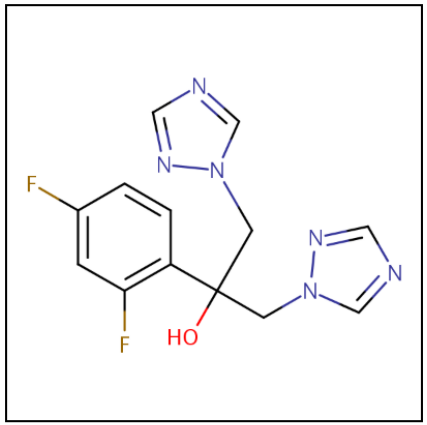
EPA United States Environmental Protection Agency

Fluconazole

86386-73-4 | DTXSID3020627

Searched by DSSTox Substance Id.

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



Wikipedia

Fluconazole is an antifungal medication used for a number of fungal infections. This includes candidiasis, blastomycosis, coccidiodomycosis, cryptococcosis, histoplasmosis, dermatophytosis, and pityriasis versicolor. It is also used to prevent candidiasis in those who are at high risk such as following organ transplantation, low birth weight babies, and those with low blood neutrophil counts. It is given either by mouth or by injection into a vein.

Common side effects include vomiting

...

Read more

Intrinsic Properties

Molecular Formula: $C_{13}H_{12}F_2N_6O$ Mol File

Find All Chemicals

Average Mass: 306.277 g/mol Isotope Mass Distribution

Monoisotopic Mass: 306.104065 g/mol

Structural Identifiers

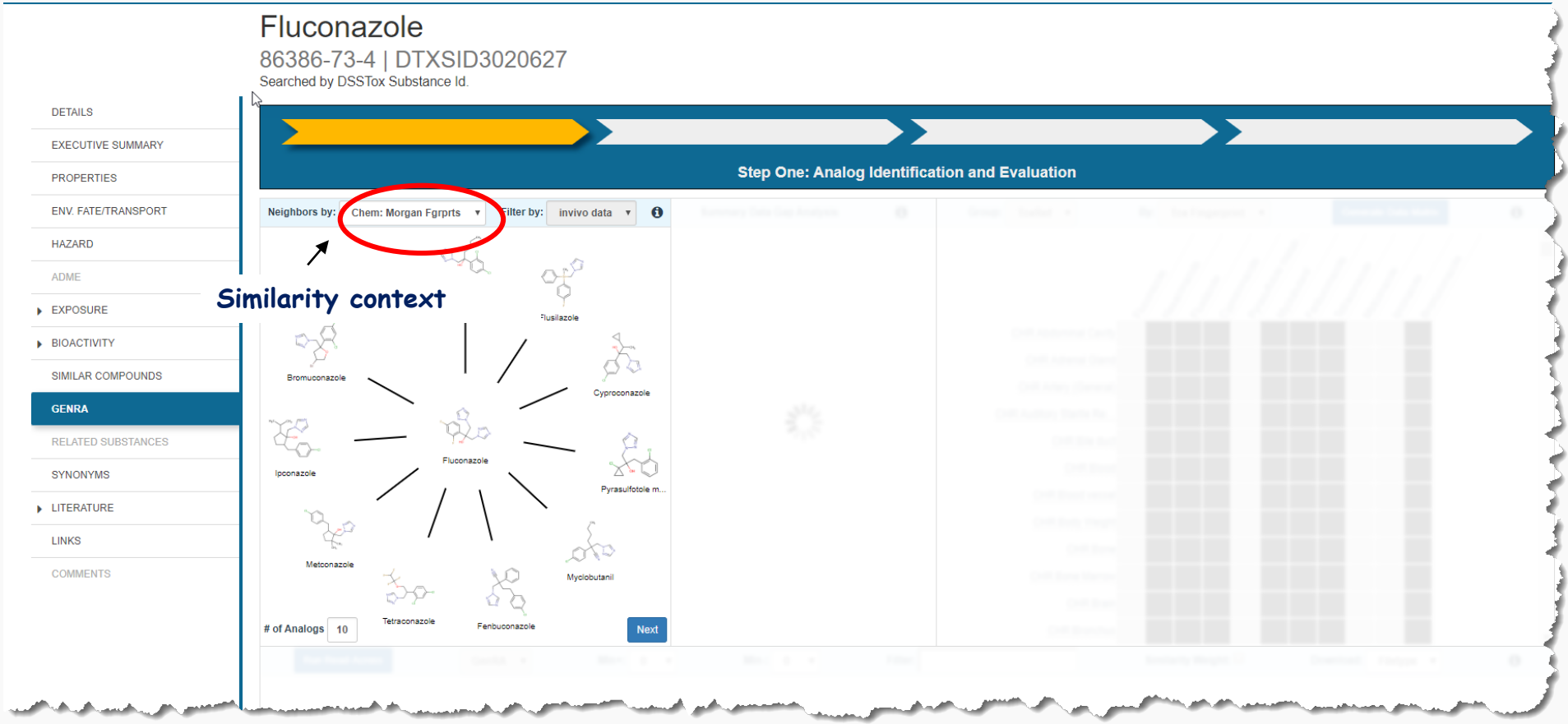
Linked Substances

Presence in Lists

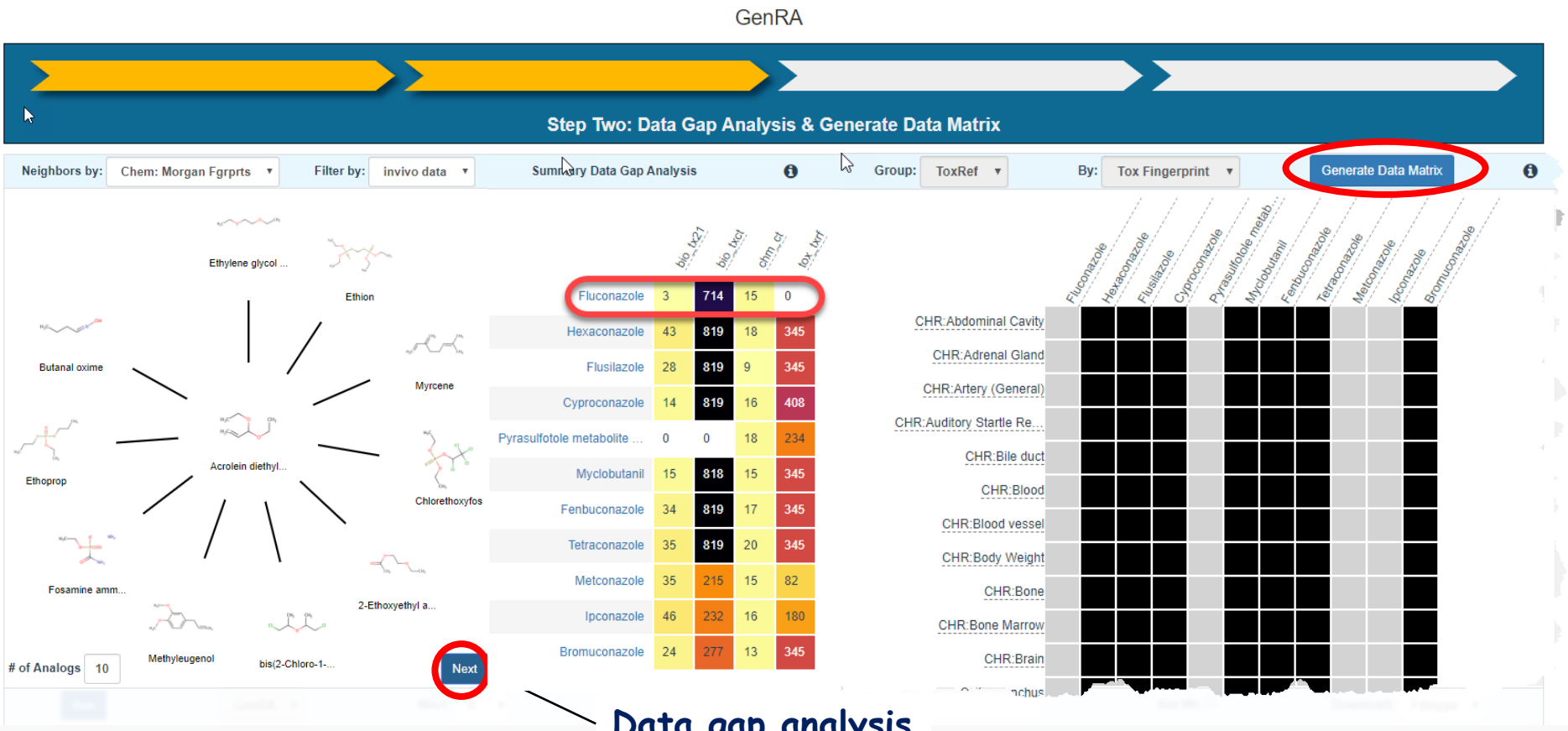
Record Information

Quality Control Notes

GenRA tool in practice



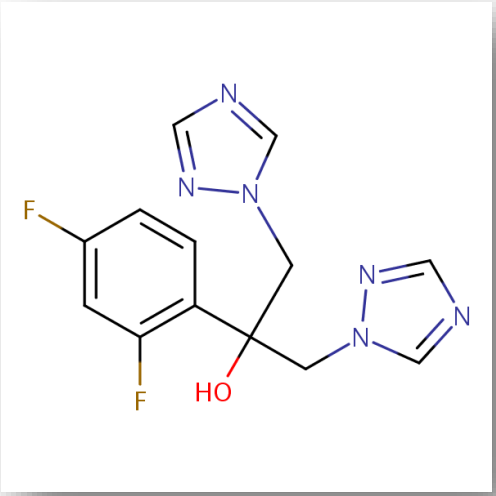
GenRA tool in practice



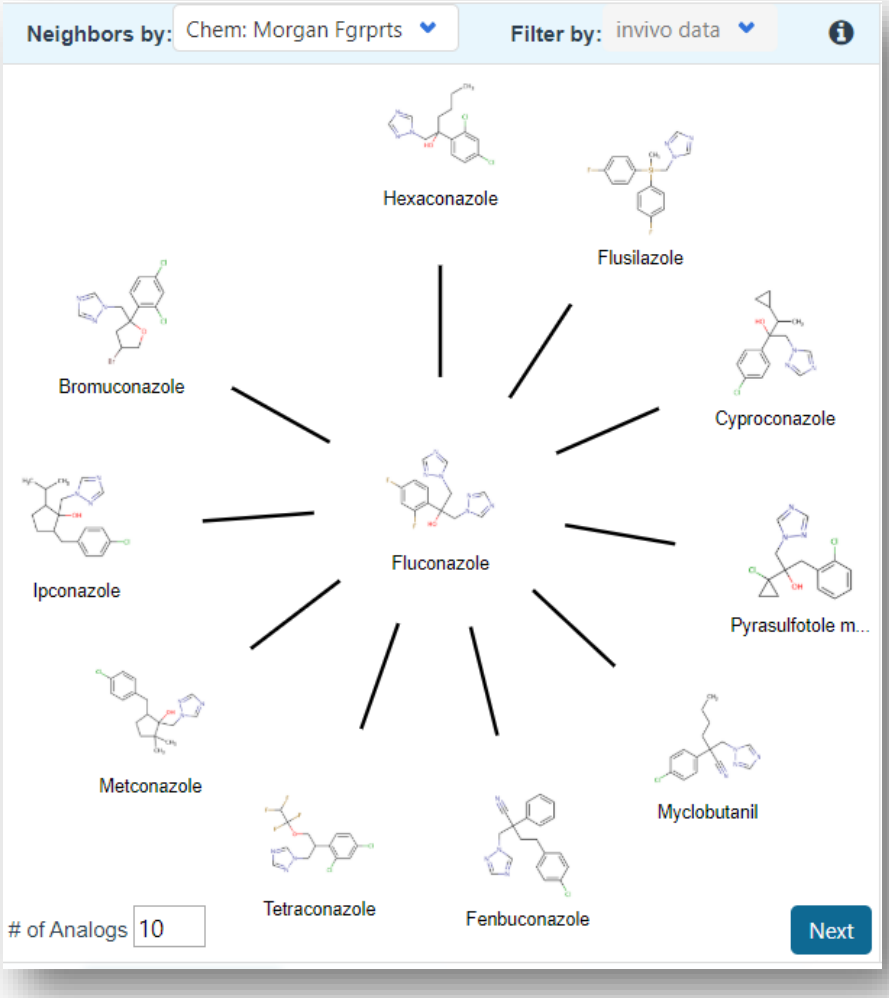
Data gap analysis

GenRA tool in practice

GenRA in practice – step by step

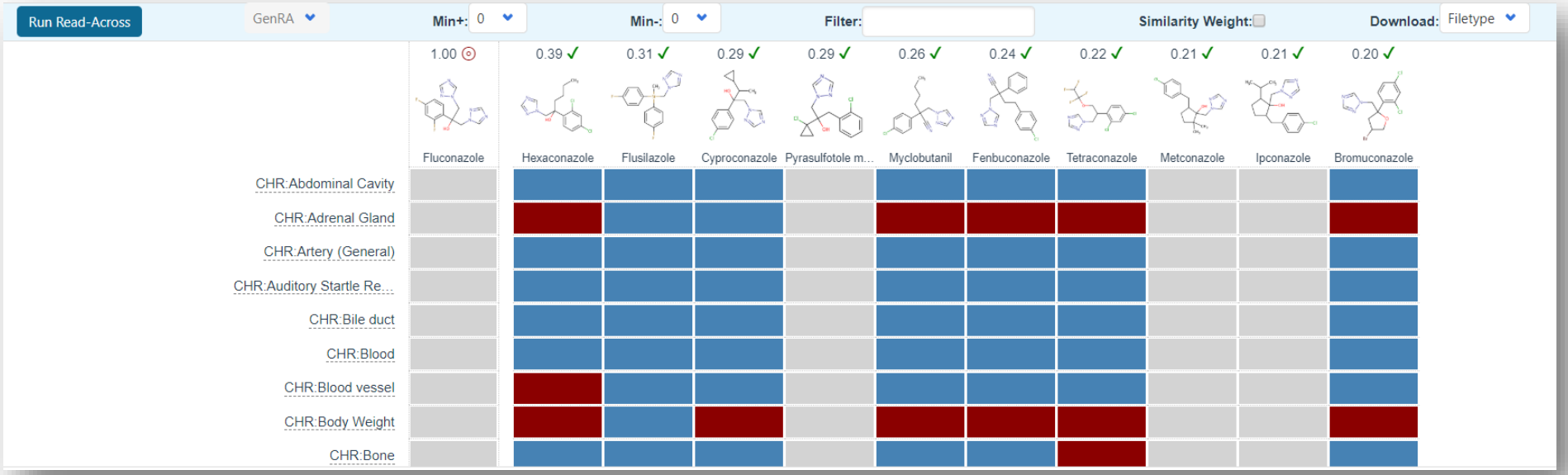


- Analogue identification:
- Similarity based on Morgan chemical fingerprints and selecting a default of 10 source analogues

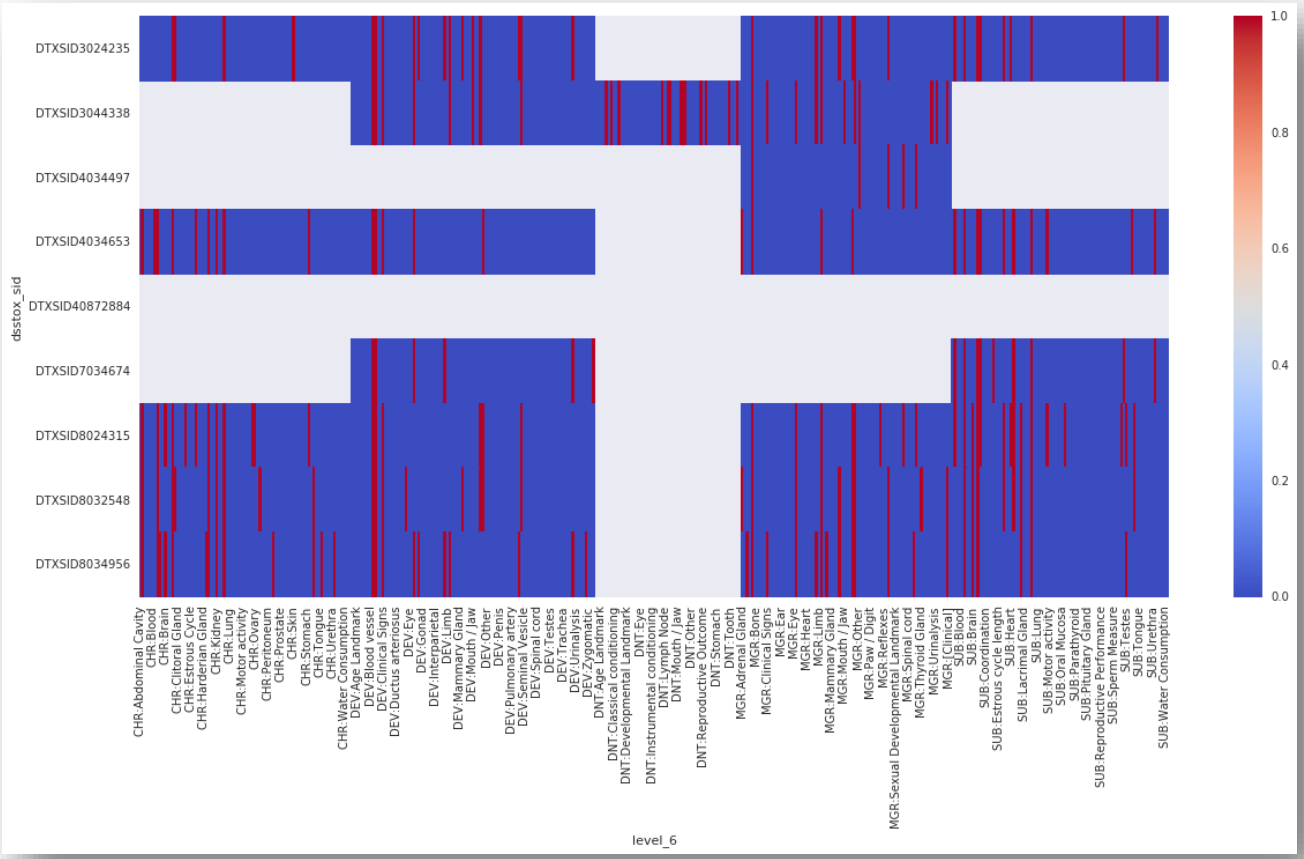


GenRA in practice – step by step

Data matrix view of source analogues relative to target chemical



Data matrix for source substances

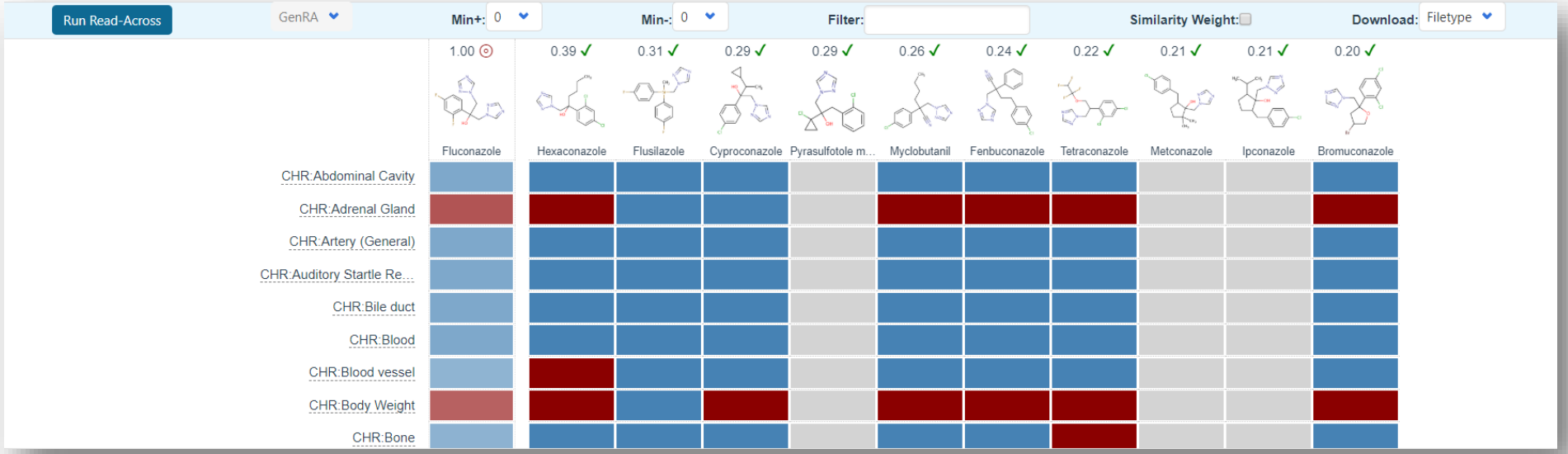


Look for commonality in profile across target effects

What are the most common effects across analogues

GenRA in practice – step by step

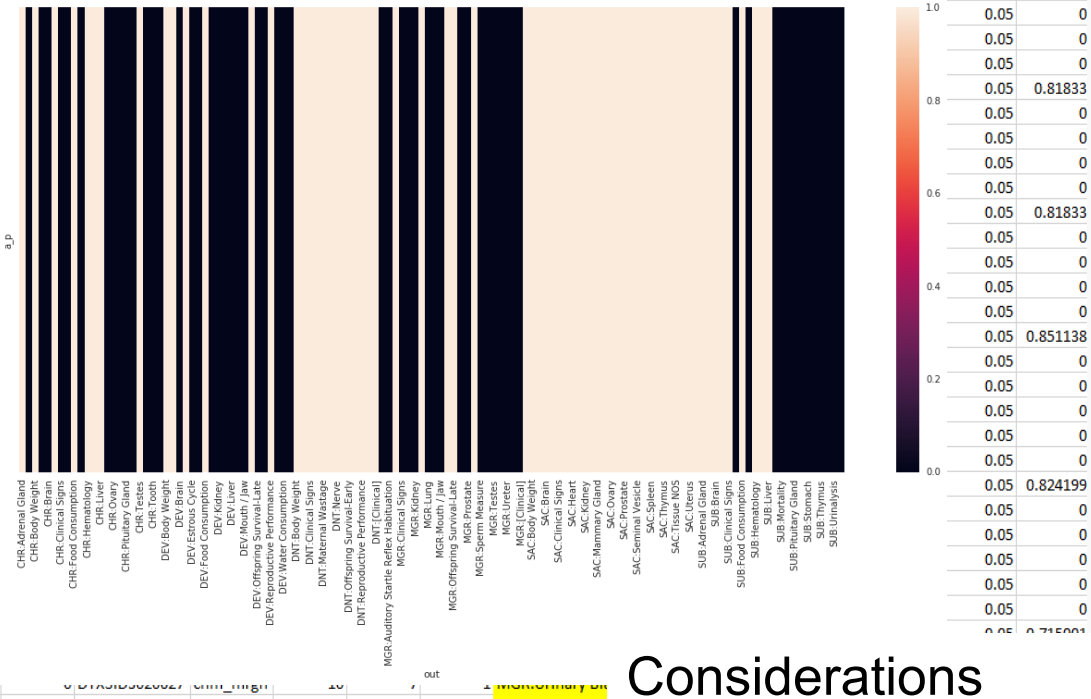
Updated Data matrix view with GenRA predictions for target chemical



- Predictions are binary (yes/no) for toxicity effects within ToxRefDB v1 studies.
- Predictions summarized on a study level basis. Red: “positive” and Blue: “negative”.

GenRA in practice: Approach

a_p	a_s	a_t	auc	dsstox_sid	fp	k0	n_neg	n_pos	out	p_val	pred	s0	t0
0	0.131		0	DTXSID3020627	chm_mrgn	10	5	1	CHR:Heart	0.75	Neg	0.05	0
0	0.108		0	DTXSID3020627	chm_mrgn	10	6	1	SUB:Esophagus	0.8	Neg	0.05	0
0	0.131		0	DTXSID3020627	chm_mrgn	10	5	1	CHR:Tooth	0.81	Neg	0.05	0
0	0.15											0.05	0
0	0.203											0.05	0
0	0.15											0.05	0
1	0.817											0.05	0.81833
0	0.131											0.05	0
0	0.139											0.05	0
0	0.131											0.05	0
0	0.101											0.05	0
1	0.817											0.05	0.81833
0	0.129											0.05	0
0	0.131											0.05	0
0	0.131											0.05	0
0	0.131											0.05	0
1	0.904											0.05	0.851138
0	0.228											0.05	0
0	0.151											0.05	0
0	0.134											0.05	0
0	0.108											0.05	0
0	0.101											0.05	0
1	0.869											0.05	0.824199
0	0.151											0.05	0
0	0.094											0.05	0
0	0.131											0.05	0
0	0.108											0.05	0
0	0.163											0.05	0
1	0.72											0.05	0
0	0.281											0.05	0.715091
0	0.129												
0	0.492		0	DTXSID3020627	chm_mrgn	10	3	3	CHR:Clinical Sig				
0	0.102		0	DTXSID3020627	chm_mrgn	10	7	1	DEV:Water Cons				
0	0.129		0	DTXSID3020627	chm_mrgn	10	7	1	MGR:Mouth / Ja				
0	0.297		0	DTXSID3020627	chm_mrgn	10	5	2	SUB:Heart				



Considerations

- Rank predictions based on the p-val and AUC values (where we have more confidence in the predictions)
- Rank based on the target organ effects observed for the source analogues

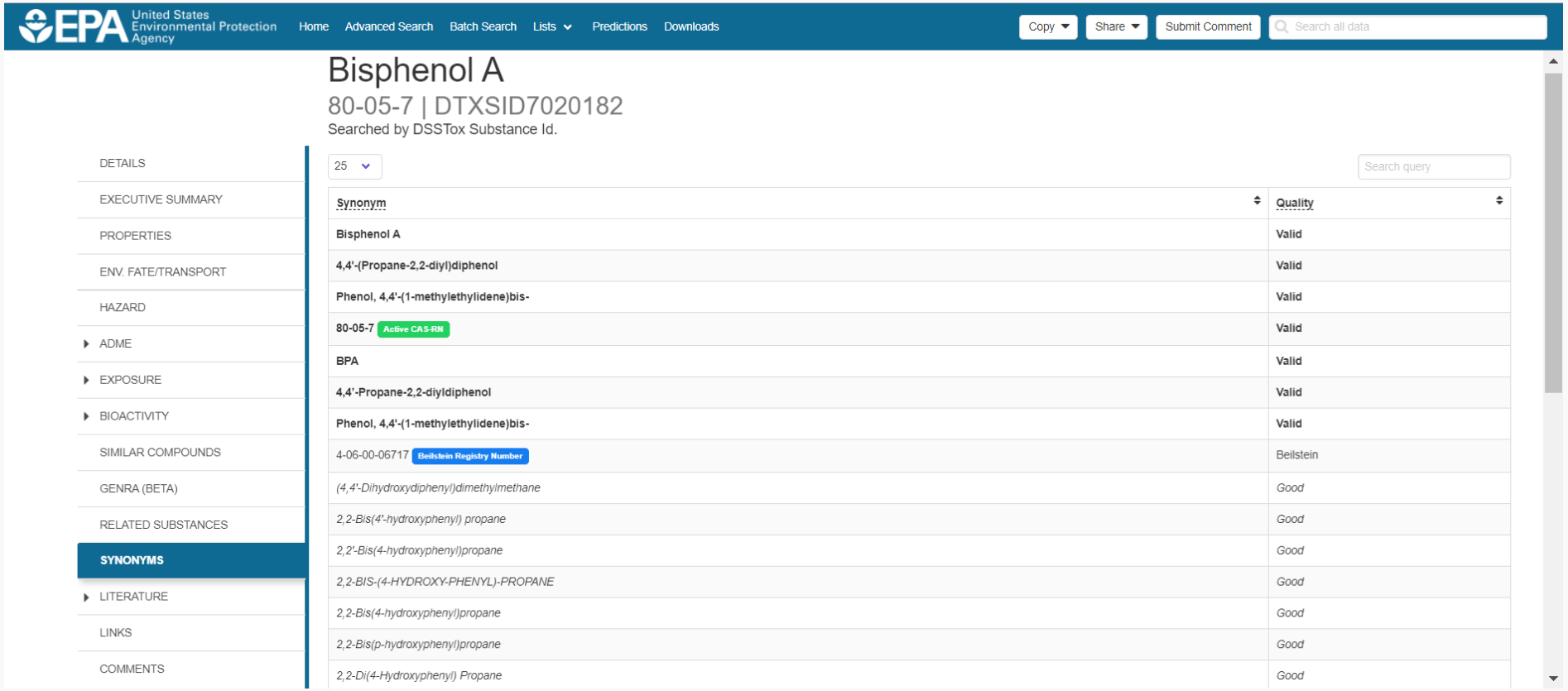
GenRA – Ongoing research

- Summarizing and aggregating the toxicity effect predictions to guide end users – what are the effects to be concerned about and which effect predictions are we most confident about
- Consideration of other information to define and refine the analogue selection – e.g. physicochemical similarity, metabolic similarity, reactivity similarity…
- EPA New Chemical Categories
- Quantifying the impact of physicochemical similarity on read-across performance
- Quantifying the impact of reactivity similarity on read-across performance

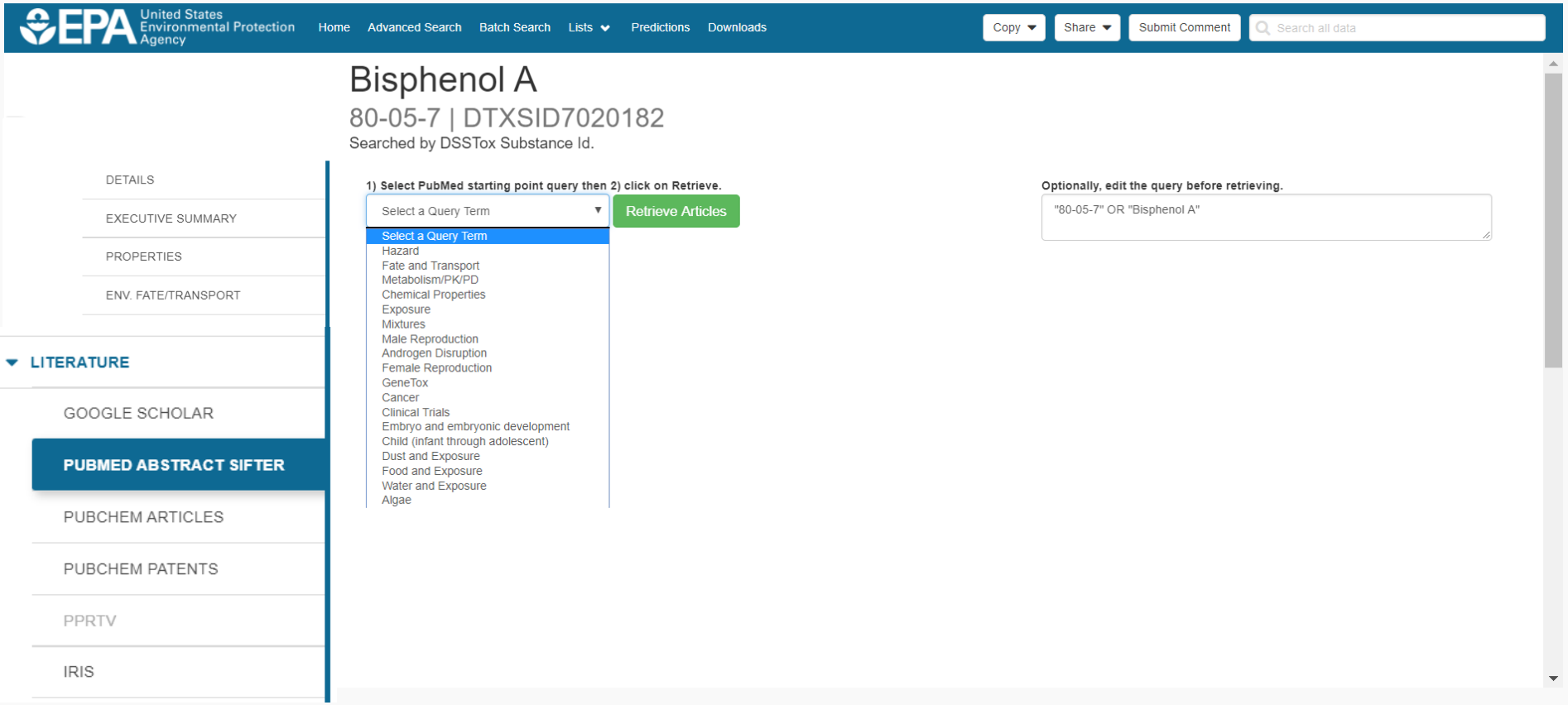
GenRA – Ongoing research

- Dose response information to refine scope of prediction beyond binary outcomes
- Transitioning from qualitative to quantitative predictions – how to apply and interpret GenRA in screening level hazard assessment
- Using quantitative data from acute rat oral toxicity, ToxRefDB v2

Names and CASRNs to Support Searches



Literature Searches - Querying 29 Million PubMed abstracts



Abstract Sifter - Querying 28 Million PubMed abstracts

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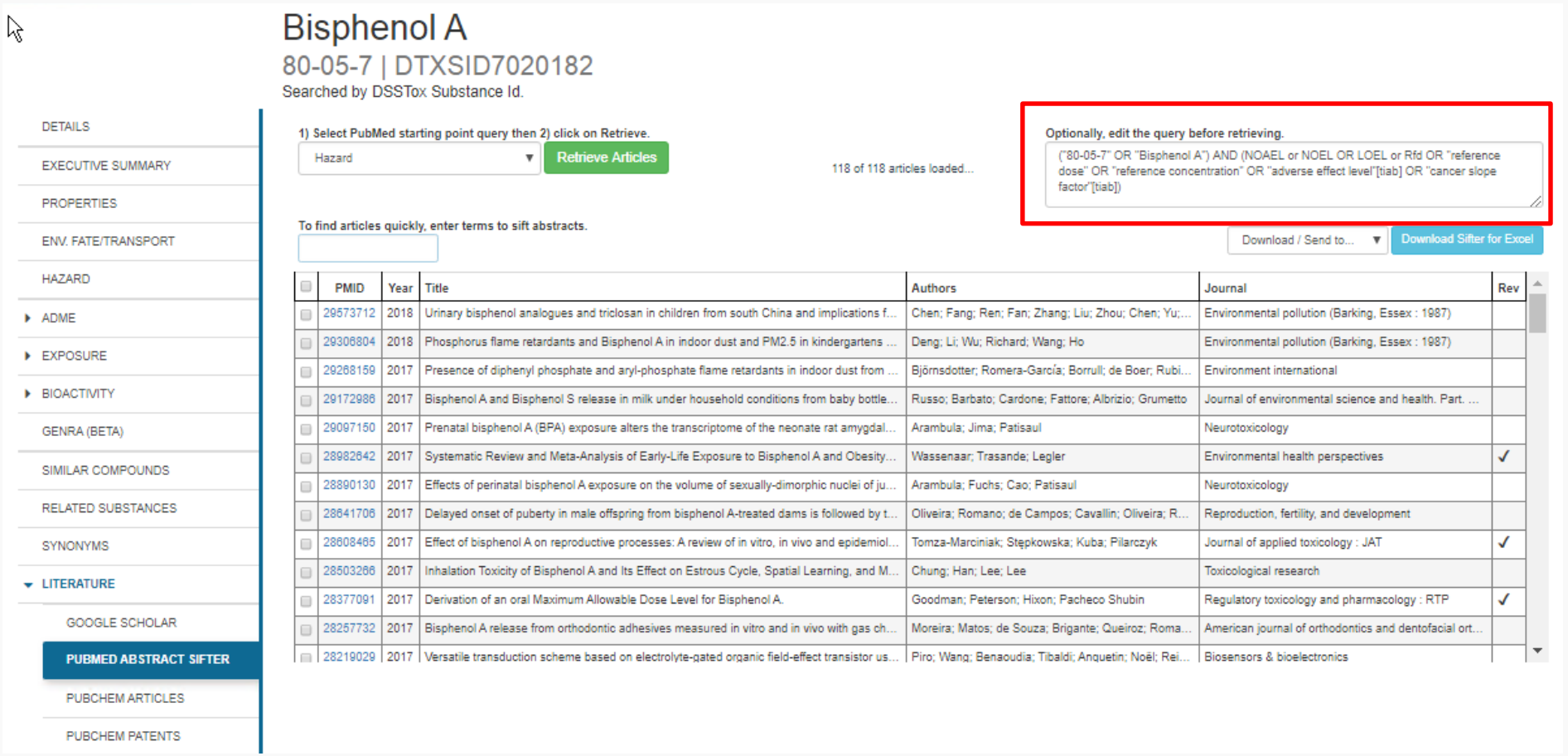

Abstract Sifter for Excel

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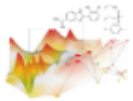
SOFTWARE TOOL ARTICLE

Abstract Sifter: a comprehensive front-end system to PubMed [version 1; referees: 2 approved]

Nancy Baker [1], Thomas Knudsen[2], Antony Williams [2]

Author details



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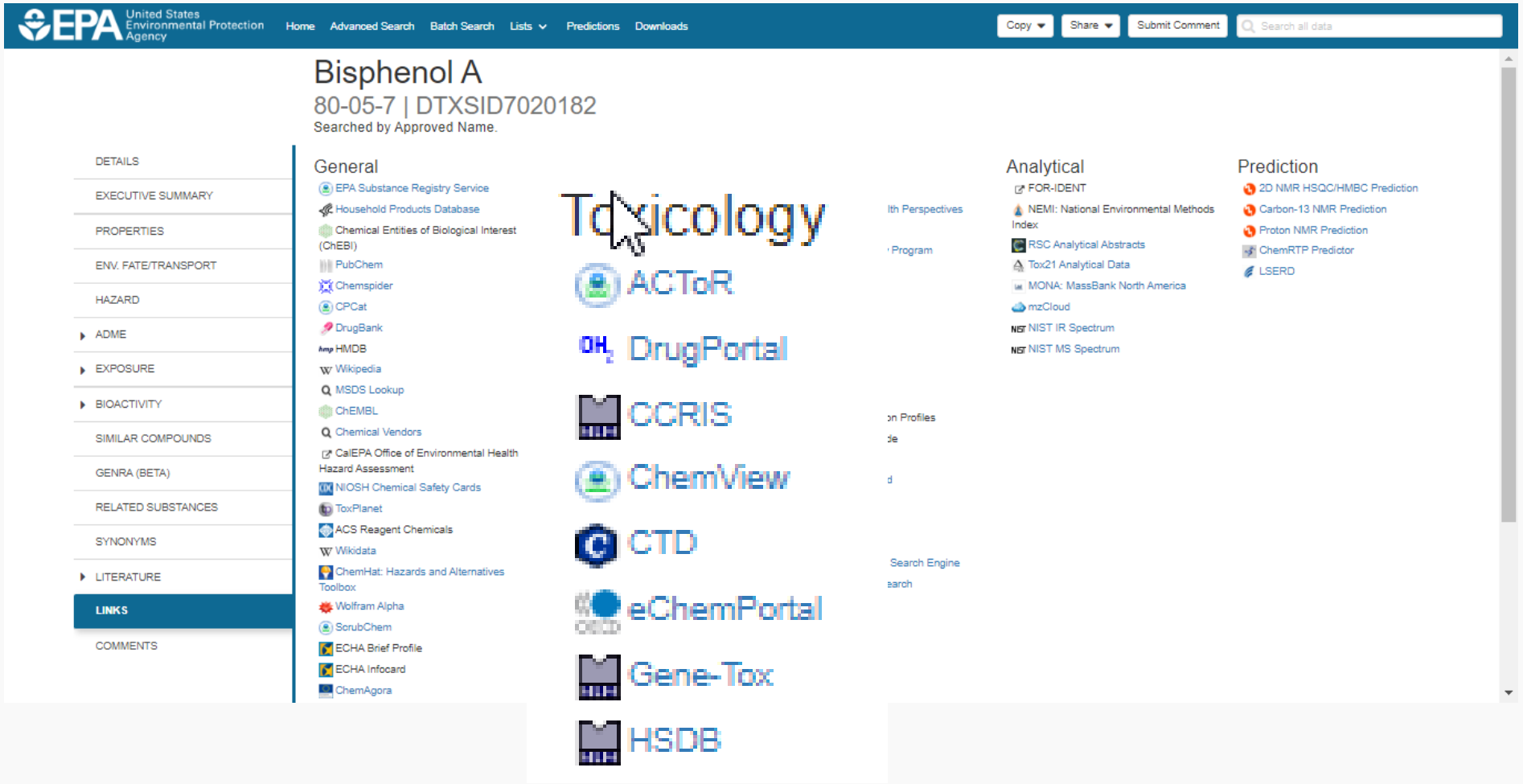
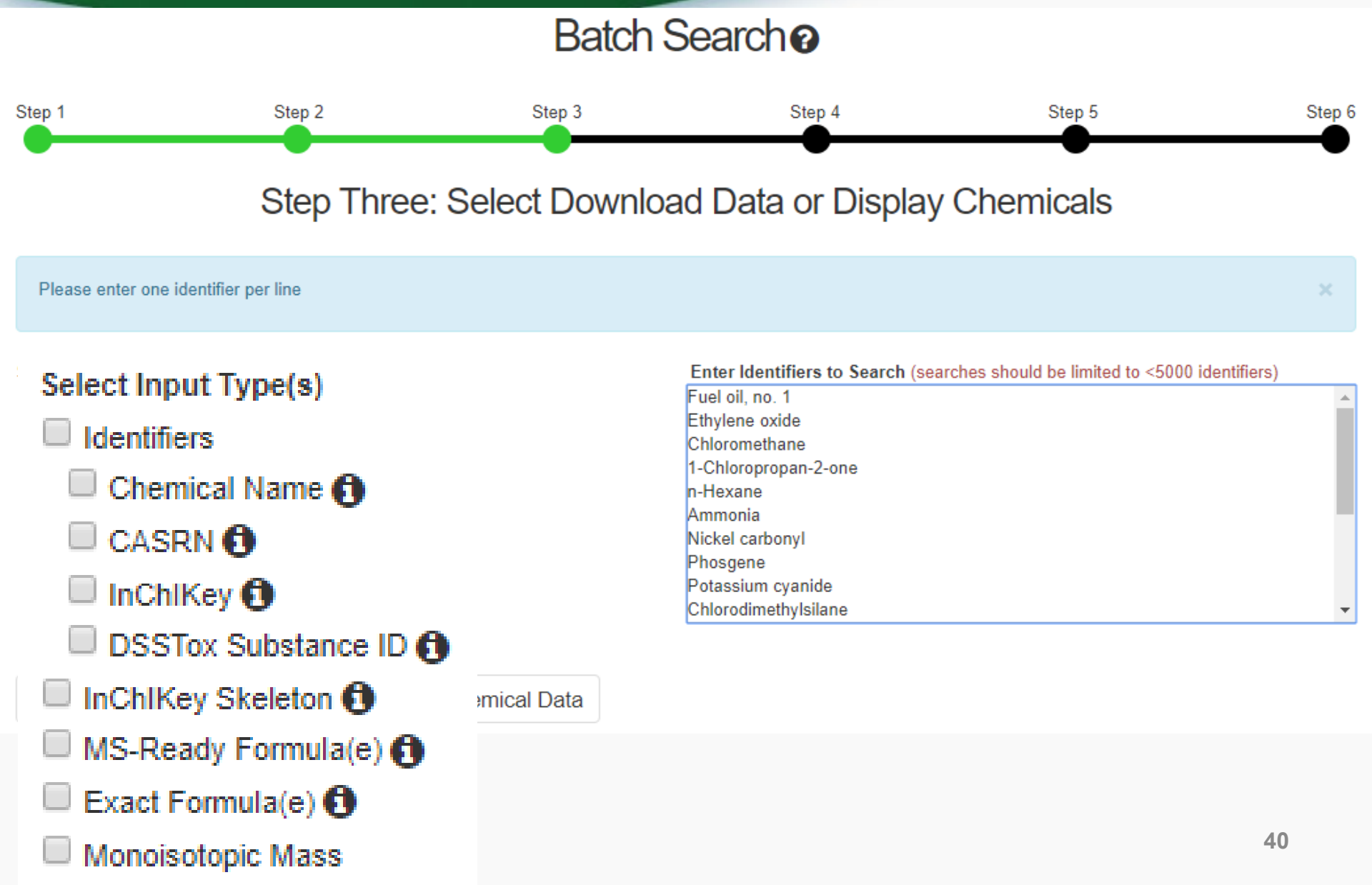
External Links to ~80 websites



Batch Searching



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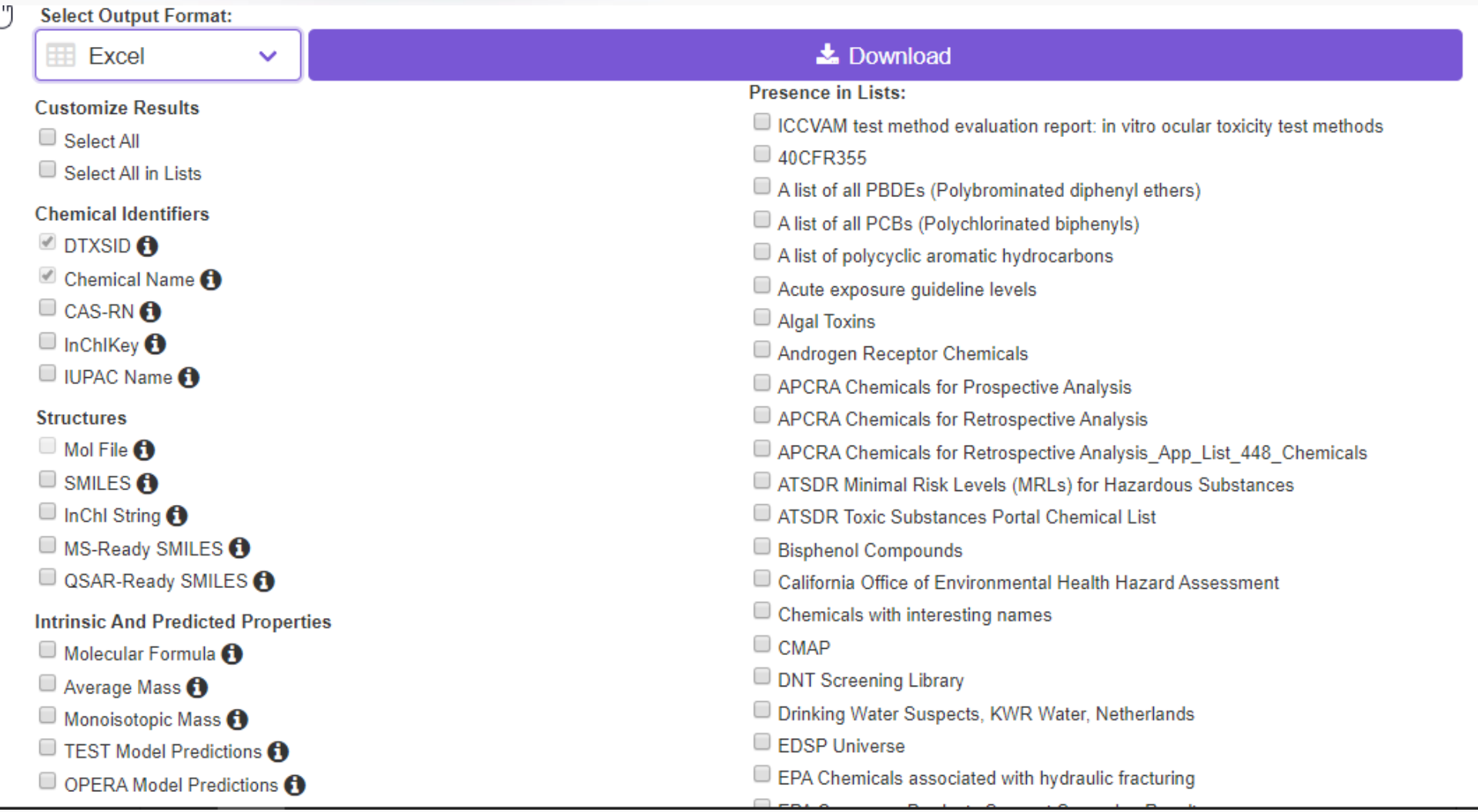
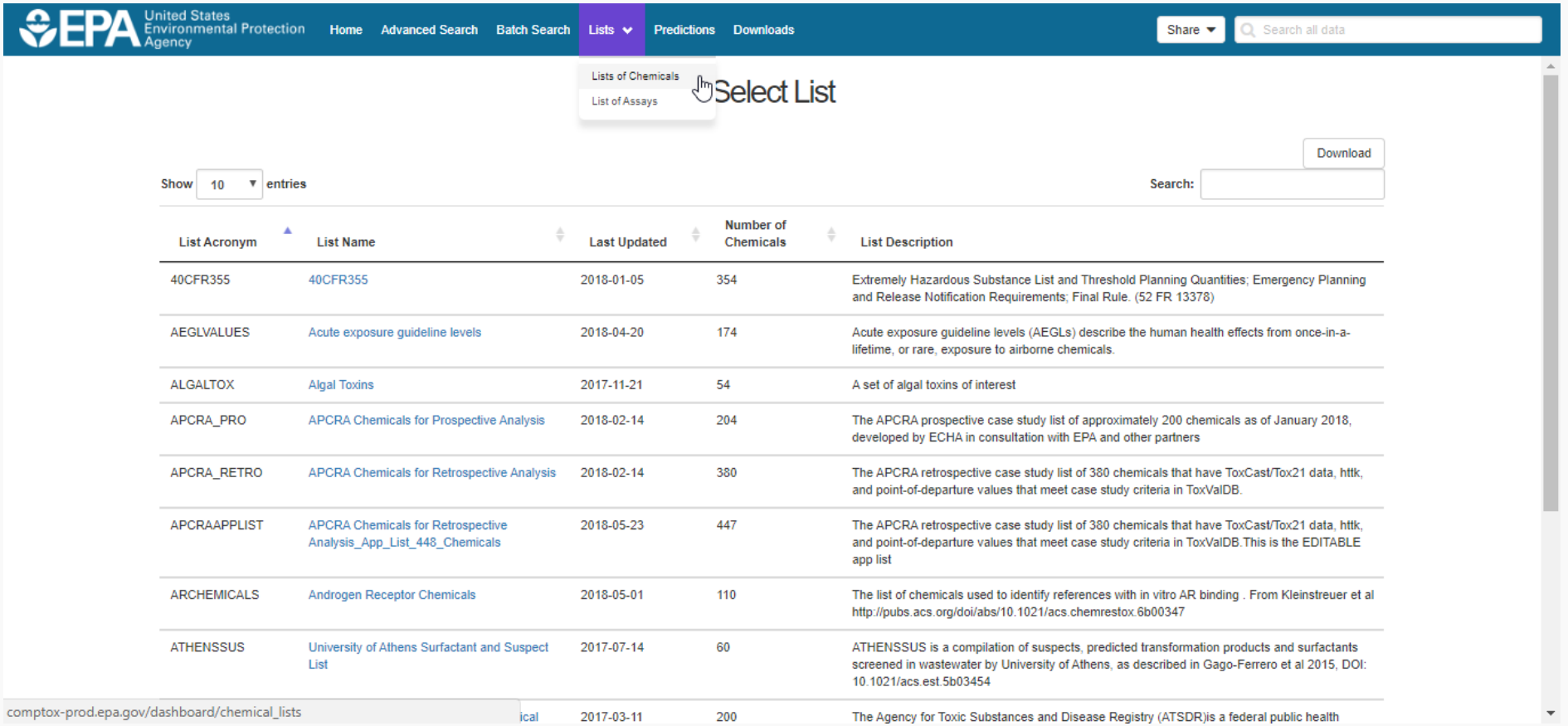


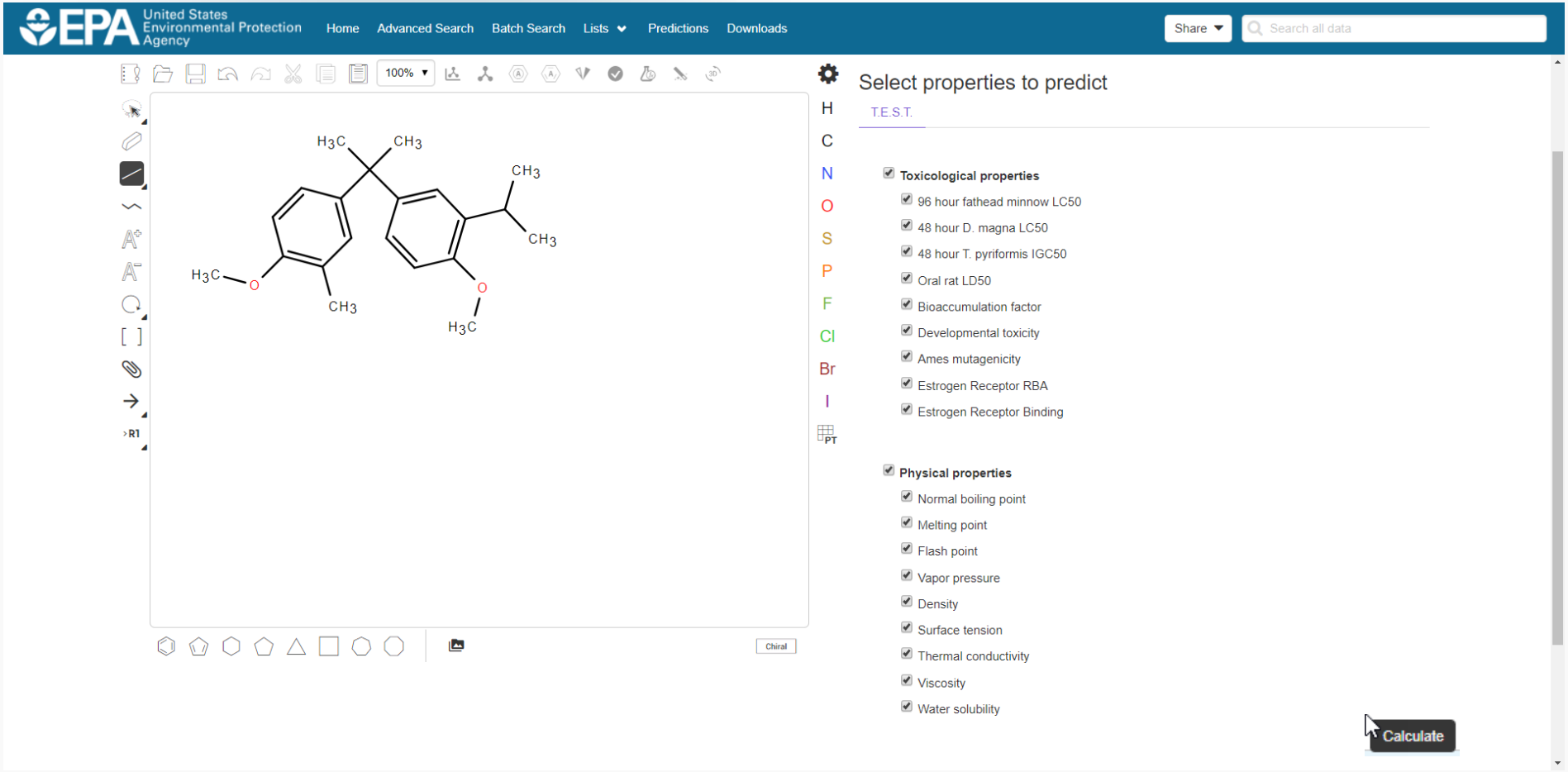
Excel Output

	A	B	C	D	E	F	G	H
1	INPUT	FOUND_BY	DTXSID	PREFERRED_NAME	EXPOCAST	EXPOCAST	NHANES	TOXVAL_D
2	1445-75-6	CAS-RN	DTXSID5024051	Diisopropyl methylpho	2.09e-08	Y	-	Y
3	50-00-0	CAS-RN	DTXSID7020637	Formaldehyde	1.32e-06	Y	-	Y
4	107-06-2	CAS-RN	DTXSID6020438	1,2-Dichloroethane	4.9e-06	Y	-	Y
5	57-12-5	CAS-RN	DTXSID6023991	Cyanide	-	-	-	Y
6	7550-45-0	CAS-RN	DTXSID8042476	Titanium tetrachloride	-	-	-	Y
7	79-01-6	CAS-RN	DTXSID0021383	Trichloroethylene	7.27e-06	Y	-	Y
8	121-82-4	CAS-RN	DTXSID9024142	Cyclonite	6.72e-08	Y	-	Y
9	108-05-4	CAS-RN	DTXSID3021431	Vinyl acetate	8.3e-05	Y	-	Y
10	7803-51-2	CAS-RN	DTXSID2021157	Phosphine	-	-	-	Y
11	122-66-7	CAS-RN	DTXSID7020710	1,2-Diphenylhydrazine	1.49e-07	Y	-	Y
12	101-77-9	CAS-RN	DTXSID6022422	4,4'-Methylenedianiline	6.08e-06	Y	-	Y
13	14017-34-6	CAS-RN	DTXSID90161250	Selenium difluoride	-	-	-	-
14	75-44-5	CAS-RN	DTXSID0024260	Phosgene	-	-	-	Y
15	621-64-7	CAS-RN	DTXSID6021032	N-Nitrosodipropylamine	4.55e-07	Y	-	Y
16	75-09-2	CAS-RN	DTXSID0020868	Dichloromethane	2.02e-06	Y	-	Y
17	100-41-4	CAS-RN	DTXSID3020596	Ethylbenzene	8.32e-05	Y	-	Y
18	7440-28-0	CAS-RN	DTXSID2036035	Thallium	-	-	-	Y
19	108-88-3	CAS-RN	DTXSID7021360	Toluene	8.61e-05	Y	-	Y
20	111-44-4	CAS-RN	DTXSID9020168	Bis(2-chloroethyl) ethe	2.82e-07	Y	-	Y
21	7440-42-8	CAS-RN	DTXSID3023922	Boron	-	-	-	Y
22	7440-29-1	CAS-RN	DTXSID6049800	Thorium	-	-	-	Y

List of Chemicals



Real-Time Predictions



Real-Time Predictions

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Download Summary

Property	Experimental Value	Consensus	Hierarchical clustering	Single model	Group contribution	Nearest neighbor
96 hour fathead minnow LC50		6.051 -Log10(mol/L) 0.278 mg/L	5.678 -Log10(mol/L) 0.656 mg/L	5.572 -Log10(mol/L) 0.836 mg/L	5.908 -Log10(mol/L) 0.386 mg/L	7.047 -Log10(mol/L) 0.028 mg/L
48 hour D. magna LC50		5.591 -Log10(mol/L) 0.802 mg/L	5.548 -Log10(mol/L) 0.884 mg/L	6.169 -Log10(mol/L) 0.212 mg/L	5.518 -Log10(mol/L) 0.948 mg/L	5.128 -Log10(mol/L) 2.329 mg/L
48 hour T. pyriformis IGC50		5.590 -Log10(mol/L) 0.804 mg/L	6.390 -Log10(mol/L) 0.127 mg/L		5.588 -Log10(mol/L) 0.806 mg/L	4.790 -Log10(mol/L) 5.068 mg/L
Oral rat LD50		2.400 -Log10(mol/kg) 1243.951 mg/kg	2.232 -Log10(mol/kg) 1829.942 mg/kg			2.568 -Log10(mol/kg) 845.609 mg/kg
Bioaccumulation factor		3.066 Log10 1164.438	3.090 Log10 1230.849	2.717 Log10 521.420	3.257 Log10 1806.262	3.200 Log10 1585.959
Developmental toxicity		true	true	true		true
Ames mutagenicity		false	false			false
Estrogen Receptor RBA		-0.710 Log10 0.195	-1.692 Log10 0.020	-1.515 Log10 0.031		1.077 Log10 11.931
Estrogen Receptor Binding		false	false	false		true
Normal boiling point		345.2 °C	306.6 °C		408.2 °C	320.7 °C
Melting point		74.3 °C	63.8 °C		41.0 °C	118.2 °C
Flash point		161.7 °C	143.5 °C		152.7 °C	188.9 °C
Vapor pressure		-5.955 Log10(mmHg) 1.109*10^-6 mmHg	-5.534 Log10(mmHg) 2.925*10^-6 mmHg		-5.903 Log10(mmHg) 1.249*10^-6 mmHg	-6.428 Log10(mmHg) 3.735*10^-7 mmHg
Density		0.959 g/cm³	0.977 g/cm³		0.843 g/cm³	1.057 g/cm³

Real-Time Predictions

EPA United States Environmental Protection Agency

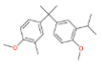
Predicted Fathead minnow LC50 (96 hr) for O(C1=CC=C(C=C1C)C(C2=CC=C(OC)C(=C2)C(C)C)(C)C)C from Consensus method

Prediction results

Endpoint	Experimental value	Predicted value
Fathead minnow LC_{50} (96 hr) -Log10(mol/L)	N/A	6.05
Fathead minnow LC_{50} (96 hr) mg/L	N/A	0.28

Individual Predictions

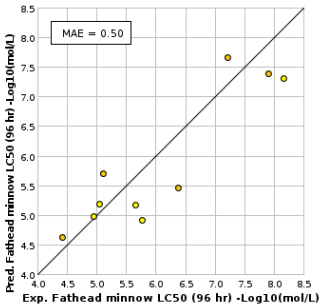
Method	Predicted value -Log10(mol/L)
Hierarchical clustering	5.68
Single model	5.57
Group contribution	5.91
Nearest neighbor	7.05



Predictions for the test chemical and for the most similar chemicals in the external test set

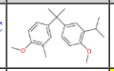
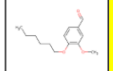
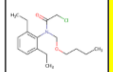
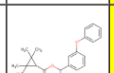
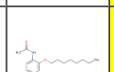
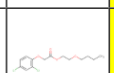
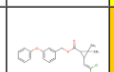
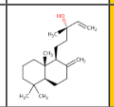
If the predicted value matches the experimental values for similar chemicals in the test set (and the similar chemicals were predicte

Prediction results (colors defined in table below)



Chemicals	MAE*
Entire set	0.55
Similarity coefficient ≥ 0.5	0.50

*Mean absolute error in -Log10(mol/L)

CAS	Structure	Similarity Coefficient	Experimental value -Log10(mol/L)	Predicted value -Log10(mol/L)
O(C1=CC=C(C=C1C)C(C2=CC=C(OC)C(=C2)C(C)C)(C)C)C (test chemical)			N/A	6.05
61096-84-2		0.74	4.95	4.97
23184-66-9		0.73	5.65	5.17
39515-41-8		0.72	8.17	7.32
55792-61-5		0.71	5.77	4.92
1929-73-3		0.71	5.05	5.19
52645-53-1		0.70	7.21	7.67
596-85-0		0.70	6.38	5.47

Not just chemical “structures”

- Chemicals in commerce, of interest to the EPA, are not all easily represented by structures

- Different chemical substances supported
  - “UVCB chemicals” - Unknown or Variable Composition, Complex Reaction Products and Biological Materials
  - Homologous series as Markush Structures

Markush Structures

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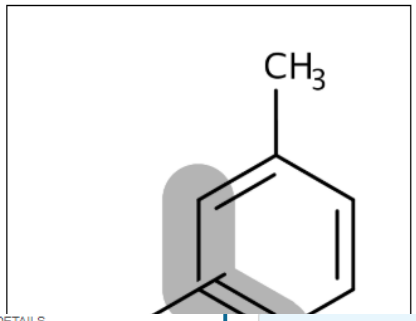
Xylenes

1330-20-7 | DTXSID2021446

Searched by DSSTox Substance Id.

DETAILS
RELATED SUBSTANCES
PROPERTIES
COMMENTS



Wikipedia

Xylene (from Greek ξύλο, *xylo*, "wood"), **xylol** or **dimethylbenzene** is any one of three isomers of dimethylbenzene, or a combination thereof. With the formula $(CH_3)_2C_6H_4$, each of the three compounds has a central benzene ring with two methyl groups attached at substituents. They are all colorless, flammable liquids, some of which are of great industrial value. The mixture is referred to as both xylene and, more precisely, xylenes

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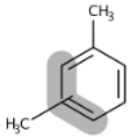


Xylenes
DTXSID: DTXSID2021446
CASRN: 1330-20-7

Predecessor: Component

4 related chemical structures with this substance

Xylenes; defined mixture 1
DTXSID: DTXSID9021421
CASRN: NOCAS_21421

Predecessor: Component

4 related chemical structures with this substance

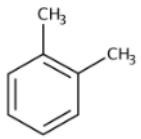
Xylenes; defined mixture 2
DTXSID: DTXSID7021447
CASRN: NOCAS_21447

Predecessor: Component

5 related chemical structures with this substance

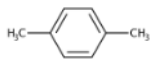
Total Petroleum Hydrocarbons (TPH)
DTXSID: DTXSID30891529
CASRN: NOCAS_891529

Markush Child



o-Xylene
DTXSID: DTXSID3021807
CASRN: 95-47-6

Markush Child



p-Xylene
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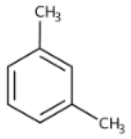
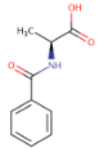
CASRN: 106-42-3

Markush Child



m-Xylene
DTXSID: DTXSID6026298
CASRN: 108-38-3

Transformation Product

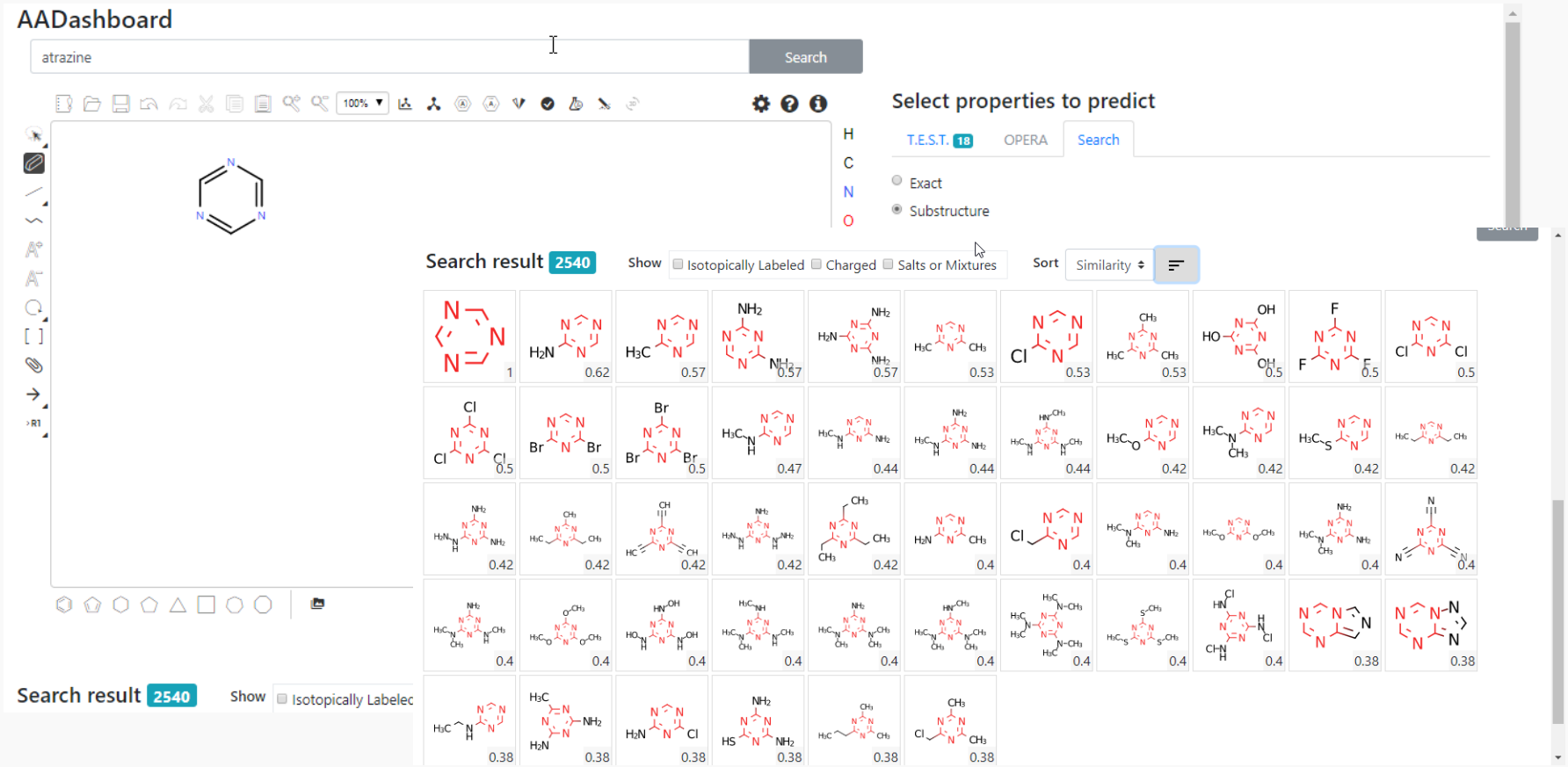


N-Benzoylalanine
DTXSID: DTXSID40176394
CASRN: 2198-64-3

Downloadable data

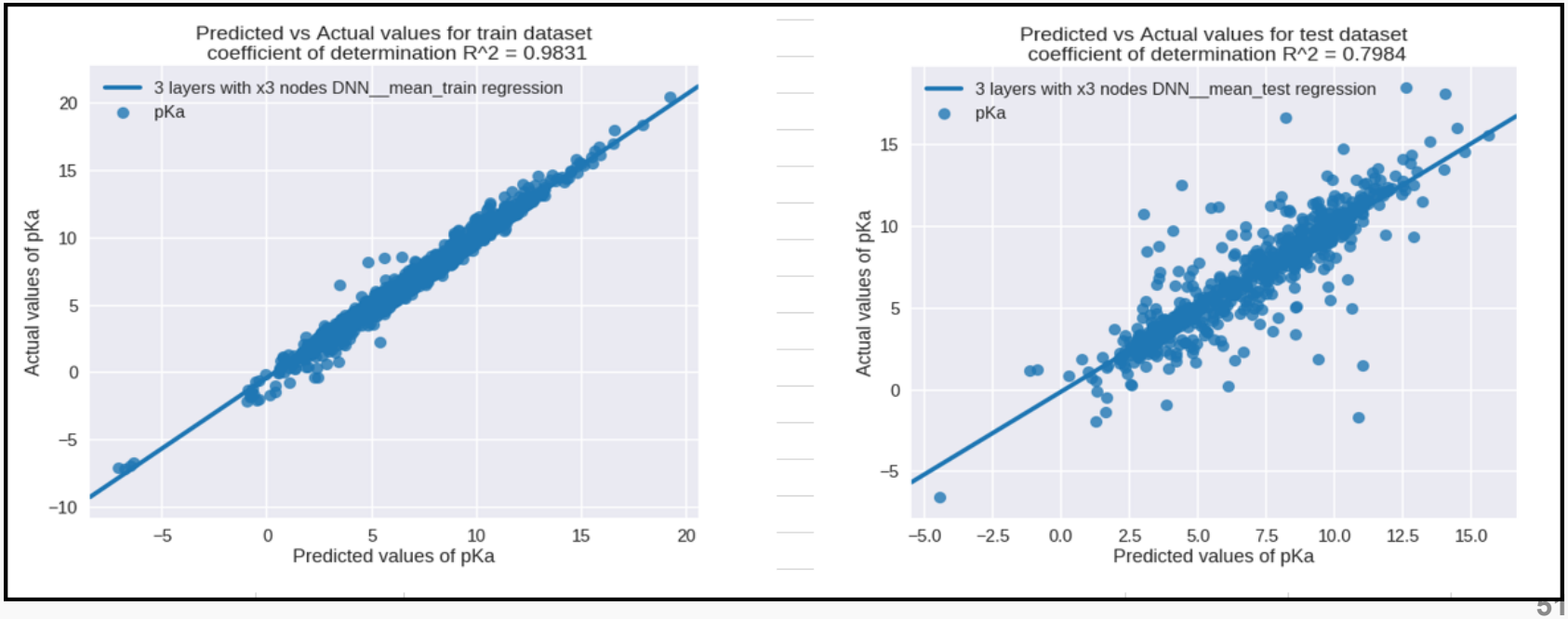
- Our data are licensed as public domain data
  - available from downloads page
  - registered to Figshare
  - SQL data dumps
- Collection of web services for old dashboards are available – API is being fully revamped

In Progress: Structure, Substructure and Similarity Searching



In Progress : pKa Prediction Model

- pKa prediction models based on Open Data Set of 8000 chemicals – acidic, basic and amphoteric chemicals



In Progress: API development
Prototype services available

https://comptox.epa.gov/dashboard/web-test/WS?smiles=CCO&method=hc

JSON Raw Data Headers

Save Copy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uuid:                "55547f4f-f966-48e8-b831-a0d217998064"
predictionTime:      1520539090089
software:            "T.E.S.T (Toxicity Estimation Software Tool)"
softwareVersion:     "5.01"
condition:           "25°C"
endpoint:            "Water solubility at 25°C"
method:              "Hierarchical clustering"
predictions:
  0:
    id:              "C_1520539090089"
    smiles:          "OCC"
    expValMolarLog:  "-1.337"
    expValMass:      "1001180.703"
    predValMolarLog: "-1.338"
    predValMass:     "1002625.241"
    molarLogUnits:   "-Log10(mol/L)"
    massUnits:       "mg/L"
```

Conclusion

- Transparent access to data supporting computational toxicology
- CompTox Chemicals Dashboard provides access to data for ~875,000 chemicals
- Ongoing expansion of functionality to serve all data streams for NCCT
- Generalized Read-Across module is an intuitive, integrated dashboard module. Showing great promise and clear development path ahead

Acknowledgements

EPA-RTP

- *An enormous team of contributors from NCCT, especially the IT software development team*
- *Multiple centers and laboratories across the EPA*
- *Special Mentions:*
- ***Dashboard**: Jeremy Dunne, Jeff Edwards and Chris Grulke*
- ***GenRA**: Imran Shah & George Helman*
- ***InvitroDB**: Katie Paul-Friedman*