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EPA United States Environmental Protection Agency

Accessing Environmental Chemistry Data via Data Dashboards

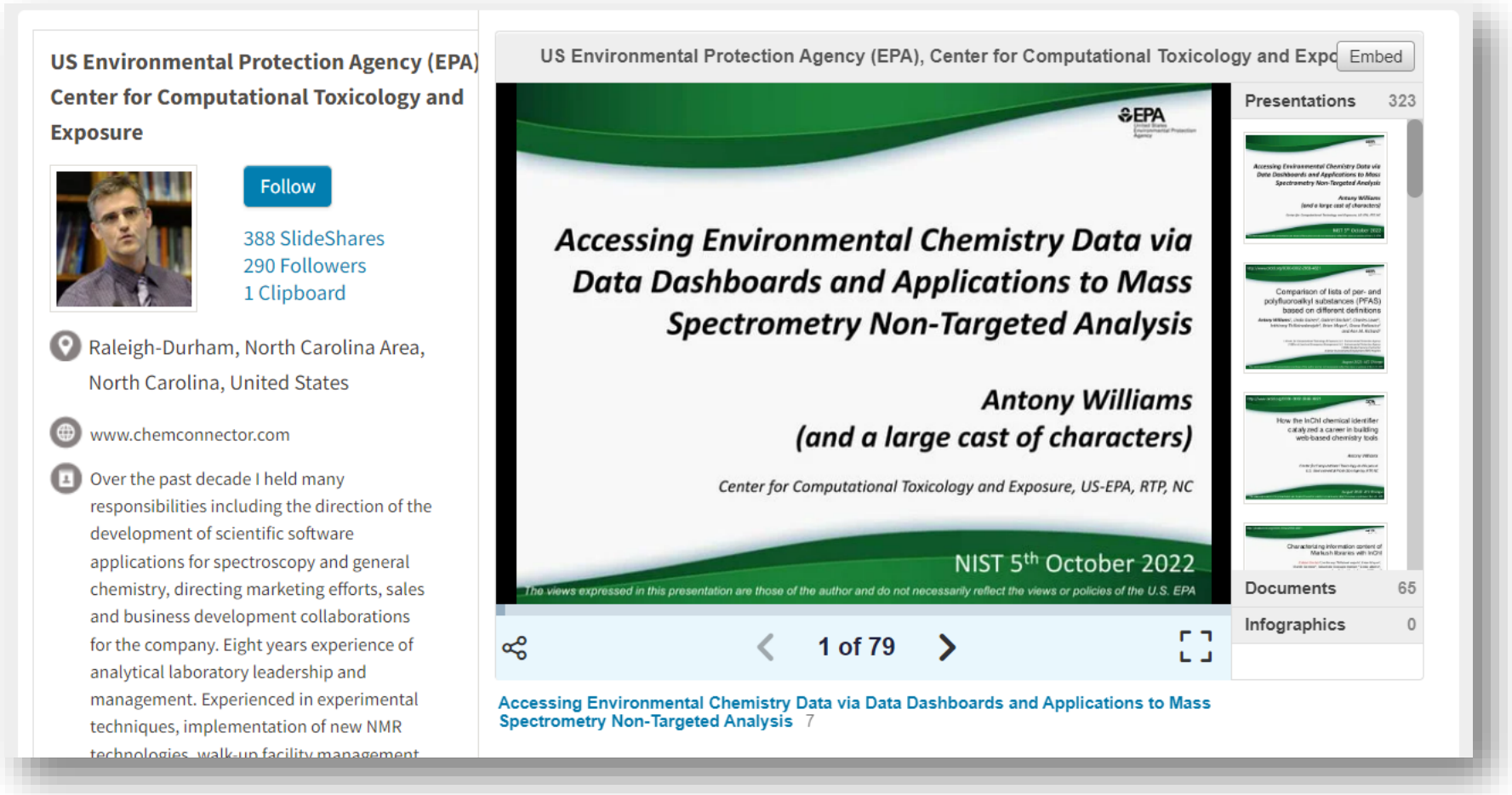
Antony J. Williams

Center for Computational Toxicology and Exposure, US-EPA, RTP, NC

BfR – German Federal Institute for Risk Assessment – April 7th 2022

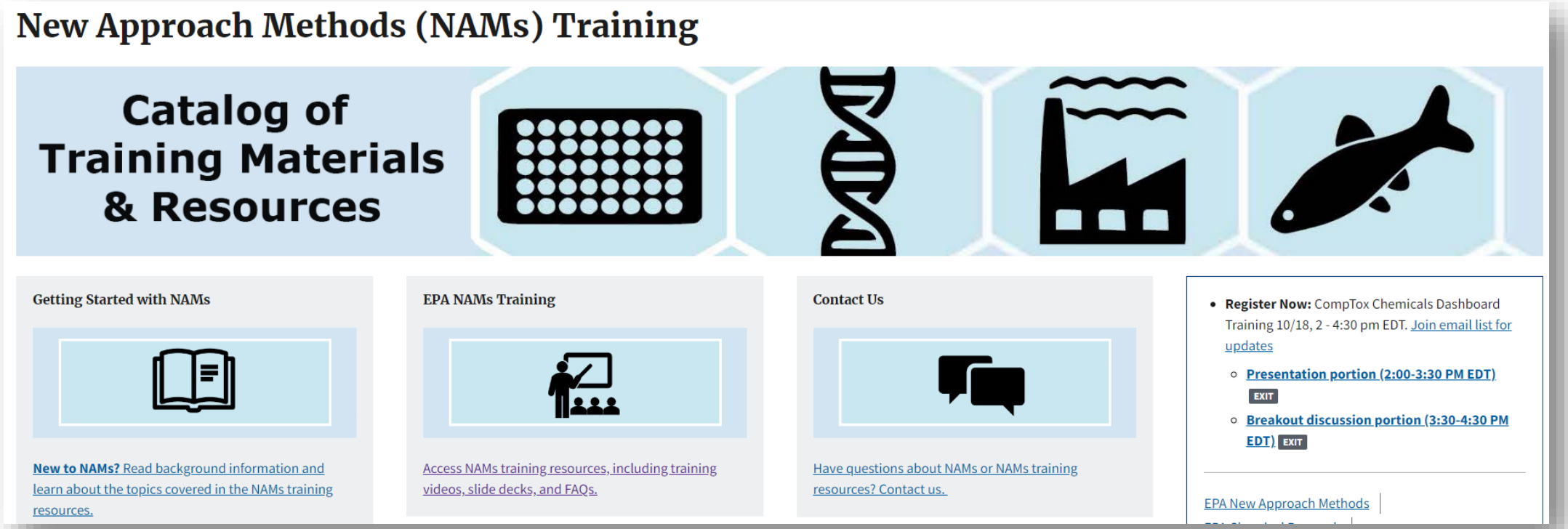
Many other talks on SlideShare
https://www.slideshare.net/AntonyWilliams/

- Slides will be circulated after the presentation



This talk is an overview

- This talk is a high-level overview only. We can provide trainings into the individual modules and data as required
- LOTS of training materials are available https://www.epa.gov/chemical-research/new-approach-methods-nams-training



20 Years of Curating Data in Our Team

EPA United States Environmental Protection Agency

ELSEVIER

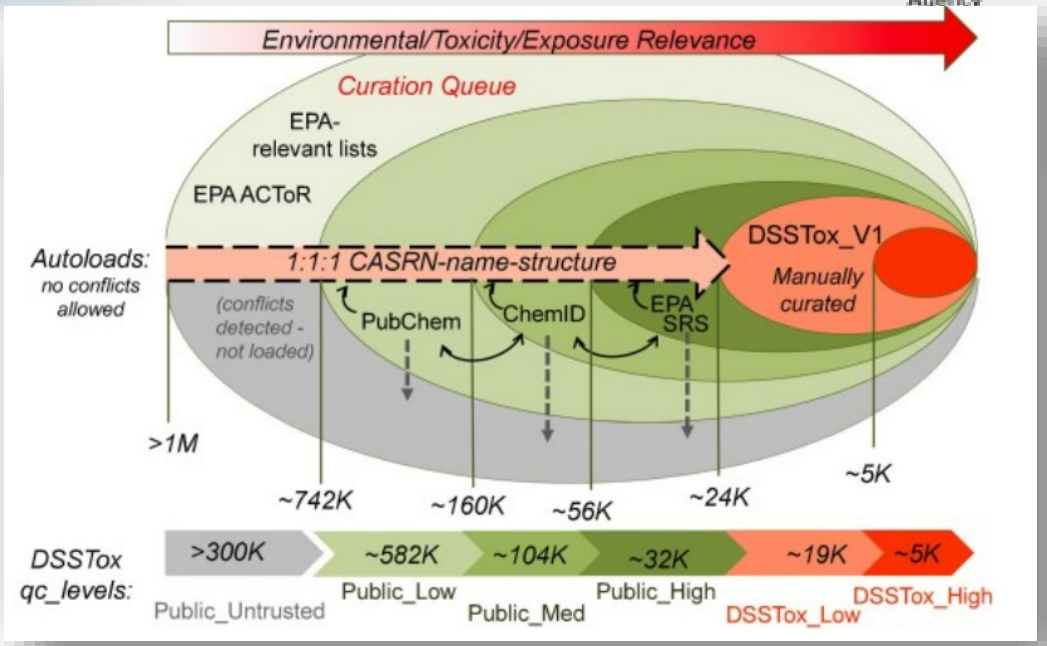
Mutation Research/Fundamental and Molecular Mechanisms of Mutagenesis

Volume 499, Issue 1, 29 January 2002, Pages 27-52

Mutation Research Frontiers

Distributed structure-searchable toxicity (DSSTox) public database network: a proposal

Ann M. Richard [a], ClarLynda R. Williams [a, b]



ELSEVIER

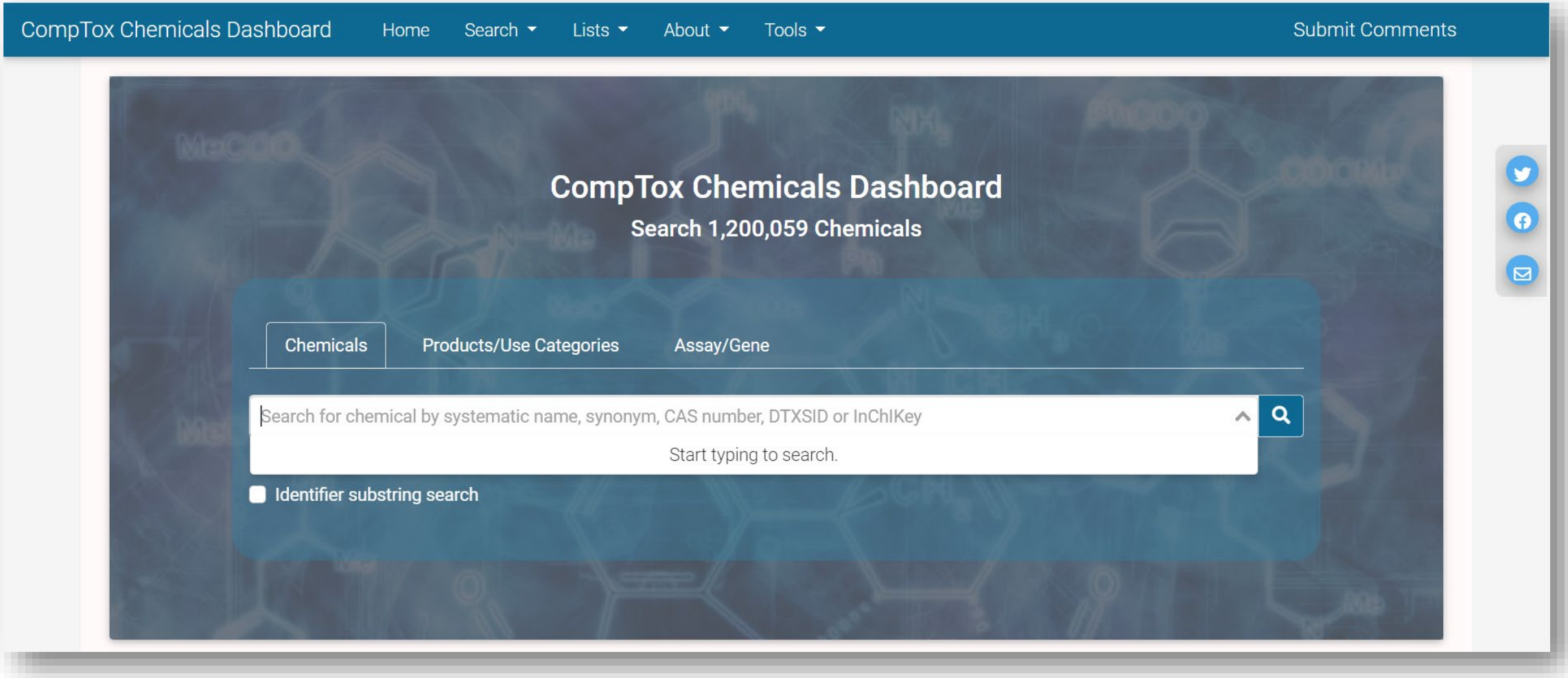
Computational Toxicology

Volume 12, November 2019, 100096

EPA's DSSTox database: History of development of a curated chemistry resource supporting computational toxicology research

Christopher M. Grulke [a], Antony J. Williams [a], Inthirany Thillanadarajah [b], Ann M. Richard [a]

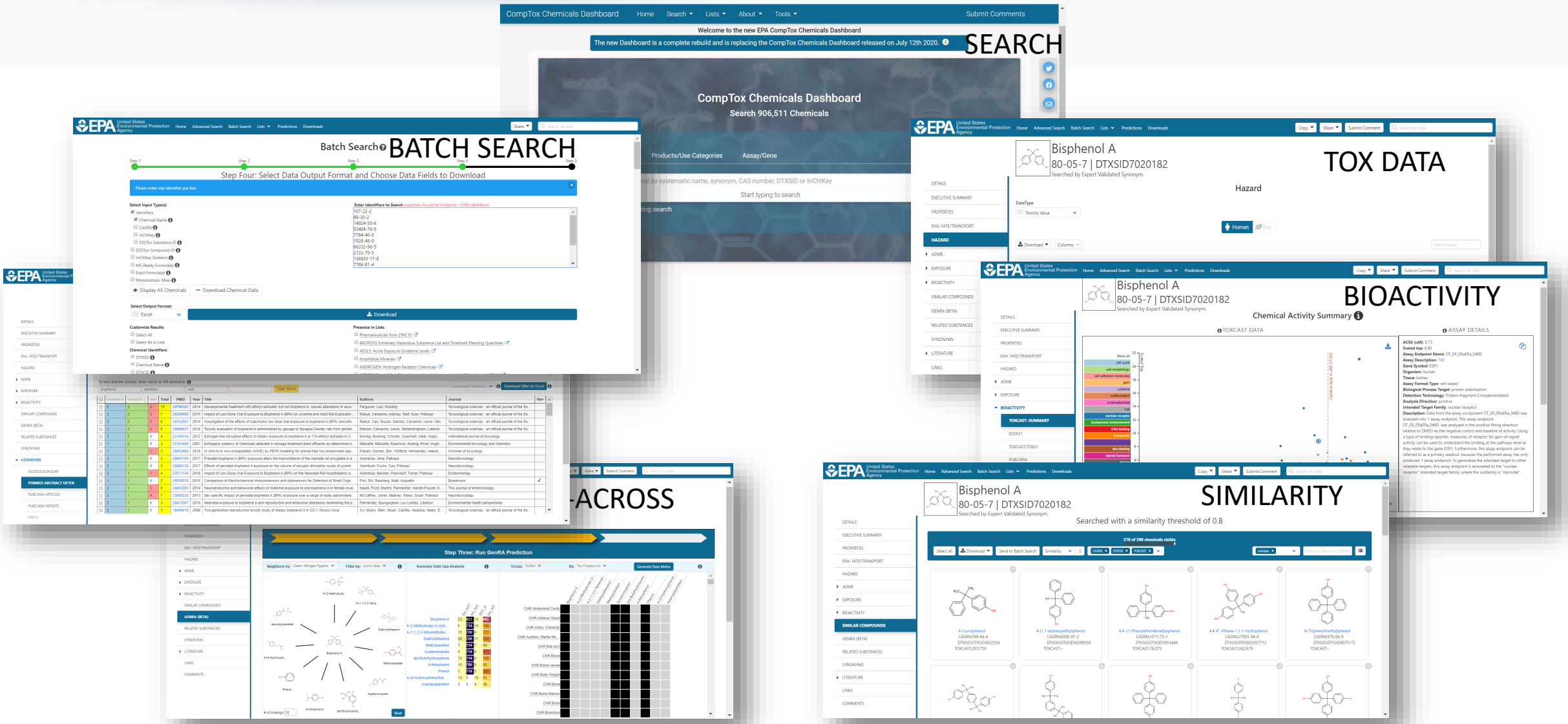
CompTox Chemicals Dashboard
>1.2 million chemicals



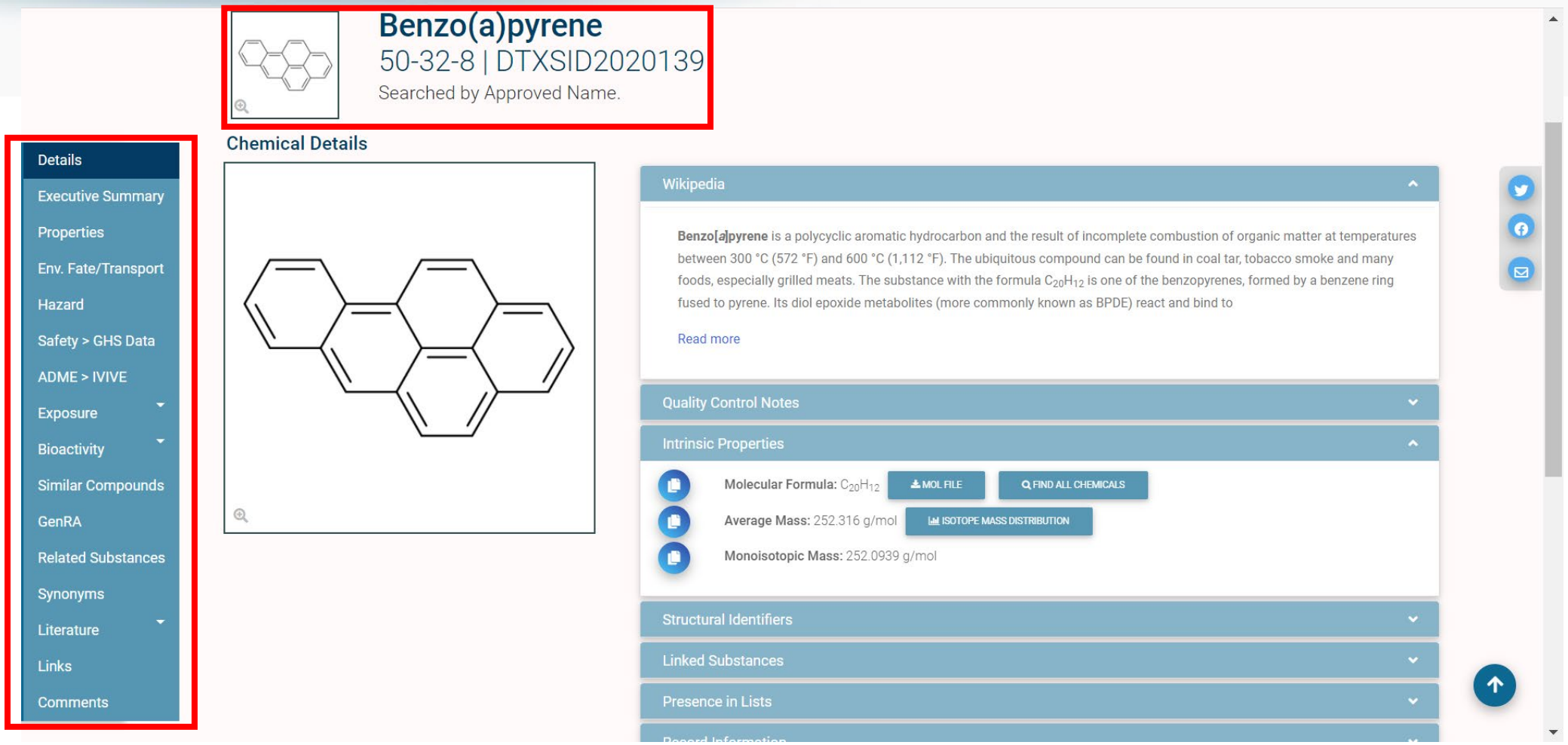
The Charge for the Dashboard

- Develop a “first-stop-shop” for environmental chemical data to support EPA and partner decision making:
  - **Centralized location** for relevant chemical data
  - Chemistry, exposure, hazard and dosimetry
  - Combination of existing data and predictive models
  - Publicly accessible, periodically updated, curated
- Easy access to data improves efficiency and ultimately accelerates chemical risk assessment

CompTox Chemicals Dashboard
https://comptox.epa.gov/dashboard

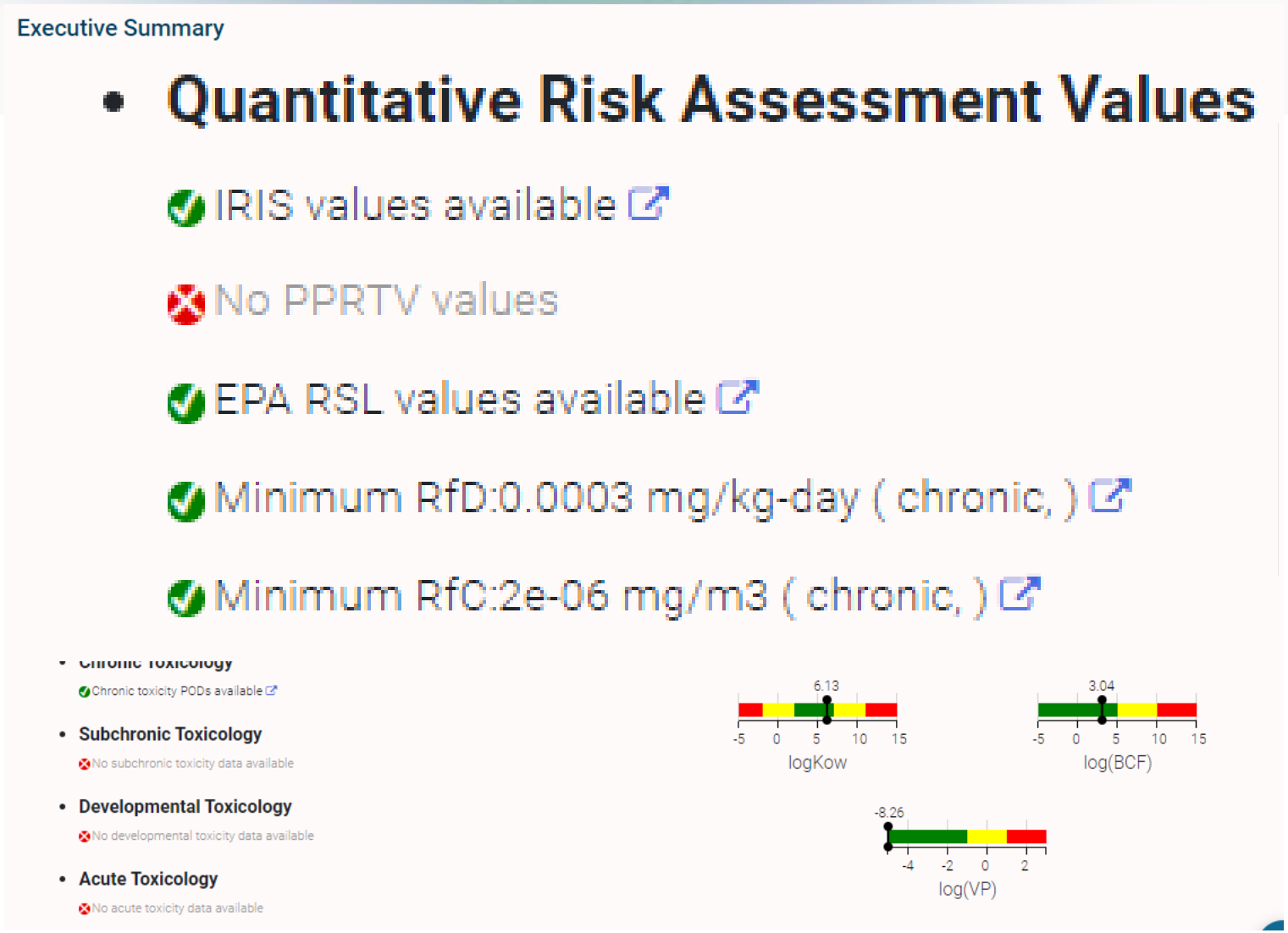


Detailed Chemical Pages



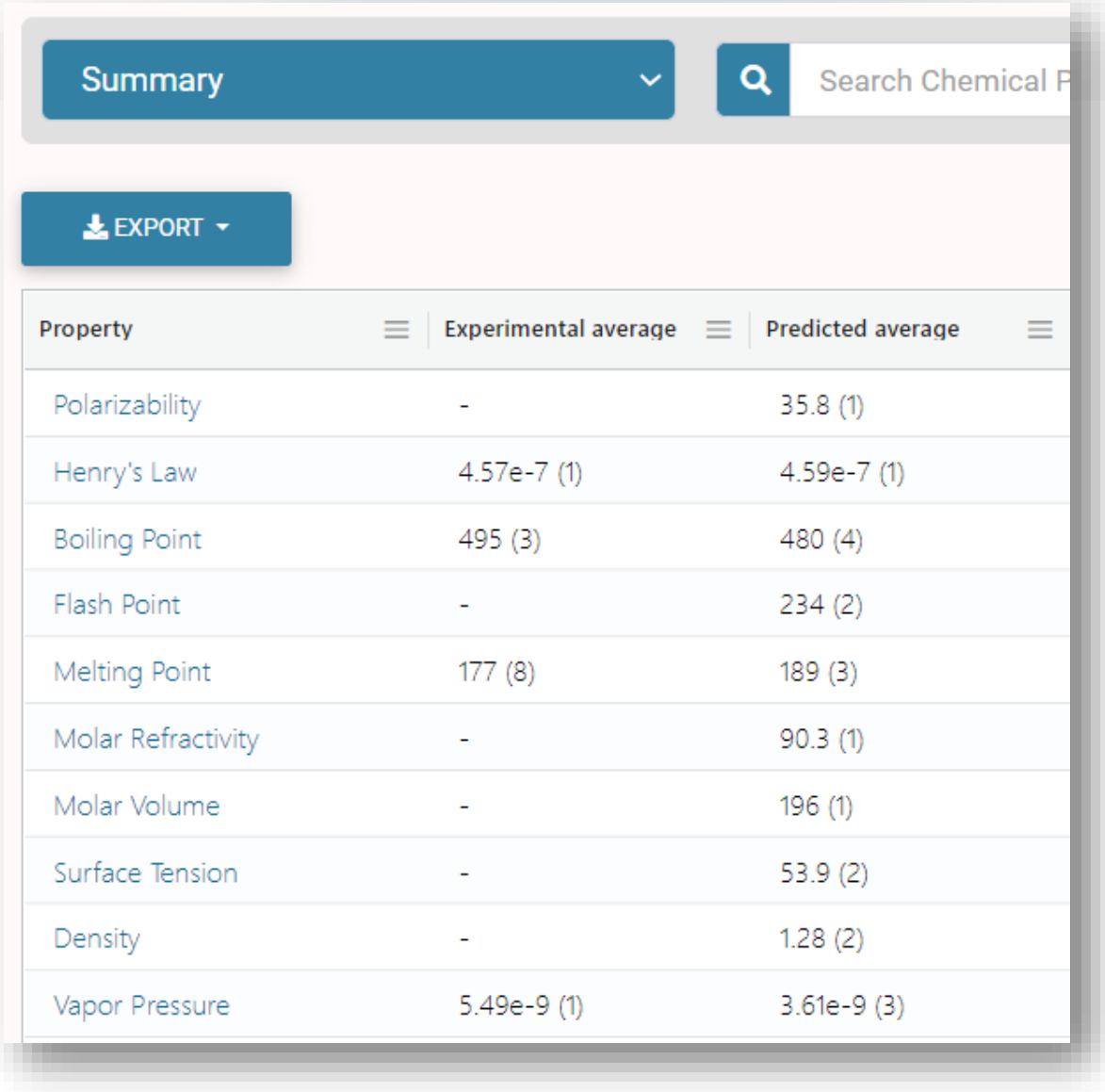
- Chemical page: Wikipedia snippet when available, intrinsic properties, structural identifiers, linked substances

“Executive Summary”



- Overview of toxicity-related info
  - Quantitative values
  - Physchem. and Fate & Transport
  - Adverse Outcome Pathway links
  - *In vitro* bioactivity summary plot

Experimental and Predicted Data



Property	Experimental average	Predicted average
Polarizability	-	35.8 (1)
Henry's Law	4.57e-7 (1)	4.59e-7 (1)
Boiling Point	495 (3)	480 (4)
Flash Point	-	234 (2)
Melting Point	177 (8)	189 (3)
Molar Refractivity	-	90.3 (1)
Molar Volume	-	196 (1)
Surface Tension	-	53.9 (2)
Density	-	1.28 (2)
Vapor Pressure	5.49e-9 (1)	3.61e-9 (3)

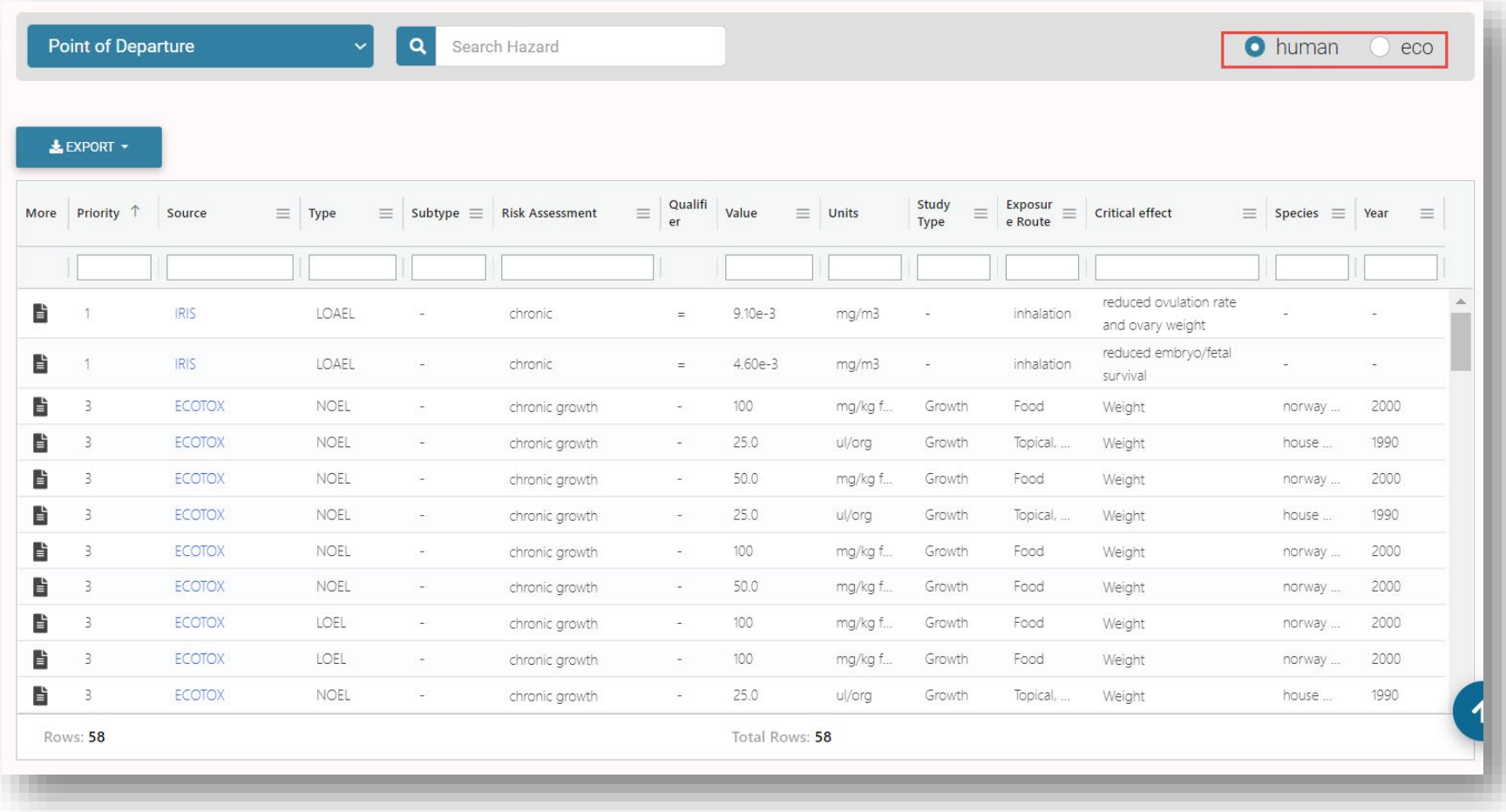
- Physchem and Fate & Transport experimental and predicted data
- Data can be downloaded as Excel, TSV and CSV files

Chemical Hazard Data

United States Environmental Protection Agency

ToxVal Database

- >50k chemicals
- >770k tox. values
- >30 sources of data
- ~5k journals cited
- ~70k citations



More	Priority	Source	Type	Subtype	Risk Assessment	Qualifier	Value	Units	Study Type	Exposure Route	Critical effect	Species	Year
	1	IRIS	LOAEL	-	chronic	=	9.10e-3	mg/m3	-	inhalation	reduced ovulation rate and ovary weight	-	-
	1	IRIS	LOAEL	-	chronic	=	4.60e-3	mg/m3	-	inhalation	reduced embryo/fetal survival	-	-
	3	ECOTOX	NOEL	-	chronic growth	-	100	mg/kg f...	Growth	Food	Weight	norway ...	2000
	3	ECOTOX	NOEL	-	chronic growth	-	25.0	ul/org	Growth	Topical, ...	Weight	house ...	1990
	3	ECOTOX	NOEL	-	chronic growth	-	50.0	mg/kg f...	Growth	Food	Weight	norway ...	2000
	3	ECOTOX	NOEL	-	chronic growth	-	25.0	ul/org	Growth	Topical, ...	Weight	house ...	1990
	3	ECOTOX	NOEL	-	chronic growth	-	100	mg/kg f...	Growth	Food	Weight	norway ...	2000
	3	ECOTOX	NOEL	-	chronic growth	-	50.0	mg/kg f...	Growth	Food	Weight	norway ...	2000
	3	ECOTOX	LOEL	-	chronic growth	-	100	mg/kg f...	Growth	Food	Weight	norway ...	2000
	3	ECOTOX	LOEL	-	chronic growth	-	100	mg/kg f...	Growth	Food	Weight	norway ...	2000
	3	ECOTOX	NOEL	-	chronic growth	-	25.0	ul/org	Growth	Topical, ...	Weight	house ...	1990

Rows: 58 Total Rows: 58

Safety Data

EPA United States Environmental Protection Agency

GHS Data

Print Page

PUBCHEM > BENZO[A]PYRENE > LABORATORY CHEMICAL SAFETY SUMMARY (LCSS) > GHS CLASSIFICATION

CID 2336

Benzo[a]pyrene

GHS Classification

Showing 6 of 6

Pictogram(s)	 Irritant, Health Hazard, Environmental Hazard
Signal	Danger
GHS Hazard Statements	H317: May cause an allergic skin reaction [Warning Sensitization, Skin] H340: May cause genetic defects [Danger Germ cell mutagenicity] H350: May cause cancer [Danger Carcinogenicity] H360FD: May damage fertility; May damage the unborn child [Danger Reproductive toxicity] H400: Very toxic to aquatic life [Warning Hazardous to the aquatic environment, acute hazard] H410: Very toxic to aquatic life with long lasting effects [Warning Hazardous to the aquatic environment, long-term hazard]
Precautionary Statement Codes	P201, P202, P261, P272, P273, P280, P281, P302+P352, P308+P313, P321, P333+P313, P363, P391, P405, and P501 (The corresponding statement to each P-code can be found at the GHS Classification page.)

Sources of Exposure to Chemicals

EPA United States Environmental Protection Agency

Chemical Weight Fractions (CWF)

Search Chemical Weight Fractions

EXPORT

Product Name	Product Use Category	Categorization Subtype	Minimum Weight Fraction	Maximum Weight Fraction	Data Type	Source	Product Count
48743 pah mixture	Not yet Categorized		-	-	reported	SIRI	1
asphalt cement penetration 60-70	Not yet Categorized		-	-	reported	SIRI	1
base-neutral 4 1ml methylene chl...	Not yet Categorized		-	-	reported	SIRI	1
base neutral calibration checkco...	Not yet Categorized		-	-	reported	SIRI	1
benzo (a) pyrene_ 98%_ b1008-0	Not yet Categorized		-	-	reported	SIRI	1
benzo (a) pyrene_ md-1956	Not yet Categorized		0.990	1.00	reported	SIRI	1
blasocut 2000 cf art no 875	Not yet Categorized		0.00	1.00e-3	reported	SIRI	1
blasocut 2000 universal_ 870	Not yet Categorized		-	-	reported	SIRI	1
blasocut 2000 universal art_ 870	Not yet Categorized		0.00	1.00e-3	reported	SIRI	1
blasocut 4000 strong_ 872	Not yet Categorized		-	-	reported	SIRI	1
blasocut 4000 universal art_ 872	Not yet Categorized		0.00	1.00e-3	reported	SIRI	1
clp-011a clp base/neutrals check ...	Not yet Categorized		-	-	reported	SIRI	1

Rows: **29**

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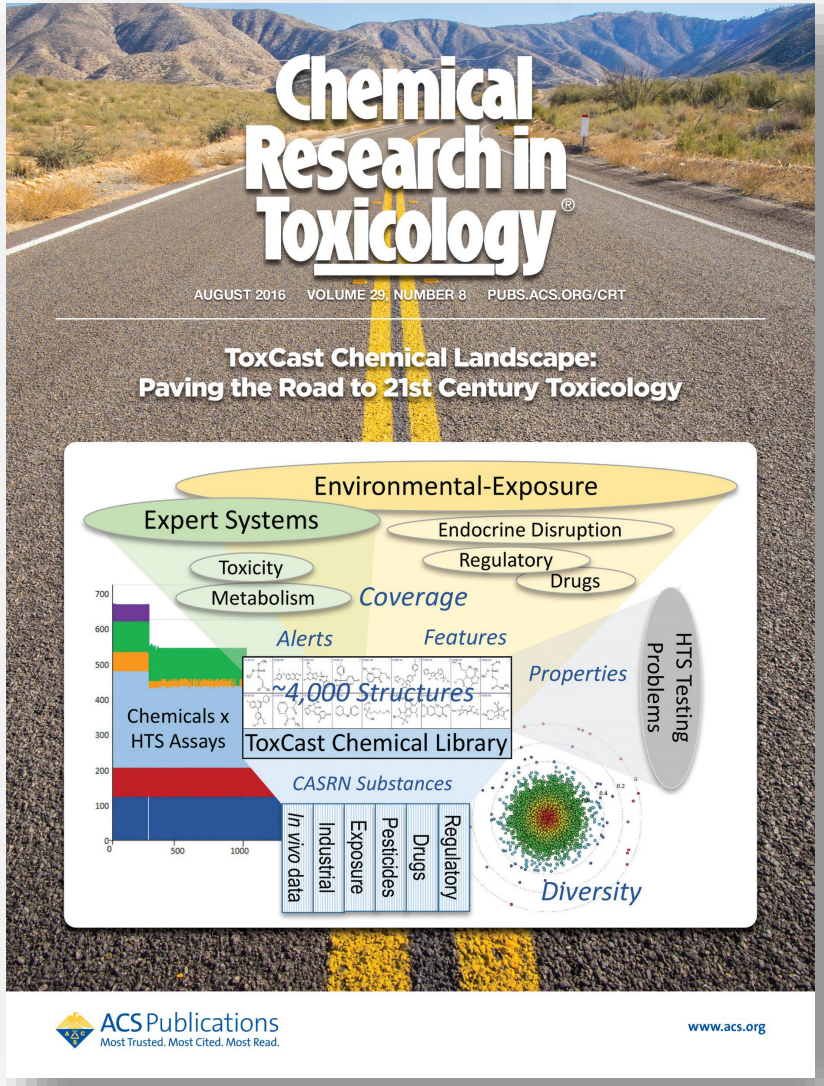
Agency

Bioactivity Data

ToxCast

EPA United States Environmental Protection Agency



ToxCast Chemical Landscape: Paving the Road to 21st Century Toxicology

Ann M. Richard[*†], Richard S. Judson[†], Keith A. Houck[†], Christopher M. Grulke[†], Patra Volarath[‡], Inthirany Thillainadarajah[§], Chihae Yang[∥⊥], James Rathman[⊥#], Matthew T. Martin[†], John F. Wambaugh[†], Thomas B. Knudsen[†], Jayaram Kancherla[▽], Kamel Mansouri[▽], Grace Patlewicz[†], Antony J. Williams[†], Stephen B. Little[†], Kevin M. Crofton[†], and Russell S. Thomas[†]

View Author Information

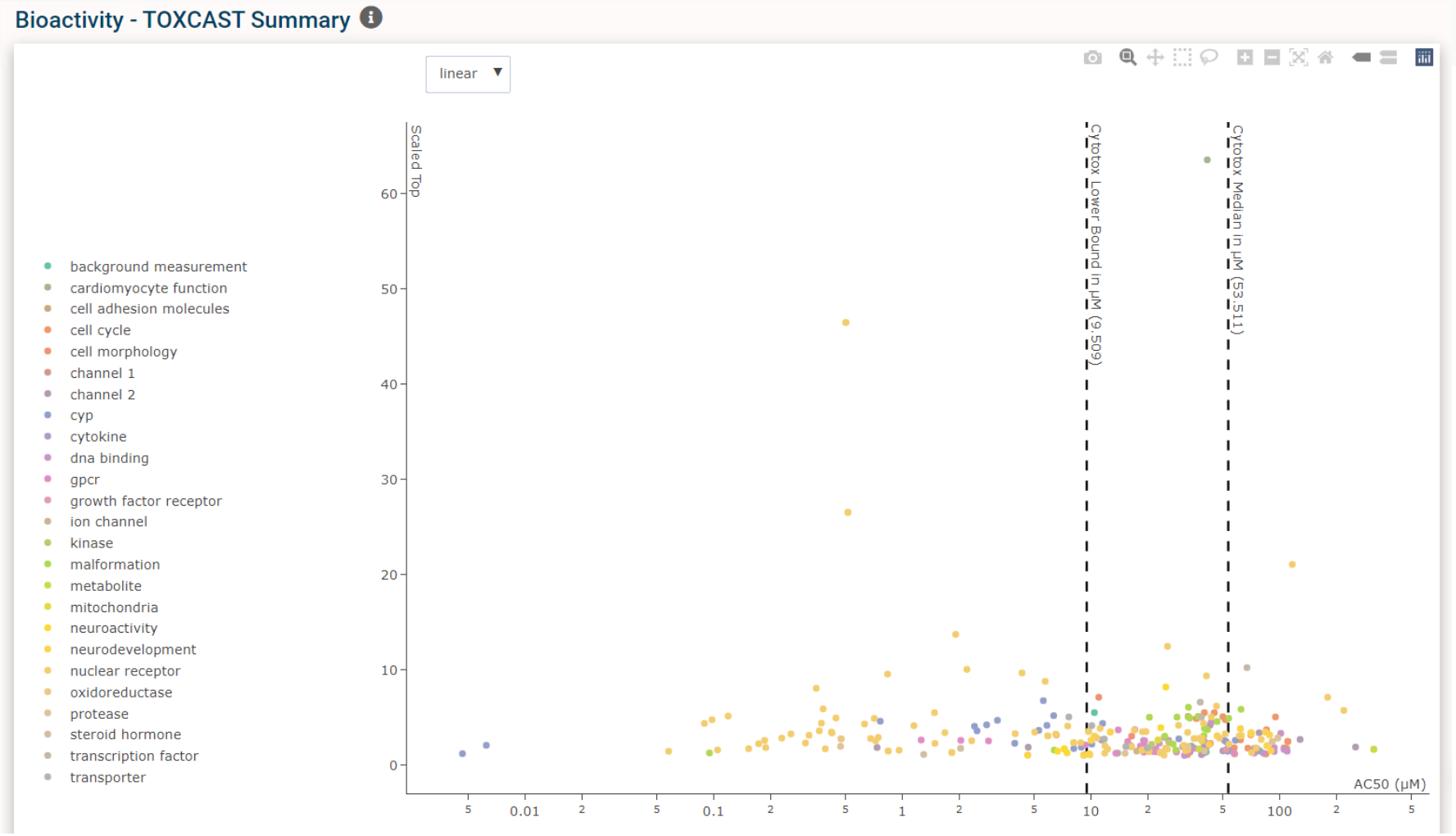
Cite this: *Chem. Res. Toxicol.* 2016, 29, 8, 1225–1251
Publication Date: July 1, 2016
https://doi.org/10.1021/acs.chemrestox.6b00135

Bioactivity Data
Summary views of >2000 Assay Endpoints

United States Environmental Protection Agency

Bioactivity

- ToxCast: Summary
- Toxcast Conc. Response Data
- HTTr: Summary
- HTPP: Summary
- PubChem
- ToxCast: Models



Bioactivity Data
Full transparency of data…

EPA United States Environmental Protection Agency

Bioactivity

- ToxCast: Summary
- Toxcast Conc. Response Data
- HTTr: Summary
- HTPP: Summary
- PubChem
- ToxCast: Models

Concentration Response Data

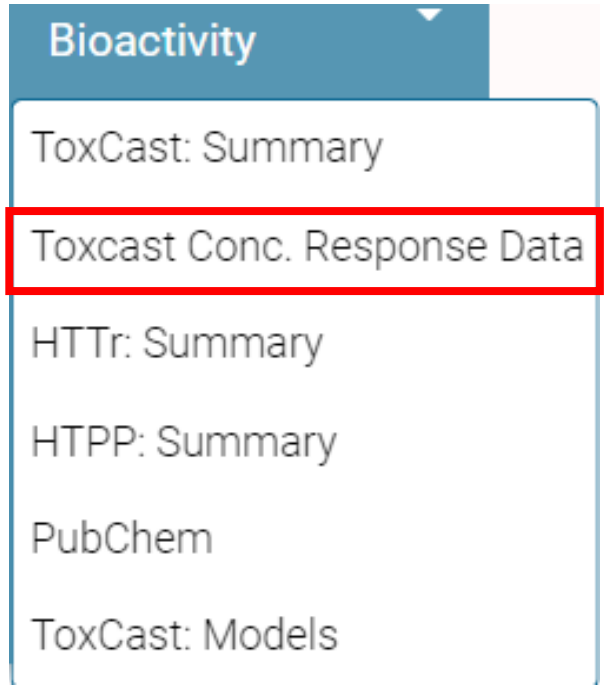
Analytical Data on Tox21 Browser

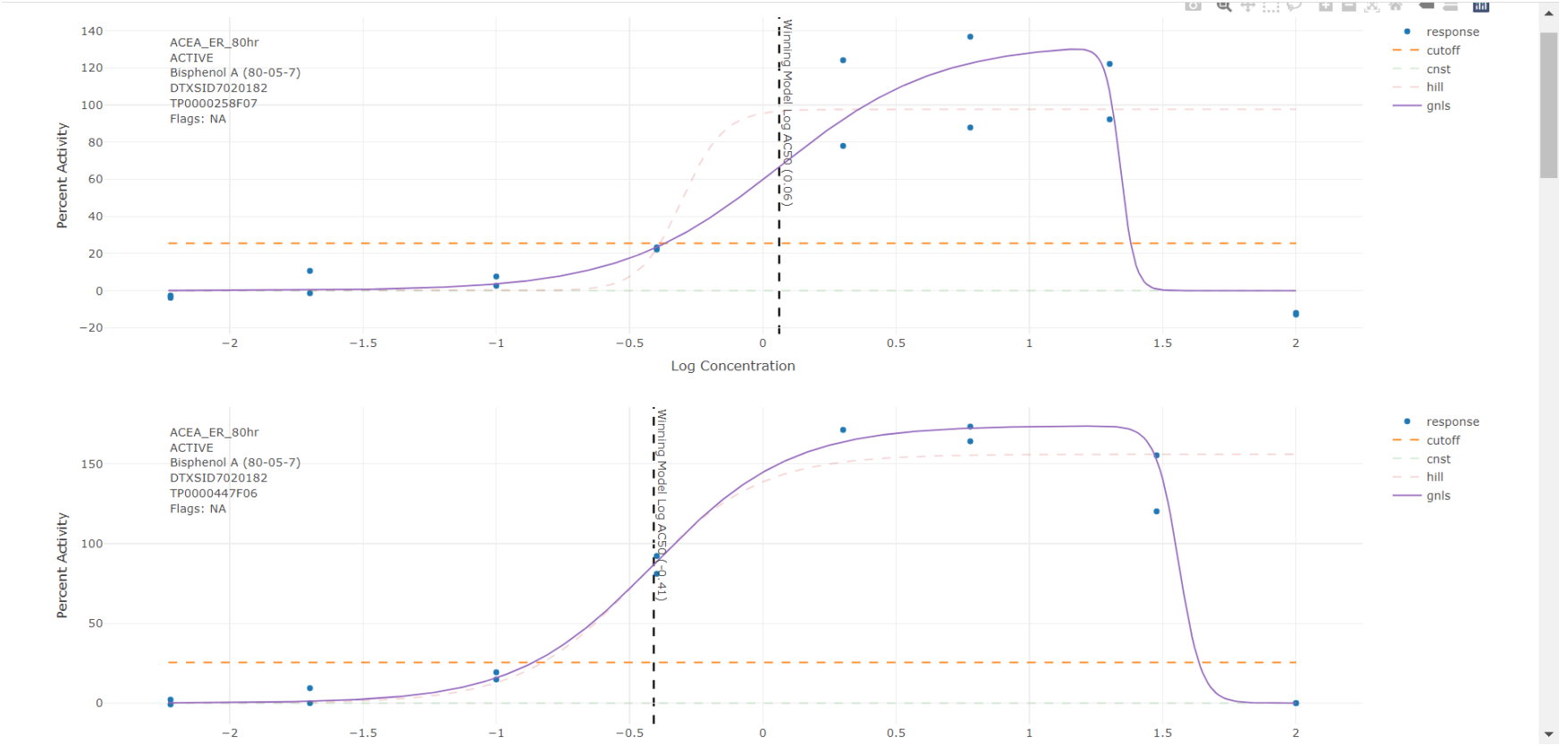
EXPORT

Name	Description	Endpoint Name	Active	Details	Rep. Plot	All Plots	Gene	Intended Target	Cell Line	Cell Format
ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_agonist_80hr	Inactive				AR	steroidal	prostate	cell line
ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_agonist_AUC_viability	Active				-	cytotoxicity	prostate	cell line
ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_antagonist_80hr	Active				AR	steroidal	prostate	cell line
ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_AR_antagonist_AUC_viability	Active				-	cytotoxicity	prostate	cell line
ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_ER_80hr	Active				ESR1	steroidal	breast	cell line
ASSAY SOURCE: ACEA	ACEA Biosciences	ACEA_ER_AUC_viability	Inactive				-	cytotoxicity	breast	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_1h_dn	Inactive				-	proliferation	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_1h_up	Inactive				-	arrest	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_24h_dn	Inactive				-	proliferation	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_24h_up	Inactive				-	arrest	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_72h_dn	Inactive				-	proliferation	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellCycleArrest_72h_up	Inactive				-	arrest	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellLoss_1h_dn	Inactive				-	cytotoxicity	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellLoss_1h_up	Inactive				-	proliferation	liver	cell line
ASSAY SOURCE: APR	Apredica	APR_HepG2_CellLoss_24h_dn	Active				-	cytotoxicity	liver	cell line

Rows: 1,398 Total Rows: 1,398

Bioactivity Data
…including concentration-response





How can these data be used? Combine *in vitro* and httk

JOURNAL ARTICLE FEATURED

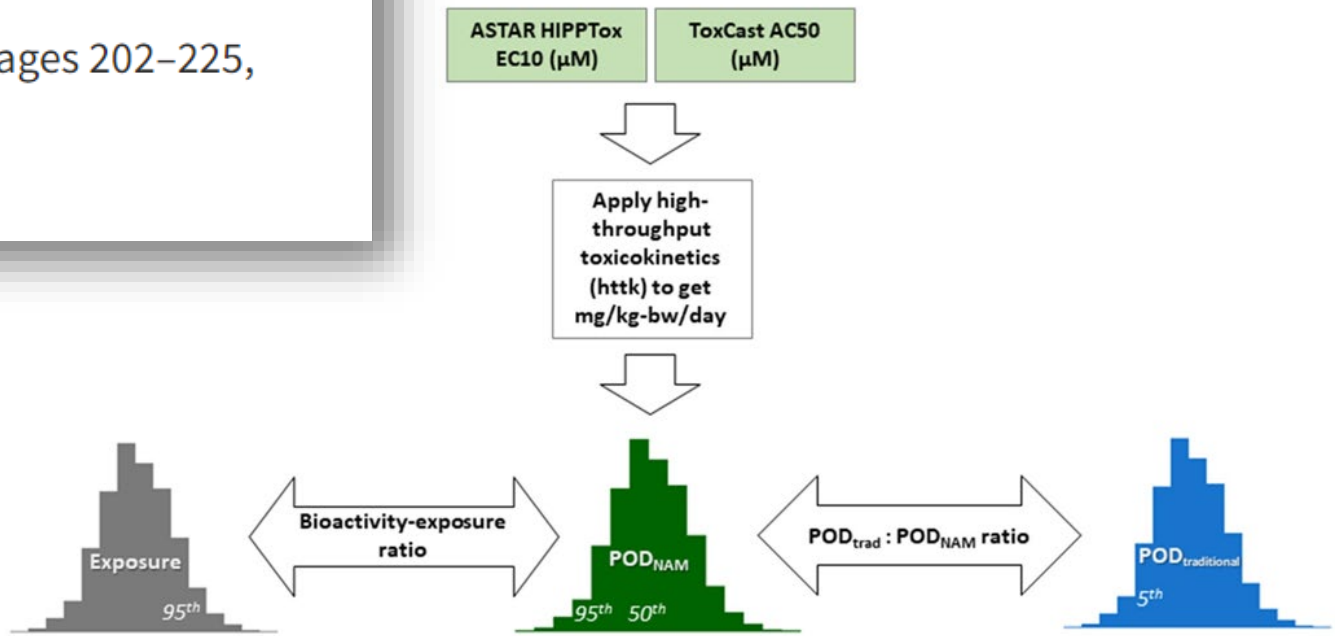
Utility of *In Vitro* Bioactivity as a Lower Bound Estimate of *In Vivo* Adverse Effect Levels and in Risk-Based Prioritization FREE

Katie Paul Friedman ✉, Matthew Gagne, Lit-Hsin Loo, Panagiotis Karamertzanis, Tatiana Netzeva, Tomasz Sobanski, Jill A Franzosa, Ann M Richard, Ryan R Lougee, Andrea Gissi ... Show more

Toxicological Sciences, Volume 173, Issue 1, January 2020, Pages 202–225, https://doi.org/10.1093/toxsci/kfz201

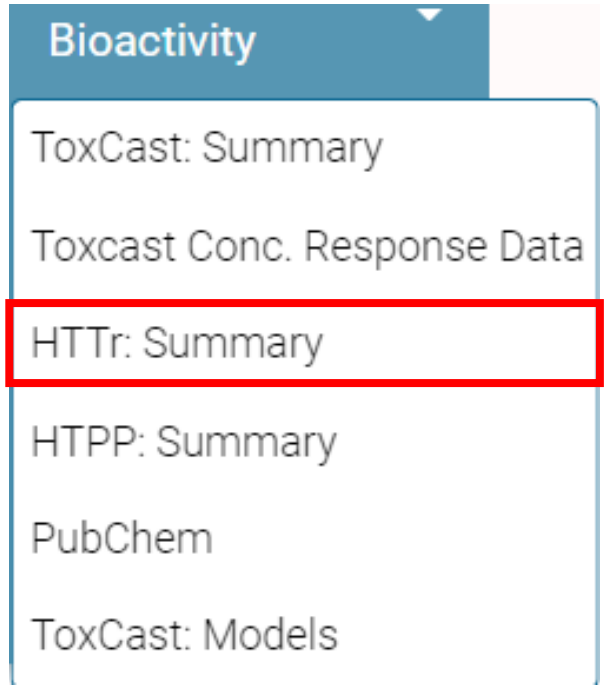
Published: 18 September 2019

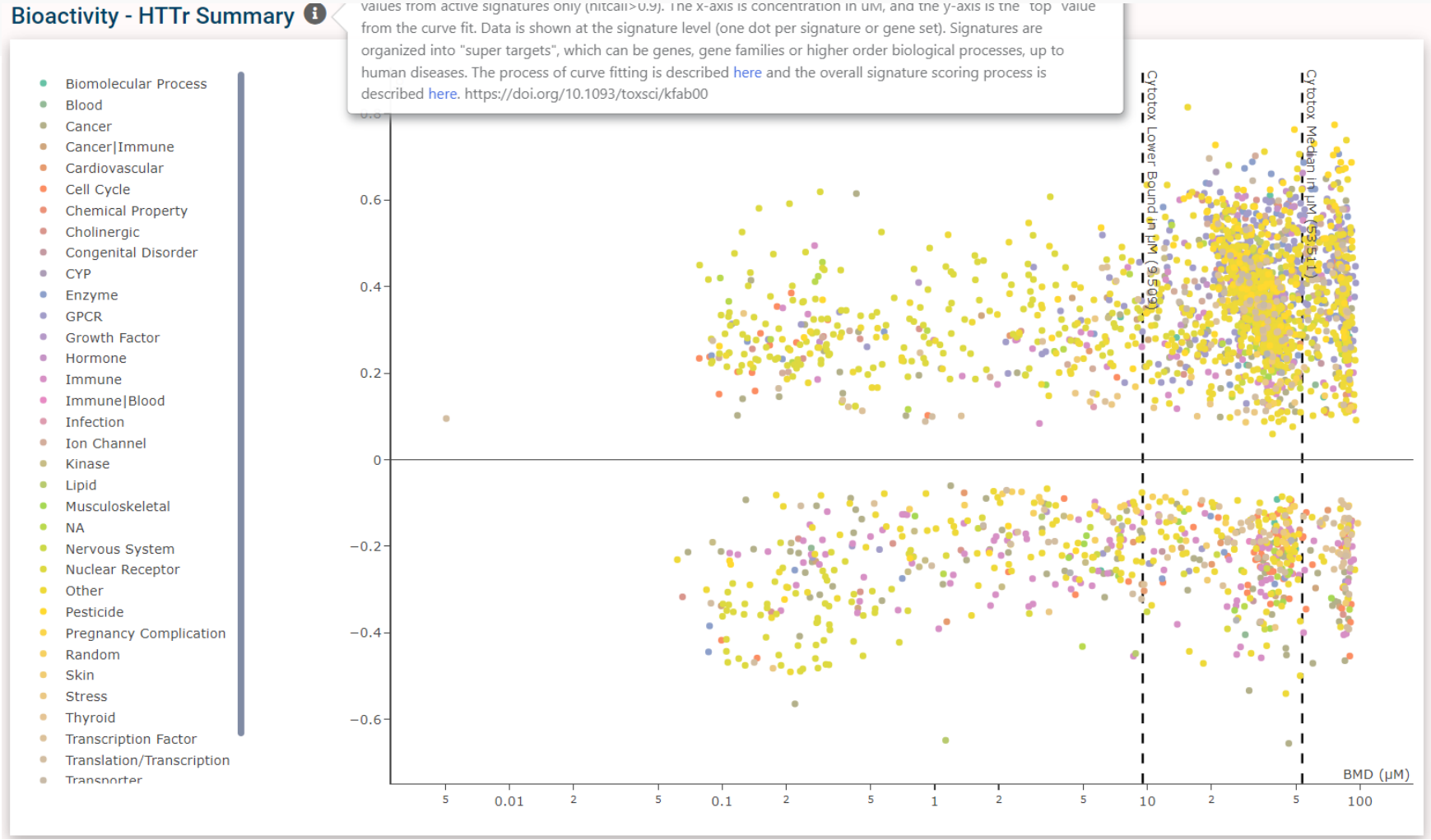
Combine *in vitro* data (AC50s in uM) with httk data to get bioactivity-exposure ratios and PODs



Bioactivity Data
NEW High-Throughput Transcriptomics

United States Environmental Protection Agency





Use Models Derived from the Data

EPA United States Environmental Protection Agency

Screening Chemicals for Estrogen Receptor Bioactivity Using a Computational Model

Patience Browne[*†], Richard S. Judson[‡], Warren M. Casey[§], Nicole C. Kleinstreuer[∥], and Russell S. Thomas[‡]

View Author Information

Cite this: *Environ. Sci. Technol.* 2015, 49, 14, 8804−8814
Publication Date: June 12, 2015
https://doi.org/10.1021/acs.est.5b02641

Article Views 3796 | Altmetric 27 | Citations 157 | Share

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CERAPP: Collaborative Estrogen Receptor Activity Prediction Project

Vol. 124, No. 7 | Research

Kamel Mansouri, Ahmed Abdelaziz, Aleksandra Rybacka, Alessandra Roncaglioni, Alexander Tropsha, Alexandre Varnek, Alexey Zakharov, Andrew Worth, Ann M. Richard, Christopher M. Grulke, Daniela Trisciuzzi, Denis Fourches, Dragos Horvath, Emilio Benfenati, Eugene Muratov, Eva Bay Wedebye, Francesca Grisoni, Giuseppe F. Mangiatordi, ... See all authors

Published: 1 July 2016 | https://doi.org/10.1289/ehp.1510267 | Cited by: 76

CERAPP and CoMPARA available in OPERA

Development and Validation of a Computational Model for Androgen Receptor Activity

Nicole C. Kleinstreuer[*†], Patricia Ceger[‡], Eric D. Watt[§], Matthew Martin[§], Keith Houck[§], Patience Browne[∥], Russell S. Thomas[§], Warren M. Casey[†], David J. Dix[⊥], David Allen[‡], Srilatha Sakamuru[#], Menghang Xia[#], Ruili Huang[#], and Richard Judson[§]

View Author Information

Cite this: *Chem. Res. Toxicol.* 2017, 30, 4, 946−964
Publication Date: November 18, 2016
https://doi.org/10.1021/acs.chemrestox.6b00347

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CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity

Vol. 128, No. 2 | Research

Kamel Mansouri, Nicole Kleinstreuer, Ahmed M. Abdelaziz, Domenico Alberga, Vinicius M. Alves, Patrik L. Andersson, Carolina H. Andrade, Fang Bai, Ilya Balabin, Davide Ballabio, Emilio Benfenati, Barun Bhhatarai, Scott Boyer, Jingwen Chen, Viviana Consonni, Sherif Farag, Denis Fourches, Alfonso T. García-Sosa, Paola Gramatica, Francesca Grisoni, ... See all authors

Published: 7 February 2020 | CID: 027002 | https://doi.org/10.1289/EHP5580 | Cited by: 2

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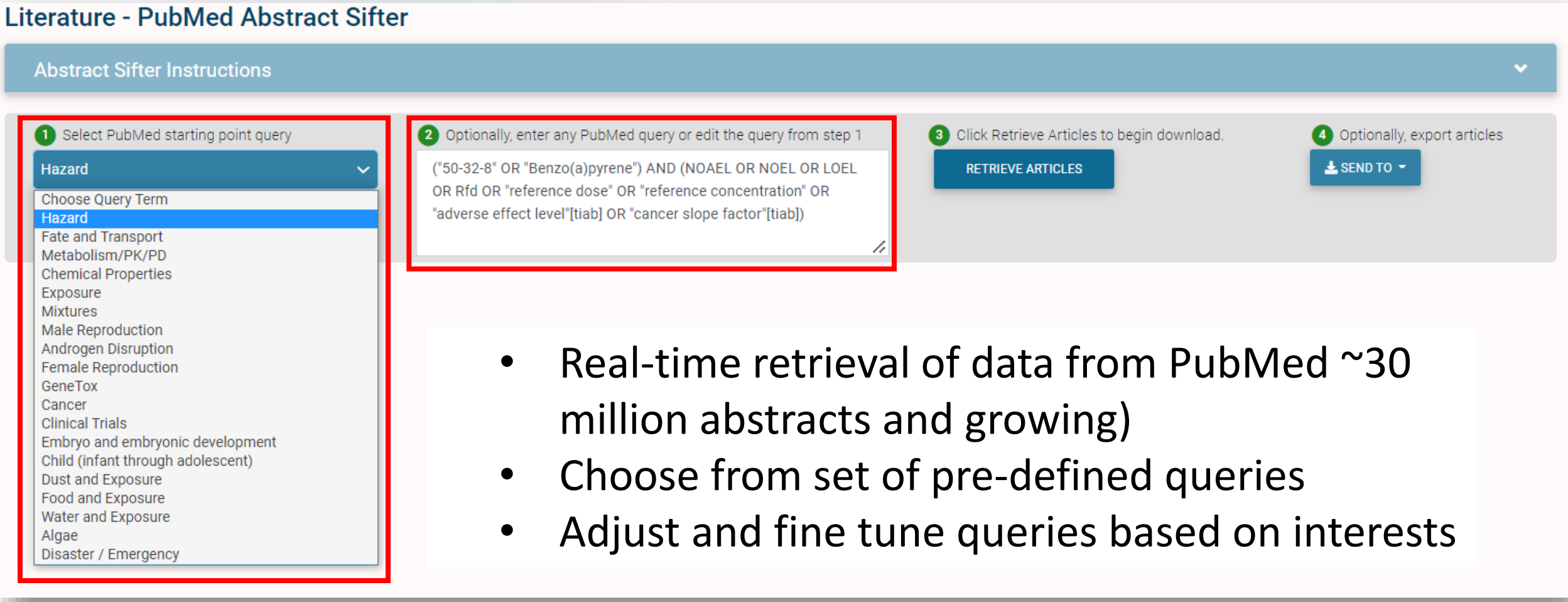
Searching Literature and the Internet

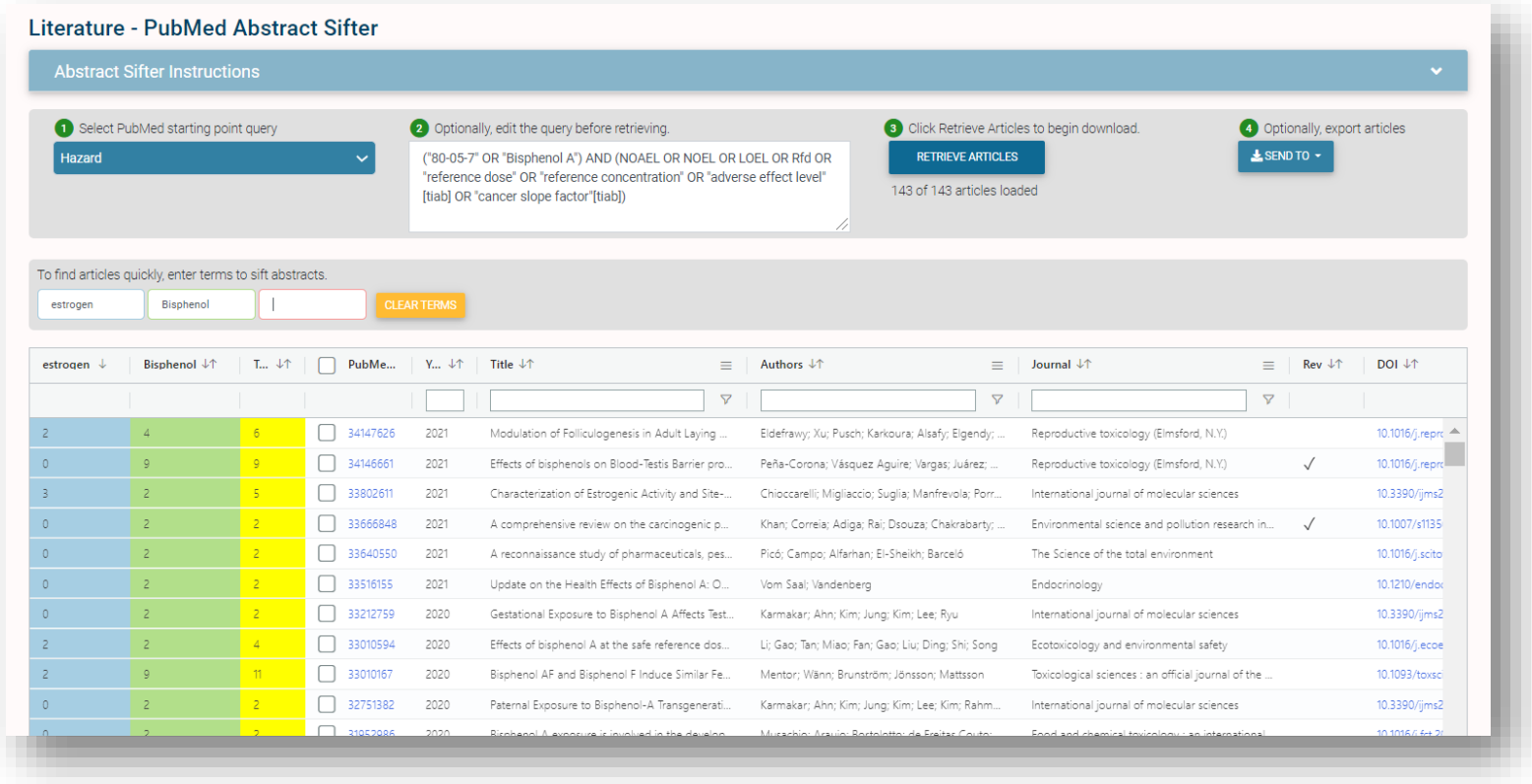
Literature Searching



- Real-time retrieval of data from PubMed ~30 million abstracts and growing)
- Choose from set of pre-defined queries
- Adjust and fine tune queries based on interests

Literature Searching

- “Sifting” of results using multiple terms
- Frequency counting terms
- Color highlighting of terms
- Download list to Excel
- Send list to PubMed for downloading ref. file
- Direct link via PubMed ID



What's the best way to search the internet for chemical data?

- We know how complex chemicals identifiers are…
  - CASRN(s)
  - Hundreds of names (maybe)
  - SMILES
  - InChIs
  - EINECS, EC numbers

- What can WE do to help you navigate the internet?

External Links – Also use Identifiers
Names, CASRN, PubChem IDs, InChIs…

Benzo(a)pyrene

50-32-8 | DTXSID2020139

Searched by DSSTox Substance Id.

General

- EPA Substance Registry Service
- PubChem
- Chemspider
- CPCat
- DrugBank
- Wikipedia
- MSDS Lookup
- ChEMBL
- ToxPlanet
- ACS Reagent Chemicals
- Wolfram Alpha
- ECHA Infocard
- ChemAgora
- Consumer Product Information Database
- ChEBI
- NIST Chemistry Webbook
- WEBWISER
- PubChem Safety Sheet
- Consumer Product Information Database
- PubChem: Chemical Vendors

Toxicology

- ACToR
- DrugPortal
- CCRIS
- ChemView
- CTD
- eChemPortal
- Gene-Tox
- HSDB
- ACToR PDF Report
- CREST
- National Air Toxics Assessment
- ECOTOX
- ChemView
- Chemical Checker
- BindingDB
- CalEPA OEHHA
- NIOSH IDLH Values
- LactMed
- ECOTOX

Publications

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

Analytical

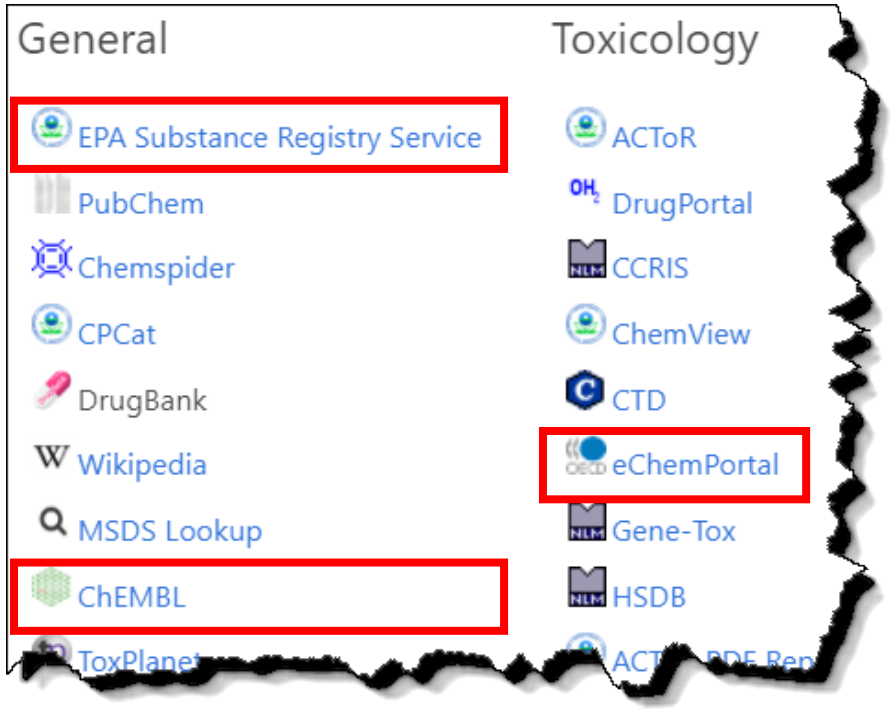
- RSC Analytical Abstracts
- Tox21 Analytical Data
- MONA: MassBank North America
- mzCloud
- NIST IR Spectrum
- NIST MS Spectrum
- MassBank
- NIST Antoine Constants
- IR Spectra on PubChem
- NIST Kovats Index values
- Protein DataBank
- National Environmental Methods Index

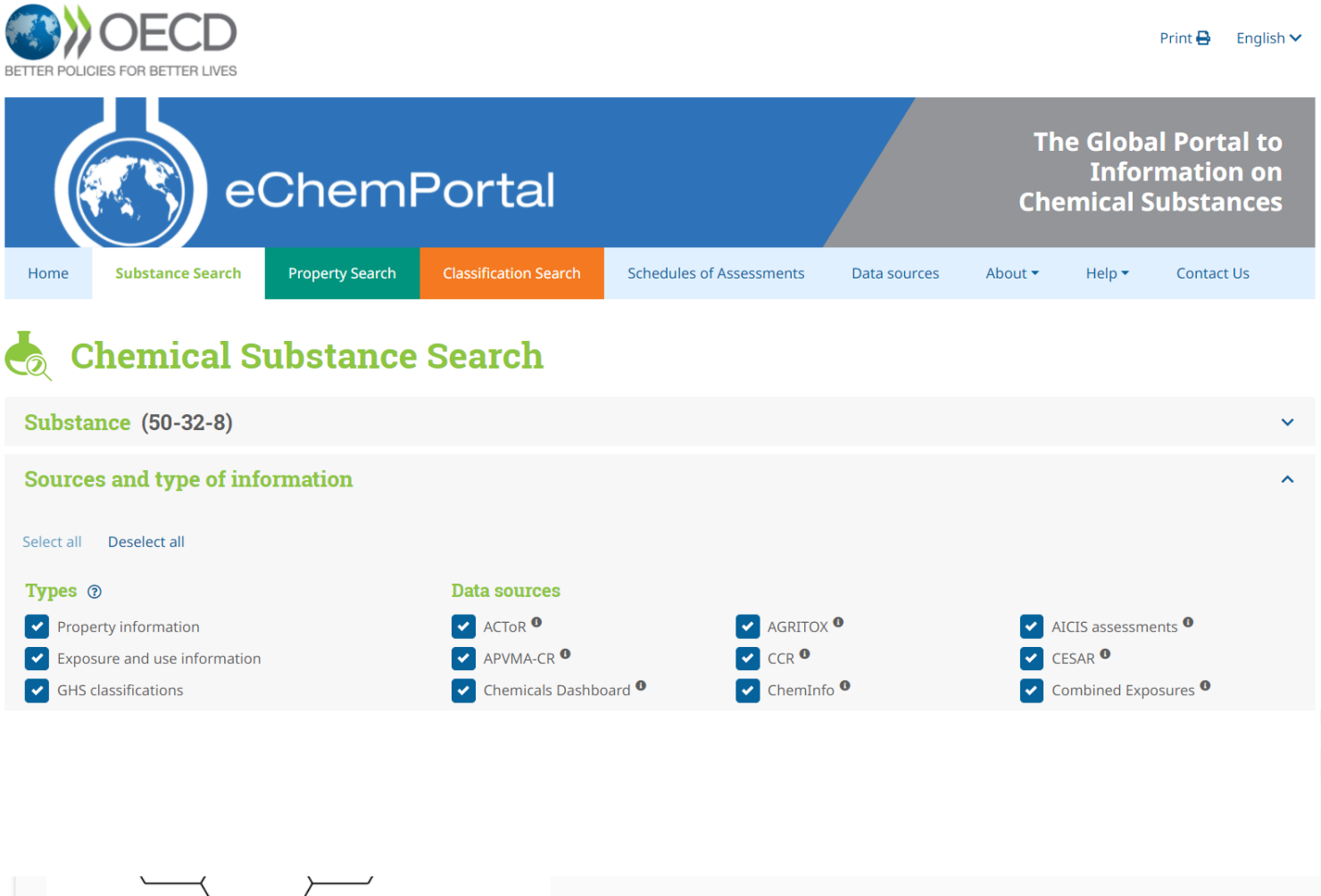
Prediction

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

External Links

- Links to ~90 websites providing access to additional data on the chemical of interest





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Chemical Lists and Categories

A List of Lists of Chemicals

https://comptox.epa.gov/dashboard/chemical_lists

EPA United States Environmental Protection Agency

Chemical Lists

Search Chemical Lists

EXPORT | COPY URL

Showing 36 of 319 Records

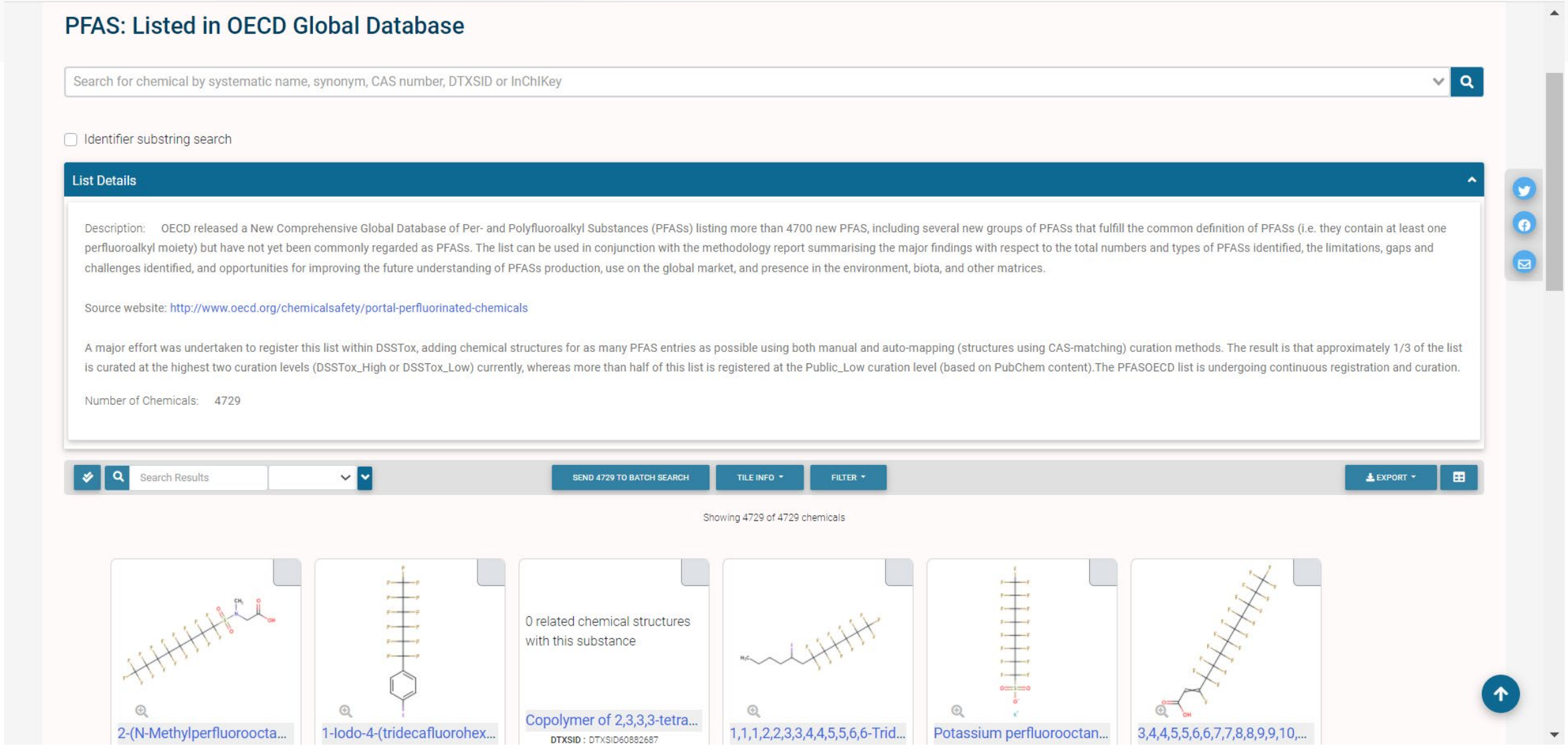
List Acronym	List Name	# Chemicals	Updated	List Description
PFAS				
EPAPFASDW537	PFAS|EPA|WATER: Existing EPA DW Method ...	19	2019-11-16	EPA has recently revised method 537.1 for the PFAS on this list to detect them in drinking water.
EPAPFASDWTREAT	PFAS|EPA|WATER: Drinking Water Treatment...	9	2019-11-16	EPA is gathering and evaluating treatment effectiveness and cost data for removing these PFAS from drinking water systems.
EPAPFASINSOL	PFAS|EPA: Chemical Inventory Insoluble in ...	43	2021-11-21	Per- and Polyfluoroalkyl Substances (PFASs) in EPA's expanded ToxCast chemical inventory that were determined to be insoluble in DMSO above 5mM concentration. These PFAS chemicals were successfully procured from commercial suppliers (with a small number provided by National Toxicology Program partners) but deemed unsuitable for testing due to limited DMSO solubility. For a complete list of solubilized PFAS in EPA's inventory, see https://comptox.epa.gov/dashboard/chemical-lists/EPAPFASINV
EPAPFASINV	PFAS|EPA: ToxCast Chemical Inventory	430	2021-11-21	Per- and Polyfluoroalkyl Substances (PFAS) included in EPA's expanded ToxCast chemical inventory and available for testing. These PFAS chemicals were successfully procured from commercial suppliers (with a small number provided by National Toxicology Program partners) and were deemed suitable for testing (i.e., solubilized in DMSO above 5mM, and not gaseous or highly reactive). All or portions of this inventory are being made available to EPA researchers and collaborators to be analyzed and tested in various high-throughput screening (HTS) and high-throughput toxicity (HTT) assays. The https://comptox.epa.gov/dashboard/chemical-lists/EPAPFAS75S1 list is a prioritized subset of this larger chemical inventory.

Rows: **36 of 319**

The OECD List of PFAS

http://www.oecd.org/chemicalsafety/portal-perfluorinated-chemicals/

EPA United States Environmental Protection Agency



PFAS List Paper

https://doi.org/10.3389/fenvs.2022.850019

frontiers in Environmental Science | Toxicology, Pollution and the Environment

SECTION ABOUT ARTICLES RESEARCH TOPICS FOR AUTHORS EDITORIAL BOARD ARTICLE ALERTS

< Articles

THIS ARTICLE IS PART OF THE RESEARCH TOPIC
Environmental Pollution and Toxicity of Emerging Per- and Polyf
View all Articles >

ORIGINAL RESEARCH article

Front. Environ. Sci., 05 April 2022 | https://doi.org/10.3389/fenvs.2022.850019

Check for updates

Assembly and Curation of Lists of Per- and Polyfluoroalkyl Substances (PFAS) to Support Environmental Science Research

Antony J. Williams[1]*, Linda G. T. Gaines[2], Christopher M. Grulke[1†], Charles N. Lowe[1], Gabriel F. B. Sinclair[3], Vicente Samano[4], Inthirany Thillainadarajah[4], Bryan Meyer[4], Grace Patlewicz[1] and Ann M. Richard[1]

- What makes our efforts different?
- MANUAL curation work
- Building lists, cross-referencing, mapping relationships, sourcing and curating data

What about PFAS?

EPA United States Environmental Protection Agency

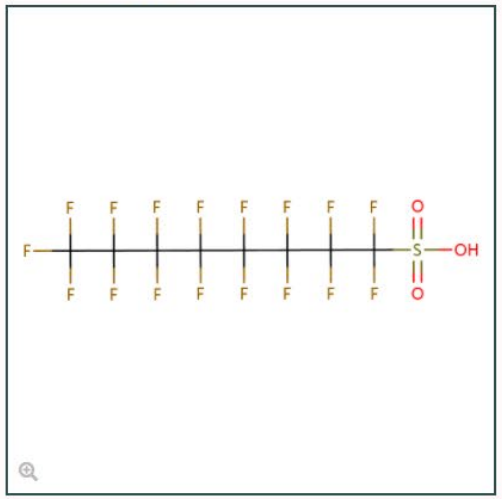
Perfluorooctanesulfonic acid

1763-23-1 | DTXSID3031864

Searched by DTXSID3031864.

- Details
- Executive Summary
- Properties
- Env. Fate/Transport
- Hazard
- Safety > GHS Data
- ADME > IVIVE
- Exposure
- Bioactivity
- Similar Compounds
- GenRA
- Related Substances
- Synonyms
- Literature
- Links
- Comments

Chemical Details



Wikipedia

Perfluorooctanesulfonic acid (**PFOS**) (conjugate base **perfluorooctanesulfonate**) is an anthropogenic (human-made) fluorosurfactant, now regarded as a global pollutant. PFOS was the key ingredient in Scotchgard, a fabric protector made by 3M, and related stain repellents. In many contexts, PFOS refers to the parent sulfonic acid and its various salts of perfluorooctanesulfonate. These are all colorless or white, water soluble solids. Although of low acute toxicity, PFOS has

Read more

Quality Control Notes

Intrinsic Properties

Molecular Formula: $C_8HF_{17}O_3S$ MOL FILE FIND ALL CHEMICALS

Average Mass: 500.13 g/mol ISOTOPE MASS DISTRIBUTION

Monoisotopic Mass: 499.937494 g/mol

Structural Identifiers

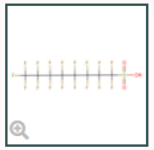
Linked Substances

Presence in Lists

Record Information

Are there Similar Compounds?

EPA United States Environmental Protection Agency



Perfluorooctanesulfonic acid

1763-23-1 | DTXSID3031864

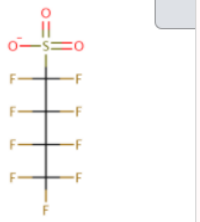
Searched by DTXSID3031864.

Searched with a similarity threshold of 0.8

- Details
- Executive Summary
- Properties
- Env. Fate/Transport
- Hazard
- Safety > GHS Data
- ADME > IVIVE
- Exposure
- Bioactivity
- Similar Compounds
- GenRA
- Related Substances
- Synonyms
- Literature
- Links
- Comments

Search Results | Similarity | SEND 127 TO BATCH SEARCH | TILE INFO | FILTER | EXPORT

Showing 127 of 127 chemicals



Perfluorobutanesulfonate
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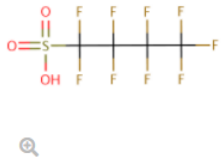
CASRN : 45187-15-3
TOXCAST :
Similarity : 1.00



Perfluorobutanesulfonic a...
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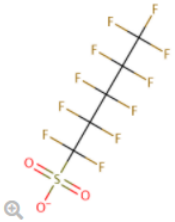
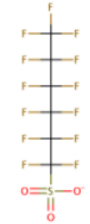
CASRN : 375-73-5
TOXCAST :
Similarity : 1.00

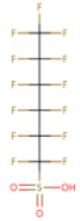


Perfluoropentanesulfonate
DTXSID : DTXSID70892479
CASRN : 175905-36-9
TOXCAST :
Similarity : 1.00

Perfluoropentanesulfonic ...
DTXSID : DTXSID8062600
CASRN : 2706-91-4
TOXCAST :
Similarity : 1.00

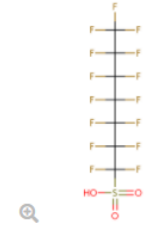


Perfluorohexanesulfonate
DTXSID : DTXSID80873012
CASRN : 108427-53-8
TOXCAST :
Similarity : 1.00



Perfluorohexanesulfonic a...
DTXSID : DTXSID7040150
CASRN : 355-46-4
TOXCAST :
Similarity : 1.00

Perfluoroheptanesulfonate
DTXSID : DTXSID20892505
CASRN : 146689-46-5
TOXCAST :
Similarity : 1.00



Perfluoroheptanesulfonic ...
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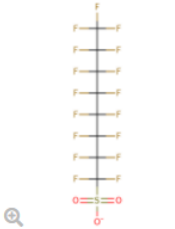
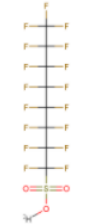
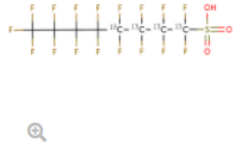
CASRN : 375-92-8
TOXCAST :
Similarity : 1.00



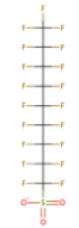
Perfluorooctanesulfonate
DTXSID : DTXSID80108992
CASRN : 45298-90-6
TOXCAST :
Similarity : 1.00



Heptadecafluorooctane-1-...
DTXSID : DTXSID00892720
CASRN : NOCAS_892720
TOXCAST :
Similarity : 1.00

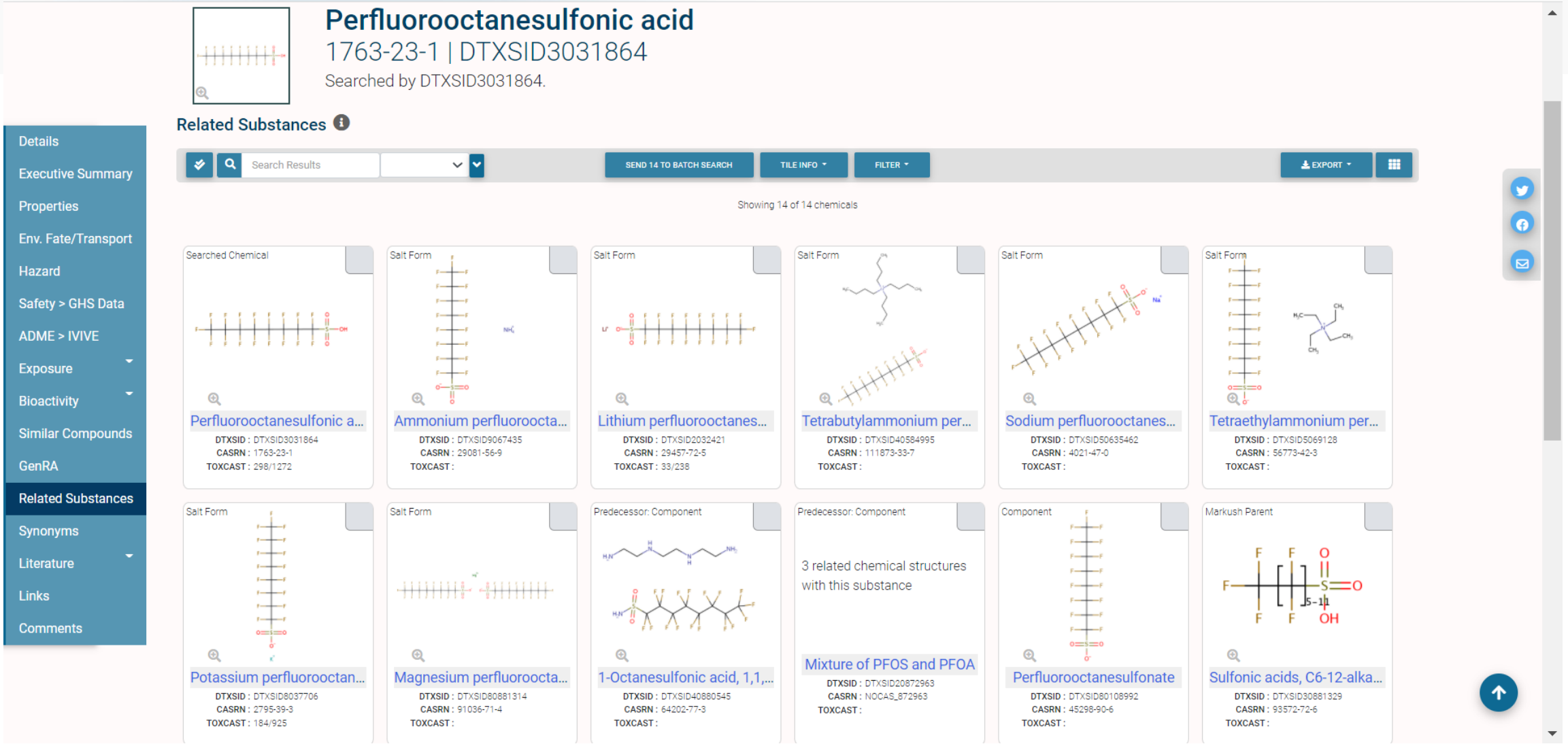


heptadecafluoro(1,2,3,4-1...
DTXSID : DTXSID80894101
CASRN : 960354-19-2
TOXCAST :
Similarity : 1.00



Perfluorononanesulfonate
DTXSID : DTXSID60873010
CASRN : 474511-07-4
TOXCAST :
Similarity : 1.00

Relationships in the data



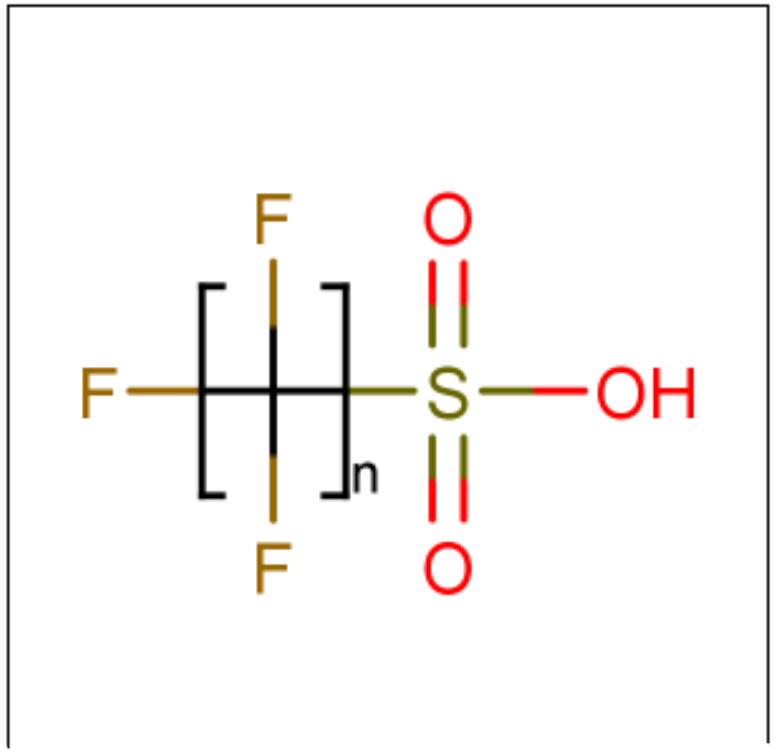
Markush Chemicals

- PFOS is a member of linear perfluoroalkyl sulfonates

Perfluoroalkyl sulfonates

NOCAS_892979 | DTXSID70892979

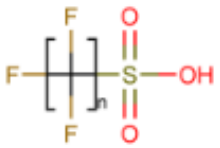
Searched by DSSTox Substance Id.



…and their Markush Children…

- Linear perfluoroalkyl sulfonates has children…

Searched Chemical



Perfluoroalkyl sulfonates
DTXSID: DTXSID70892979
CASRN: NOCAS_892979

Markush Child

Perfluorobutanesulfonic acid
DTXSID: DTXSID5030030
CASRN: 375-73-5

Markush Child

Perfluorooctanesulfonic acid
DTXSID: DTXSID3031864
CASRN: 1763-23-1

Markush Child

Perfluorodecanesulfonic acid
DTXSID: DTXSID3040148
CASRN: 335-77-3

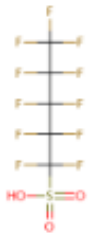
Markush Child

Perfluorohexanesulfonic acid
DTXSID: DTXSID7040150
CASRN: 355-46-4

Markush Child

Perfluoroheptanesulfonic acid
DTXSID: DTXSID8059920
CASRN: 375-92-8

Markush Child



Perfluoropentanesulfonic acid
DTXSID: DTXSID8062600
CASRN: 2706-91-4

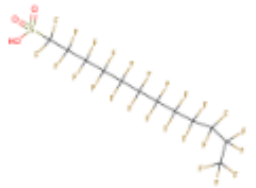
Markush Child

Perfluorononanesulfonic acid
DTXSID: DTXSID8071356
CASRN: 68259-12-1

Markush Child

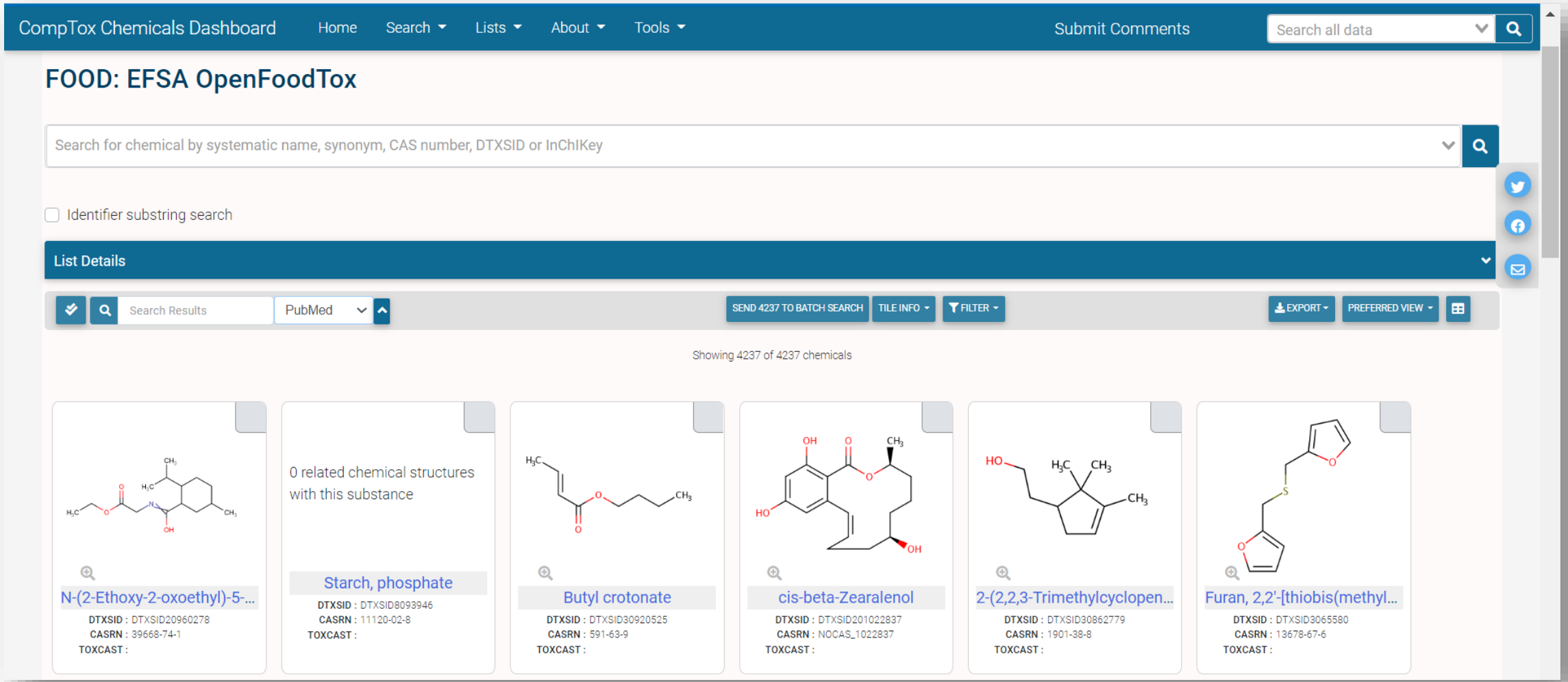
Perfluoropropanesulfonic acid
DTXSID: DTXSID30870531
CASRN: 423-41-6

Markush Child



Perfluorododecanesulfonic acid (PFDOS)
DTXSID: DTXSID20873011
CASRN: 79780-39-5

EFSA List


CompTox Chemicals Dashboard
Home
Search
Lists
About
Tools
Submit Comments
Search all data
FOOD: EFSA OpenFoodTox
Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey
Identifier substring search
List Details
Search Results
PubMed
SEND 4237 TO BATCH SEARCH
TILE INFO
FILTER
EXPORT
PREFERRED VIEW
Showing 4237 of 4237 chemicals
N-(2-Ethoxy-2-oxoethyl)-5-...
DTXSID : DTXSID20960278
CASRN : 39668-74-1
TOXCAST :
0 related chemical structures with this substance
Starch, phosphate
DTXSID : DTXSID8093946
CASRN : 11120-02-8
TOXCAST :
Butyl crotonate
DTXSID : DTXSID30920525
CASRN : 591-63-9
TOXCAST :
cis-beta-Zearalenol
DTXSID : DTXSID201022837
CASRN : NOCAS_1022837
TOXCAST :
2-(2,2,3-Trimethylcyclopen...
DTXSID : DTXSID30862779
CASRN : 1901-38-8
TOXCAST :
Furan, 2,2'-[thiobis(methyl...
DTXSID : DTXSID3065580
CASRN : 13678-67-6
TOXCAST :

MTOX biomarkers

EPA United States Environmental Protection Agency

MTox700+ metabolic biomarkers

Search for chemical by systematic name, synonym, CAS number, DTXSID or InChIKey

Identifier substring search

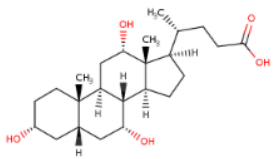
List Details

Description: List of metabolic biomarkers associated with the publication "Knowledge-Driven Approaches to Create the MTox700+ Metabolite Panel for Predicting Toxicity" authored by Viant et al.

Number of Chemicals: 627

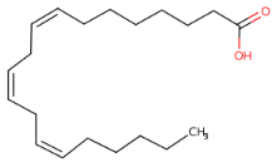
Search Results | SEND 1000 TO BATCH SEARCH | TILE INFO | FILTER | EXPORT | PREFERRED VIEW

Showing 1254 of 1254 chemicals



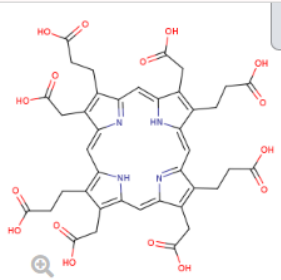
Cholic acid

DTXSID : DTXSID6040660



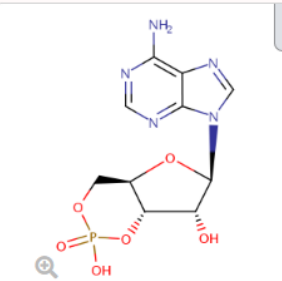
(8Z,11Z,14Z)-8,11,14-Eico...

DTXSID : DTXSID00912351



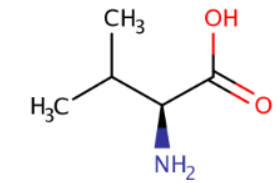
Uroporphyrin III

DTXSID : DTXSID70896977



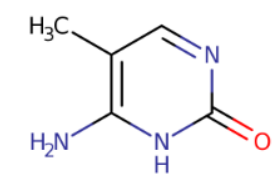
Cyclic AMP

DTXSID : DTXSID8040436



L-Valine

DTXSID : DTXSID40883233



5-Methylcytosine

DTXSID : DTXSID50203948

Batch Searching

Batch Searching

- Singleton searches are great but…
- …we generally want data on LOTS of chemicals!

- Typical questions
  - What are the structures for a set of chemical names? Set of CASRNs?
  - Can I get chemical lists in Excel files? As a list of SMILES strings? Can I get an SDF file?
  - Can I include predicted properties? OPERA? TEST?
  - Are “these chemicals” screened in Toxcast?
  - I need masses and formulae for a list of chemicals

Batch Search

EPA United States Environmental Protection Agency

Batch Search

1 Select Input Type(s)

- [x] Substance Identifiers
  - [x] Chemical Name
  - [x] CASRN
  - [x] InChIKey
  - [x] DSSTox Substance ID
- [ ] DSSTox Compound ID
- [ ] InChIKey Skeleton
- [ ] MS-Ready Formula(e)
- [ ] Exact Formula(e)
- [ ] Monoisotopic Mass

2 Enter Identifiers to Search

(Please enter one identifier per line. Processing time increases with number of inputs.)

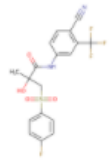
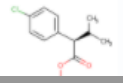
```
DTXSID9020374
DTXSID9020827
DTXSID2022678
DTXSID4023381
DTXSID9044164
DTXSID7032004
DTXSID4022361
DTXSID8021771
```

3 DISPLAY ALL CHEMICALS or CHOOSE EXPORT OPTIONS

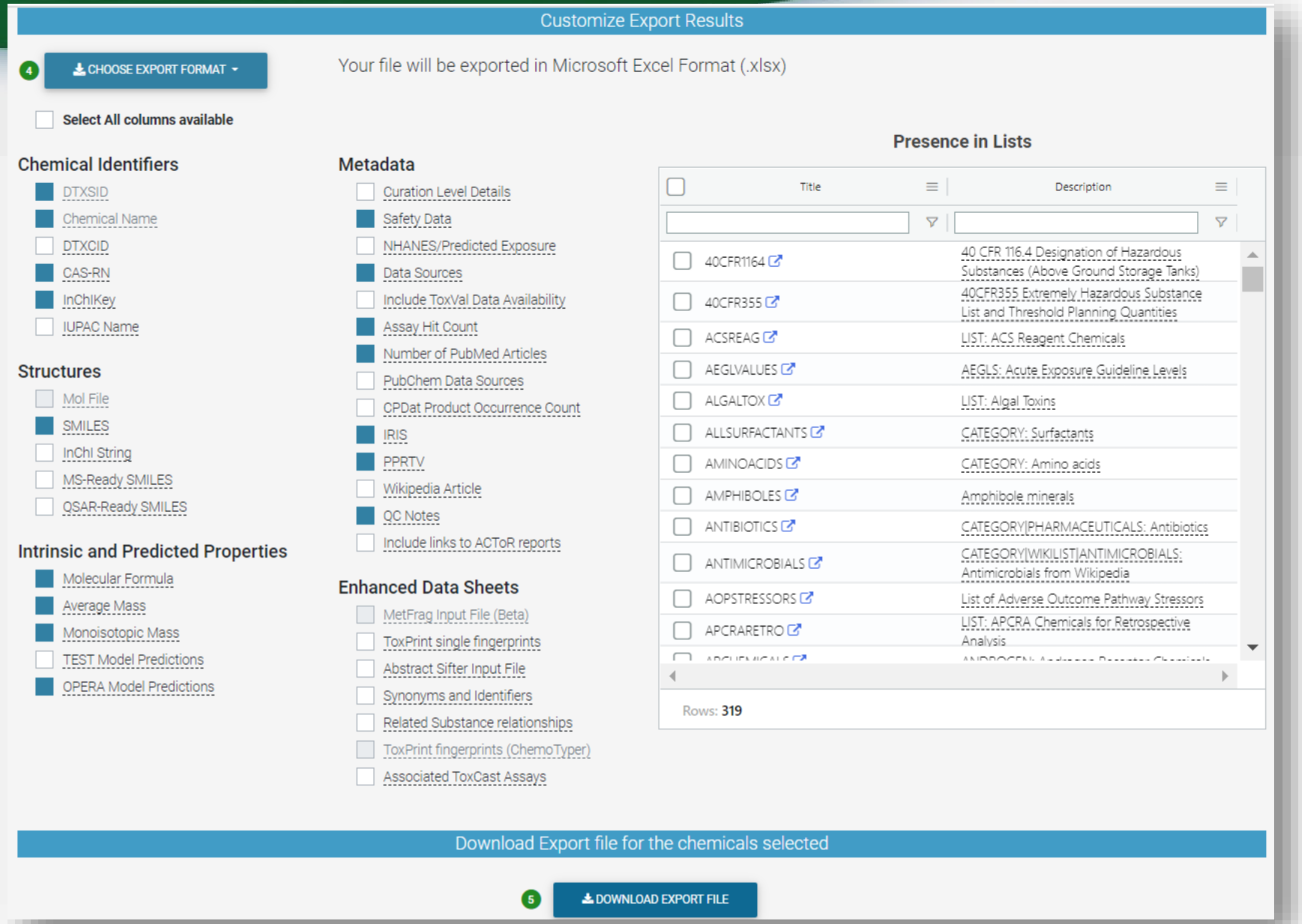
45% loaded

45 Chemicals Found from 110 Input(s)

REPLACE IDENTIFIERS WITH SELECTED CHEMICALS

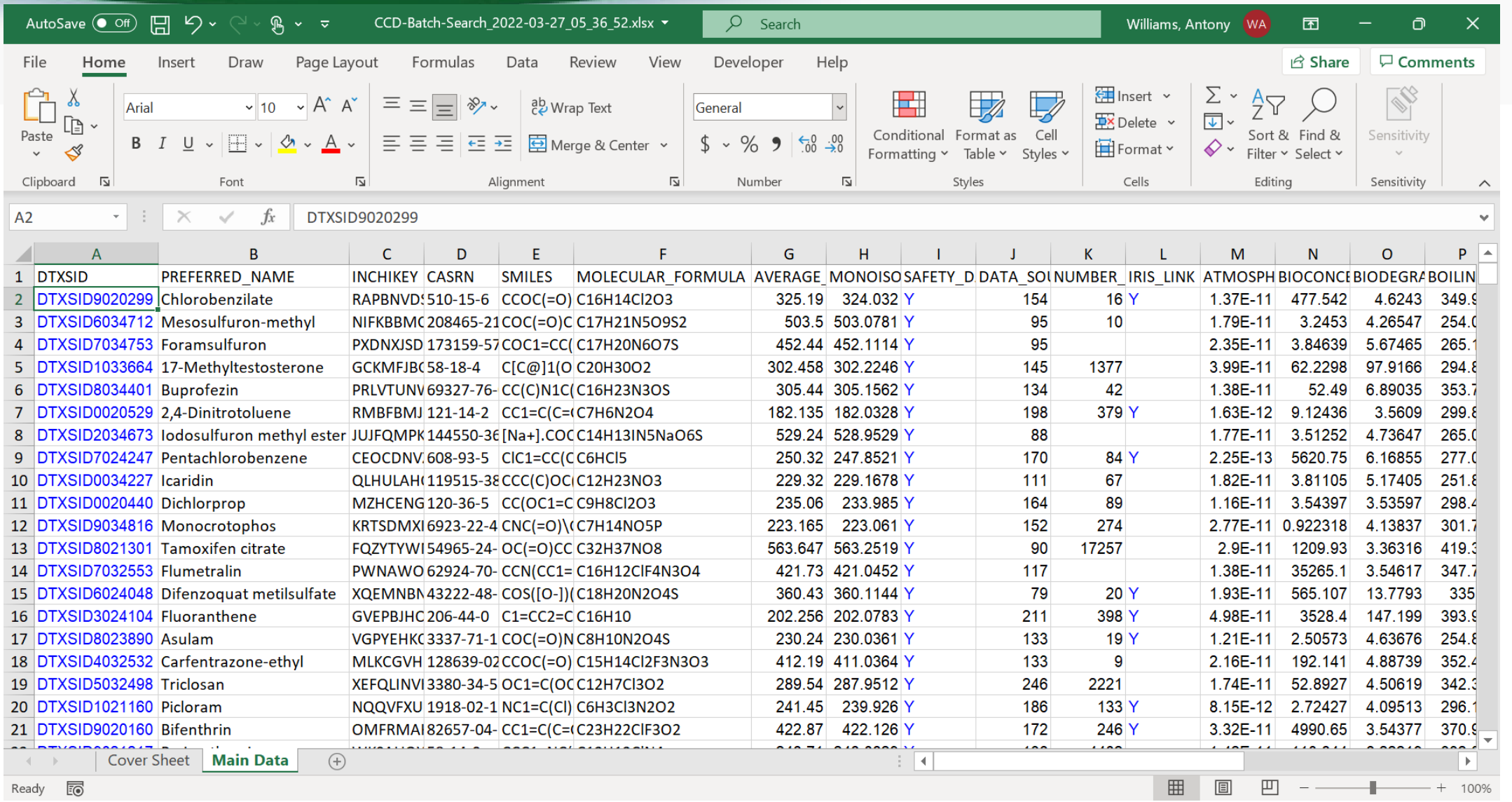
Structure	DTXSID	Preferred Name	CASRN	Mono. Mass	Mol. Formula
	DTXSID2022678	Bicalutamide	90357-06-5	430.061041	C18H14F4N2O4S
	DTXSID3020621	(R,R)-Fenvalerate	67614-33-9	419.128821	C25H22ClNO3

Batch Search – Excel, CSV, SDF file



Batch Search

United States Environmental Protection Agency



	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	DTXSID	PREFERRED_NAME	INCHIKEY	CASRN	SMILES	MOLECULAR_FORMULA	AVERAGE_	MONOISO	SAFETY_D	DATA_SOU	NUMBER_	IRIS_LINK	ATMOSPH	BIOCONCE	BIODEGRA	BOILIN
2	DTXSID9020299	Chlorobenzilate	RAPBNVDS	510-15-6	CCOC(=O)	C16H14Cl2O3	325.19	324.032	Y	154	16	Y	1.37E-11	477.542	4.6243	349.9
3	DTXSID6034712	Mesosulfuron-methyl	NIFKBBMC	208465-21	COC(=O)C	C17H21N5O9S2	503.5	503.0781	Y	95	10		1.79E-11	3.2453	4.26547	254.0
4	DTXSID7034753	Foramsulfuron	PXDNXJSD	173159-57	COC1=CC(	C17H20N6O7S	452.44	452.1114	Y	95			2.35E-11	3.84639	5.67465	265.1
5	DTXSID1033664	17-Methyltestosterone	GCKMFJBC	58-18-4	C[C@]1(O	C20H30O2	302.458	302.2246	Y	145	1377		3.99E-11	62.2298	97.9166	294.8
6	DTXSID8034401	Buprofezin	PRLVTUNV	69327-76-	CC(C)N1C(	C16H23N3OS	305.44	305.1562	Y	134	42		1.38E-11	52.49	6.89035	353.7
7	DTXSID0020529	2,4-Dinitrotoluene	RMBFBMJ	121-14-2	CC1=C(C=(	C7H6N2O4	182.135	182.0328	Y	198	379	Y	1.63E-12	9.12436	3.5609	299.8
8	DTXSID2034673	Iodosulfuron methyl ester	JUJFQMPK	144550-36	[Na+].COC	C14H13IN5NaO6S	529.24	528.9529	Y	88			1.77E-11	3.51252	4.73647	265.0
9	DTXSID7024247	Pentachlorobenzene	CEOCDNV	608-93-5	ClC1=CC(C	C6HCl5	250.32	247.8521	Y	170	84	Y	2.25E-13	5620.75	6.16855	277.0
10	DTXSID0034227	Icaridin	QLHULAH(	119515-38	CCC(C)OC(	C12H23NO3	229.32	229.1678	Y	111	67		1.82E-11	3.81105	5.17405	251.8
11	DTXSID0020440	Dichlorprop	MZHCENG	120-36-5	CC(OC1=C	C9H8Cl2O3	235.06	233.985	Y	164	89		1.16E-11	3.54397	3.53597	298.4
12	DTXSID9034816	Monocrotophos	KRTSDMXI	6923-22-4	CNC(=O)\(	C7H14NO5P	223.165	223.061	Y	152	274		2.77E-11	0.922318	4.13837	301.7
13	DTXSID8021301	Tamoxifen citrate	FQZYTYWI	54965-24-	OC(=O)CC	C32H37NO8	563.647	563.2519	Y	90	17257		2.9E-11	1209.93	3.36316	419.3
14	DTXSID7032553	Flumetralin	PWNAWO	62924-70-	CCN(CC1=	C16H12ClF4N3O4	421.73	421.0452	Y	117			1.38E-11	35265.1	3.54617	347.7
15	DTXSID6024048	Difenzoquat metilsulfate	XQEMNBN	43222-48-	COS([O-])(	C18H20N2O4S	360.43	360.1144	Y	79	20	Y	1.93E-11	565.107	13.7793	335
16	DTXSID3024104	Fluoranthene	GVEPBJHC	206-44-0	C1=CC2=C	C16H10	202.256	202.0783	Y	211	398	Y	4.98E-11	3528.4	147.199	393.9
17	DTXSID8023890	Asulam	VGPYEHKC	3337-71-1	COC(=O)N	C8H10N2O4S	230.24	230.0361	Y	133	19	Y	1.21E-11	2.50573	4.63676	254.8
18	DTXSID4032532	Carfentrazone-ethyl	MLKCGVH	128639-02	CCOC(=O)	C15H14Cl2F3N3O3	412.19	411.0364	Y	133	9		2.16E-11	192.141	4.88739	352.4
19	DTXSID5032498	Triclosan	XEFQLINVI	3380-34-5	OC1=C(OC	C12H7Cl3O2	289.54	287.9512	Y	246	2221		1.74E-11	52.8927	4.50619	342.3
20	DTXSID1021160	Picloram	NQQVFXU	1918-02-1	NC1=C(Cl)	C6H3Cl3N2O2	241.45	239.926	Y	186	133	Y	8.15E-12	2.72427	4.09513	296.1
21	DTXSID9020160	Bifenthrin	OMFRMAI	82657-04-	CC1=C(C=(	C23H22ClF3O2	422.87	422.126	Y	172	246	Y	3.32E-11	4990.65	3.54377	370.9

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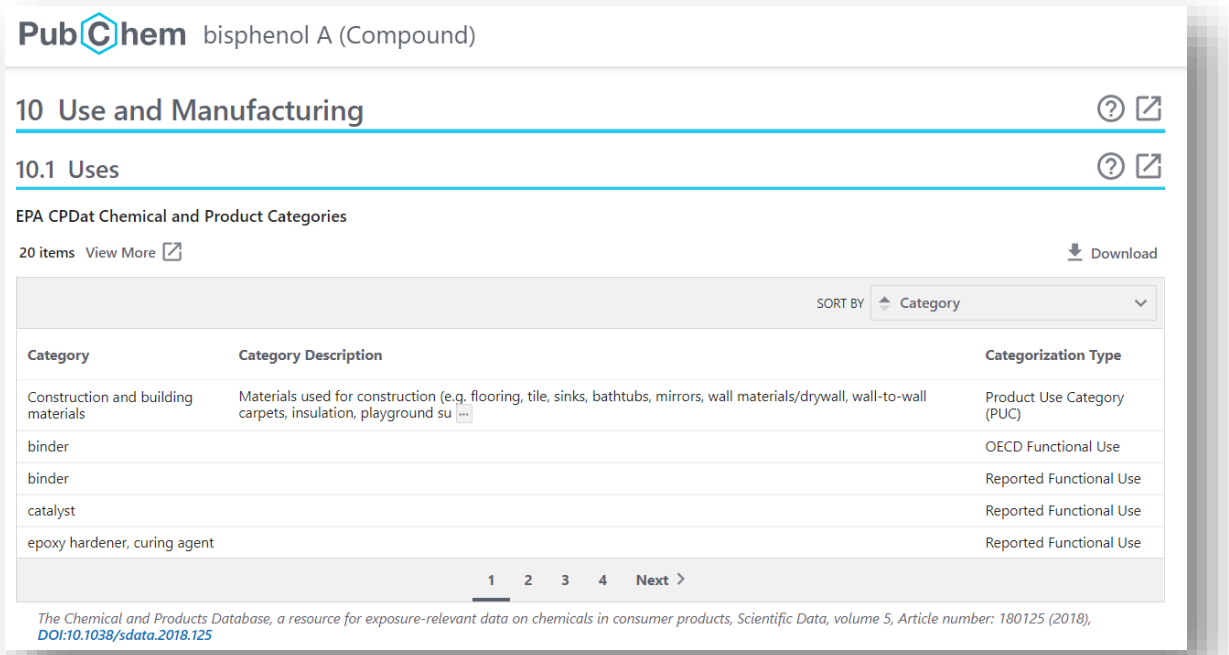
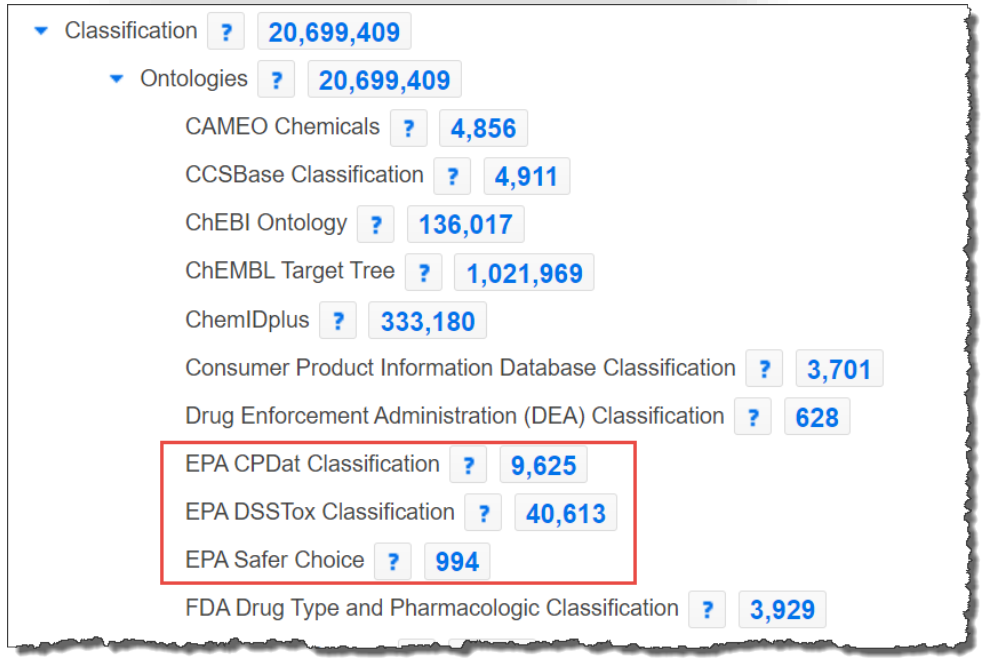
Open Data Exchange

Since our data are Open…

- They flow into other systems for benefit …
  - ECHA eChemPortal
  - ChemSpider
  - EBI's UniChem
  - PubChem





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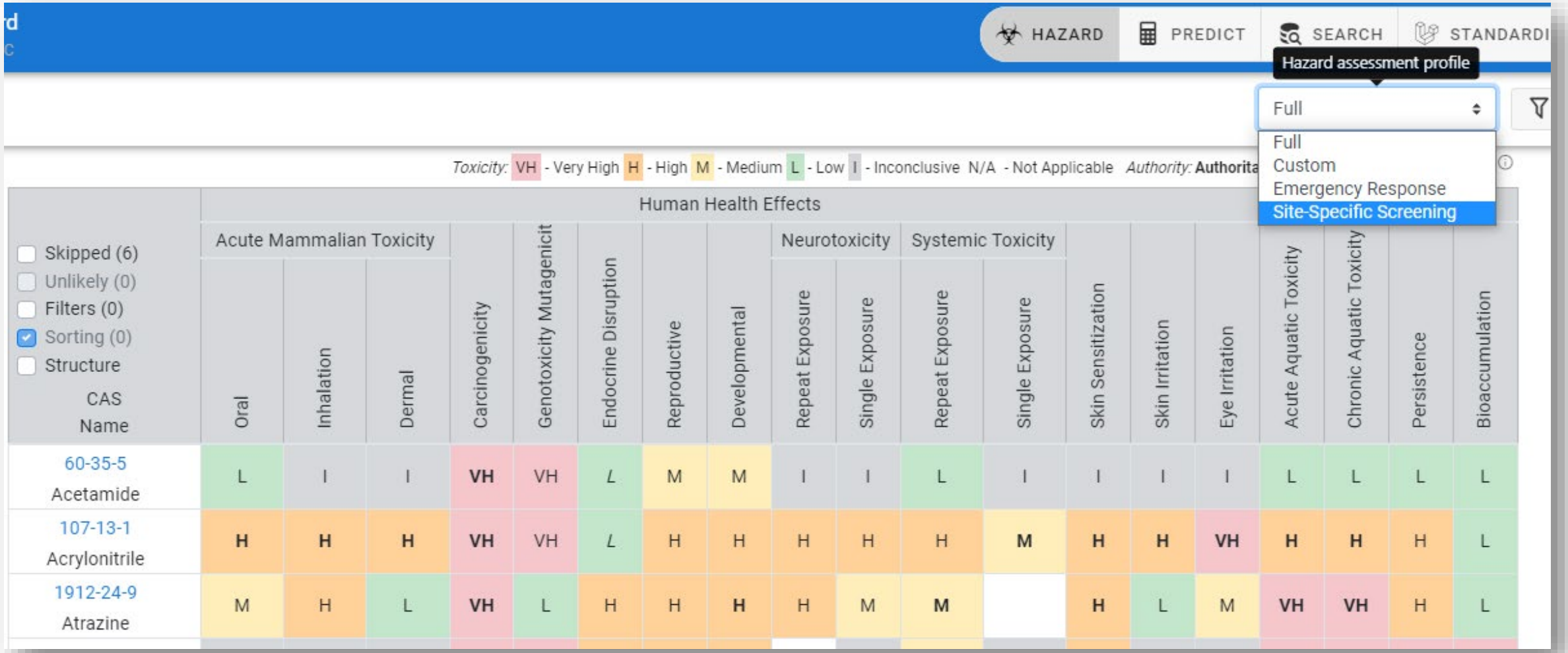
Cheminformatics "PoC Modules"

https://www.epa.gov/chemical-research/cheminformatics

Six Modules

- Hazard Comparison Profiling – profile chemicals based on hazard
- Alerts – structure, substructure, SMARTS based alerts and flags
- Predict – batch prediction using WebTEST (100s of structures)
- Search – structure/substructure/similarity searches
- Standardize – convert structures into QSAR/MS-Ready forms
- ToxPrints – generate ToxPrint substructural fragments and profile

Module 1: Hazard Module



Module 2: Alerts

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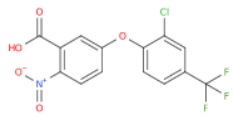
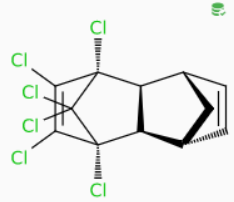
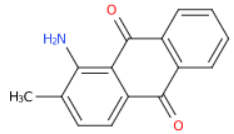
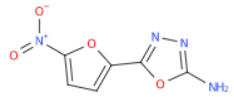
Hazard Comparison Dashboard
version: UAT, build: 2021-10-26 21:27:37 UTC

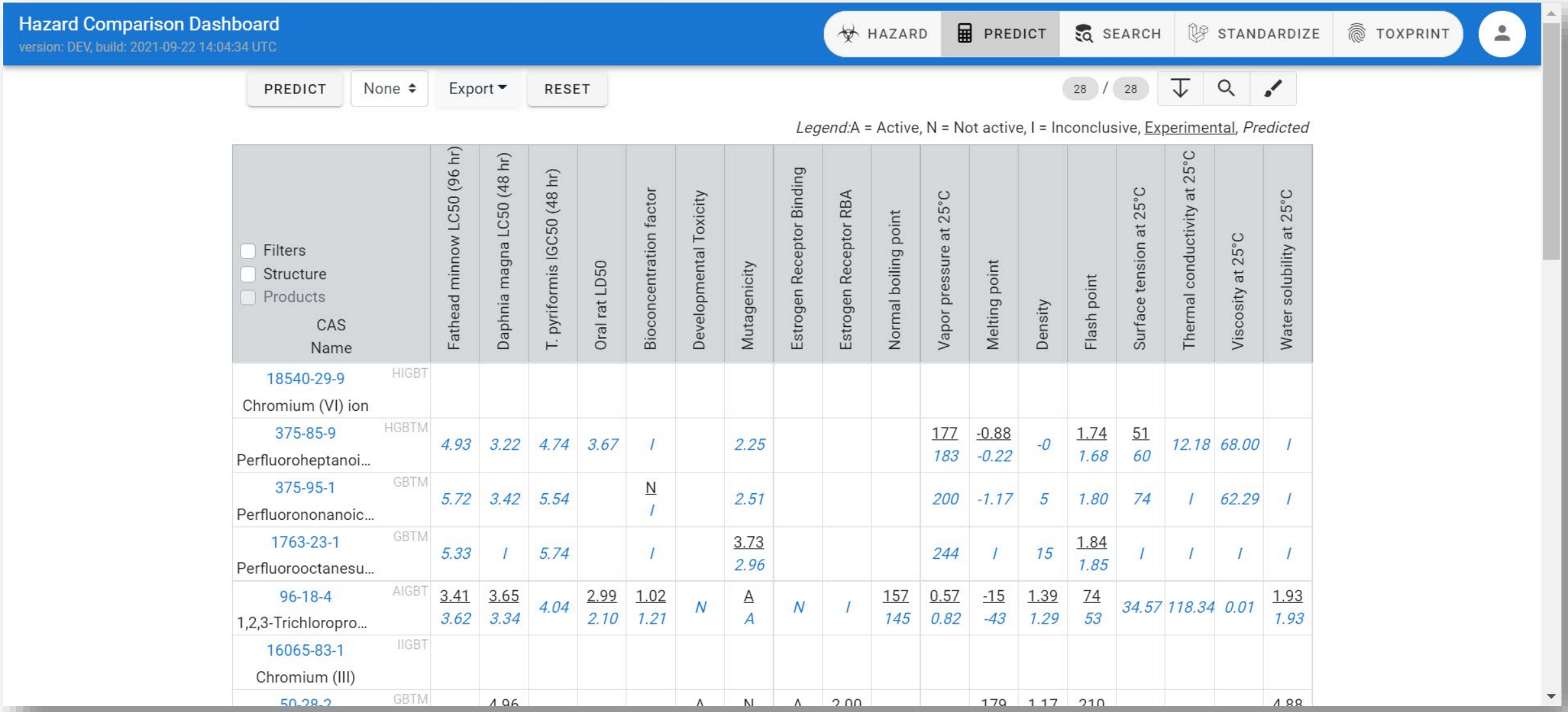
HAZARD | ALERTS | PREDICT | SEARCH | STANDARDIZE | TOXPRINTS

Search in any field

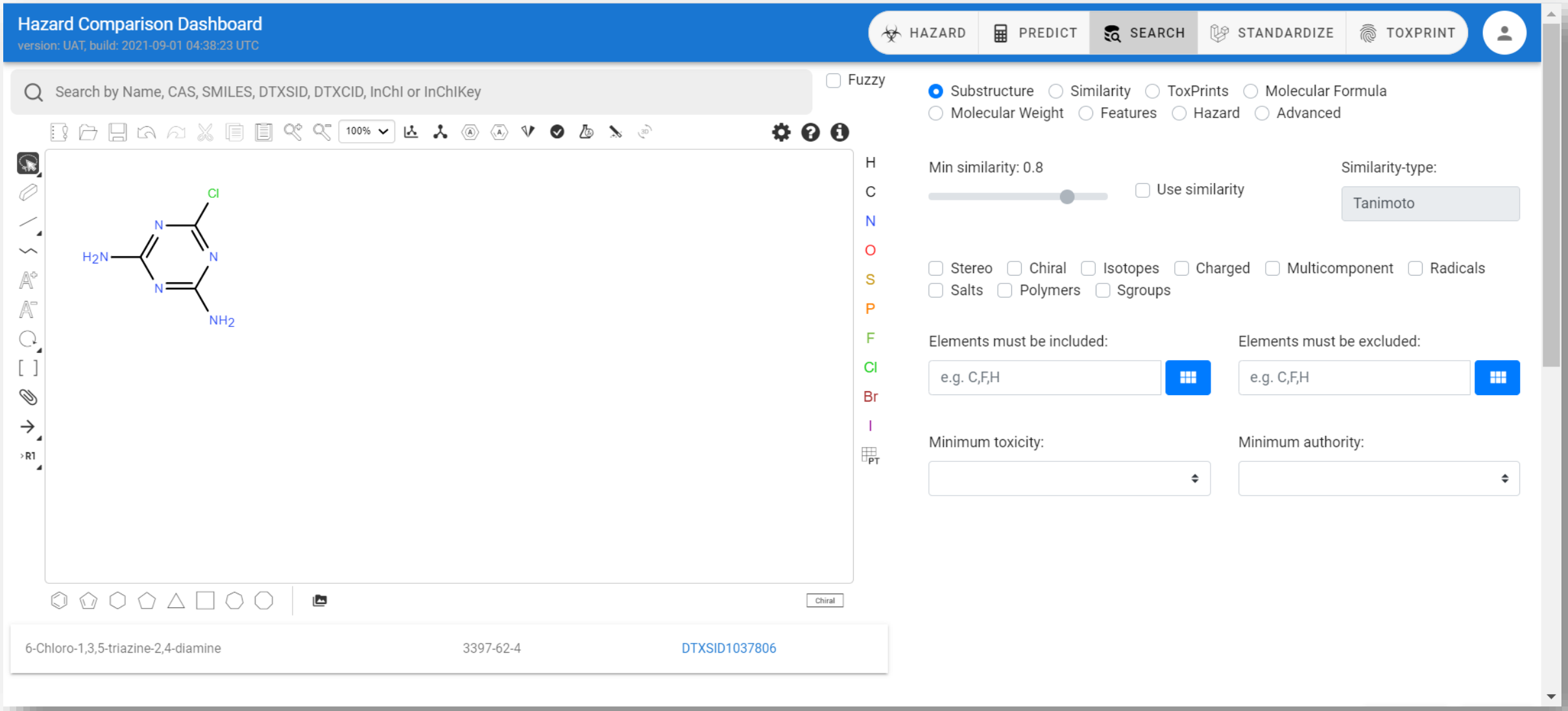
Collapse Details

#	ID	Chemical	ashby	ttc
6	50594-66-6			
10	309-00-2			bond:CX_halide_alkenyl-X_dihalo_(1_2-), bond:CX_halide_alkyl-Cl_dichloro_(1_1-), bond:CX_halide_alkyl-X_dihalo_(1_3), bond:CX_halide_generic-X_dihalo_(1_2-) 4
14	82-28-0			
15	3775-55-1		2	2

Module 3: WebTEST Batch Prediction



Module 4: Structure/Substructure/Similarity



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Chemical Transformation Database

(Work in Progress)

Chemical Transformation Database

EPA United States Environmental Protection Agency

Environmental Topics | Laws & Regulations | About EPA | Search EPA.gov

Contact Us

CTS: Chemical Transformation Simulator 1.2.3

About

- CTS Home
- CTS Basic Information

Execute CTS Workflows

- Calculate Chemical Speciation
- Calculate Physicochemical

Chemical Transformation Database

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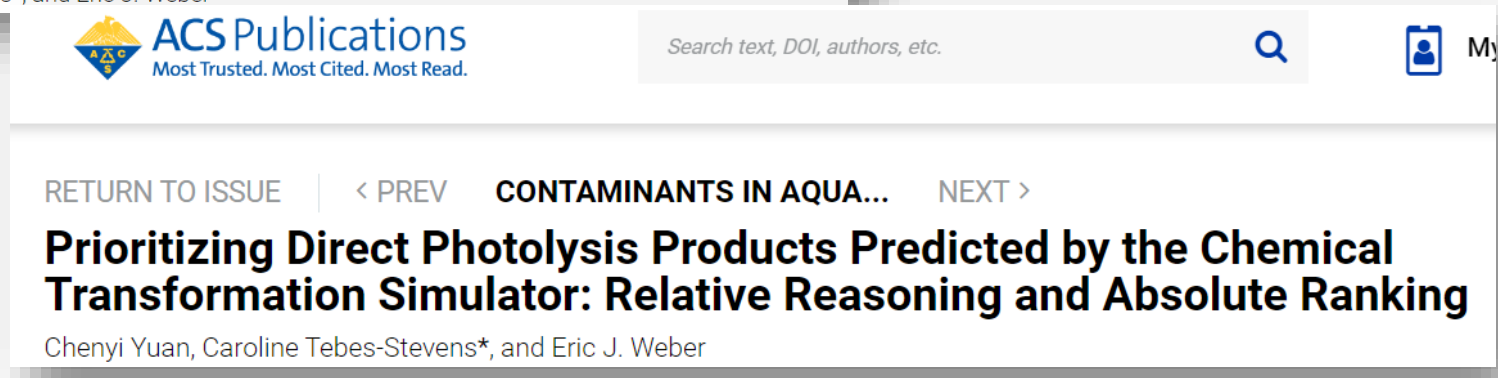
- The database of reactions under the Chemical Transformation Simulator



Chemical Transformation Database

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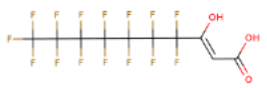
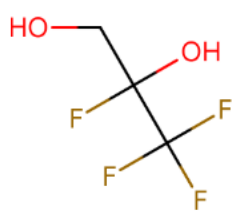
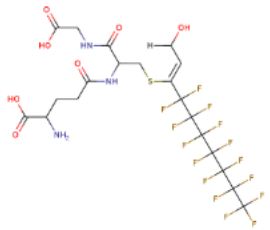
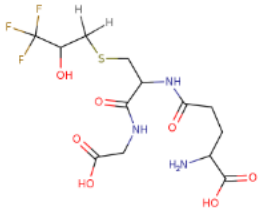
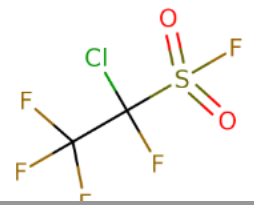
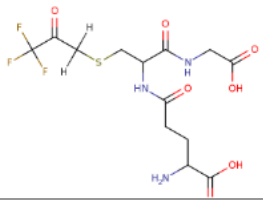
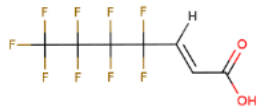
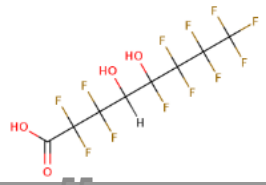
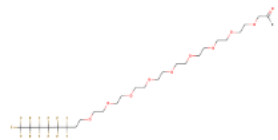
Show EPA Header and Footer

Chemical Transformations Database | Search Chemicals | Reaction Lists | Tools | About | Submit Comments | Contact Us

Search: Name, DTXSID, CASRN, InChI key

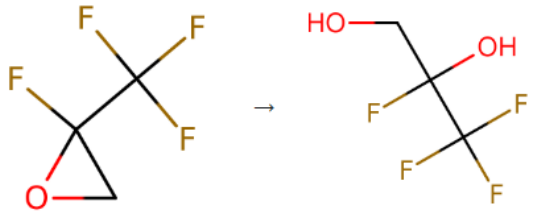
Table View | Export Chemical List

Name: (2Z)-4,4,5,5,6,6,7,7,8,...  DTXSID: DTXSID301348999 ↗	Name: 2,3,3,3-tetrafluoropr...  DTXSID: DTXSID201349001 ↗	Name: γ-glutamyl-S-[(2Z)-4,...  DTXSID: DTXSID601349003 ↗	Name: γ-glutamyl-S-(3,3,3-t...  DTXSID: DTXSID001349005 ↗	Name: 4,4,5,5,6,6,7,7,8,8,9,9,...  DTXSID: DTXSID301349004 ↗	Name: (2E)-4,4,5,5,6,6,7,7,8,...  DTXSID: DTXSID901349002 ↗
Name: 1-chloro-1,2,2,2-tetr... 	Name: γ-glutamyl-S-(3,3,3-t... 	Name: (2E)-4,4,5,5,6,6,7,7,7-... 	Name: 3,4,4,5,5,6,6,7,7,8,8,9,... 	Name: 2,2,3,3,5,6,6,7,7,8,8,8-... 	Name: 30,30,31,31,32,32,33,... 

Reaction, Original References etc

Chemical Transformations Database | Search Chemicals | Reaction Lists | Tools | About | Submit Comments | Contact Us

2-Fluoro-2-(trifluoromethyl)oxirane → 2,3,3,3-tetrafluoropropane-1,2-diol



Reaction Process:

Reaction Type: Hydrolysis

Reaction Scheme: Epoxide to diol_PTP

Reaction Details

T...	Half Life (days)	Reaction System	Metabolic	Environmental	Notes	Reference	Delete
		rat	1			Schuster et al., 2008	Delete

Export Reaction Details

Migrating MetaPath data

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ELSEVIER

Regulatory Toxicology and Pharmacology

Volume 63, Issue 1, June 2012, Pages 84-96

MetaPath: An electronic knowledge base for collating, exchanging and analyzing case studies of xenobiotic metabolism

Richard C. Kolanczyk [a], Patricia Schmieder [a], William J. Jones [b], Ovanes G. Mekenyan [c], Atanas Chapkanov [c], Stanislav Temelkov [c], Stefan Kotov [c],

METAPATH

Consolidation and management of metabolism data

The MetaPath platform is developed to collect, organize and analyze experimental data on metabolism or catabolism, observed biotransformation pathways and crucial supporting metadata. Thus, the results from metabolism studies are compiled and organized into a systematic database. The system provides a set of tools for managing and accessing the information, including powerful search engine that can extract information based on chemical structure, biotransformation, experimental metadata and specific proteins responsible for a given biotransformation.

Work in Progress: MetaPath migration

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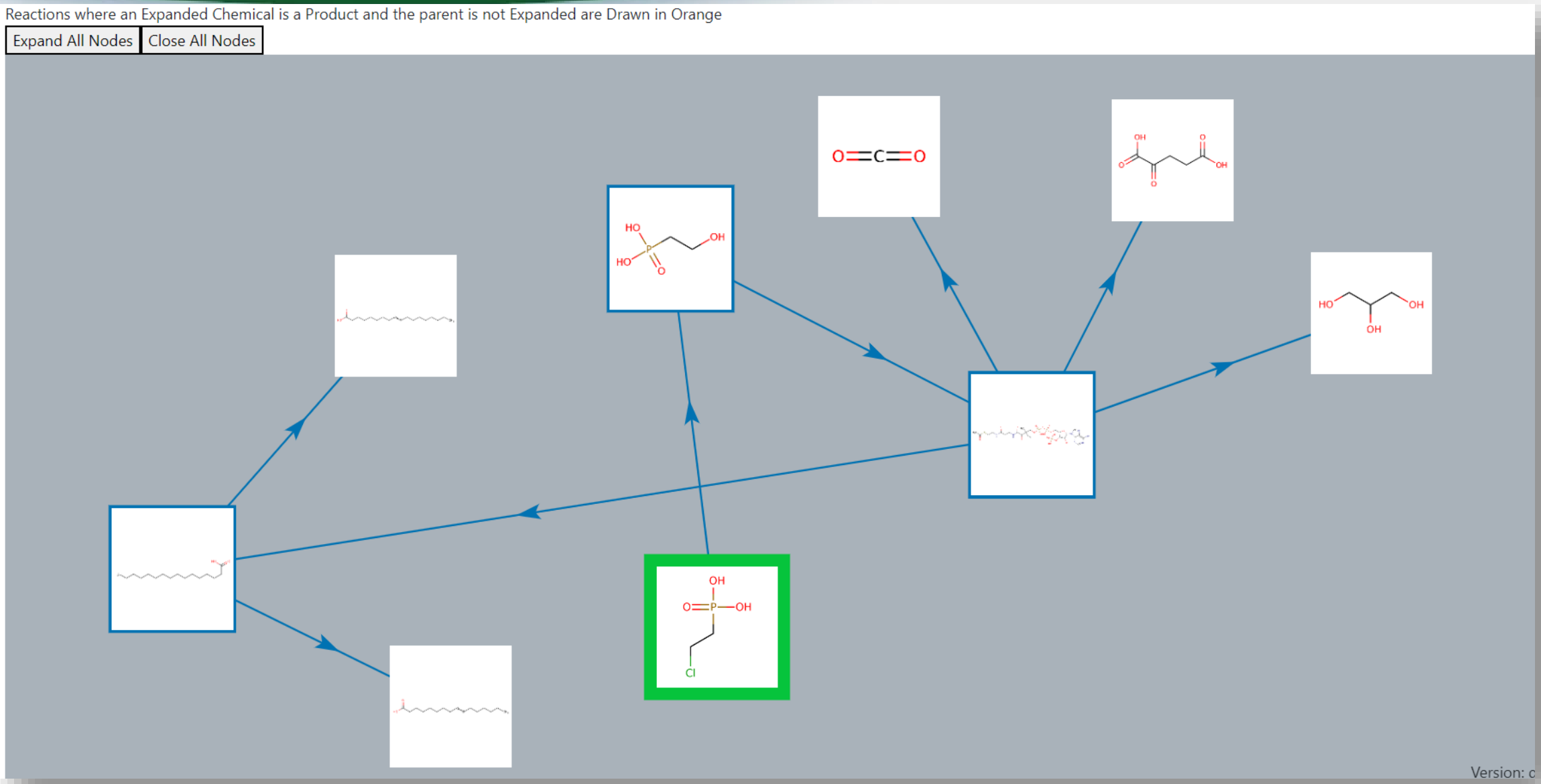
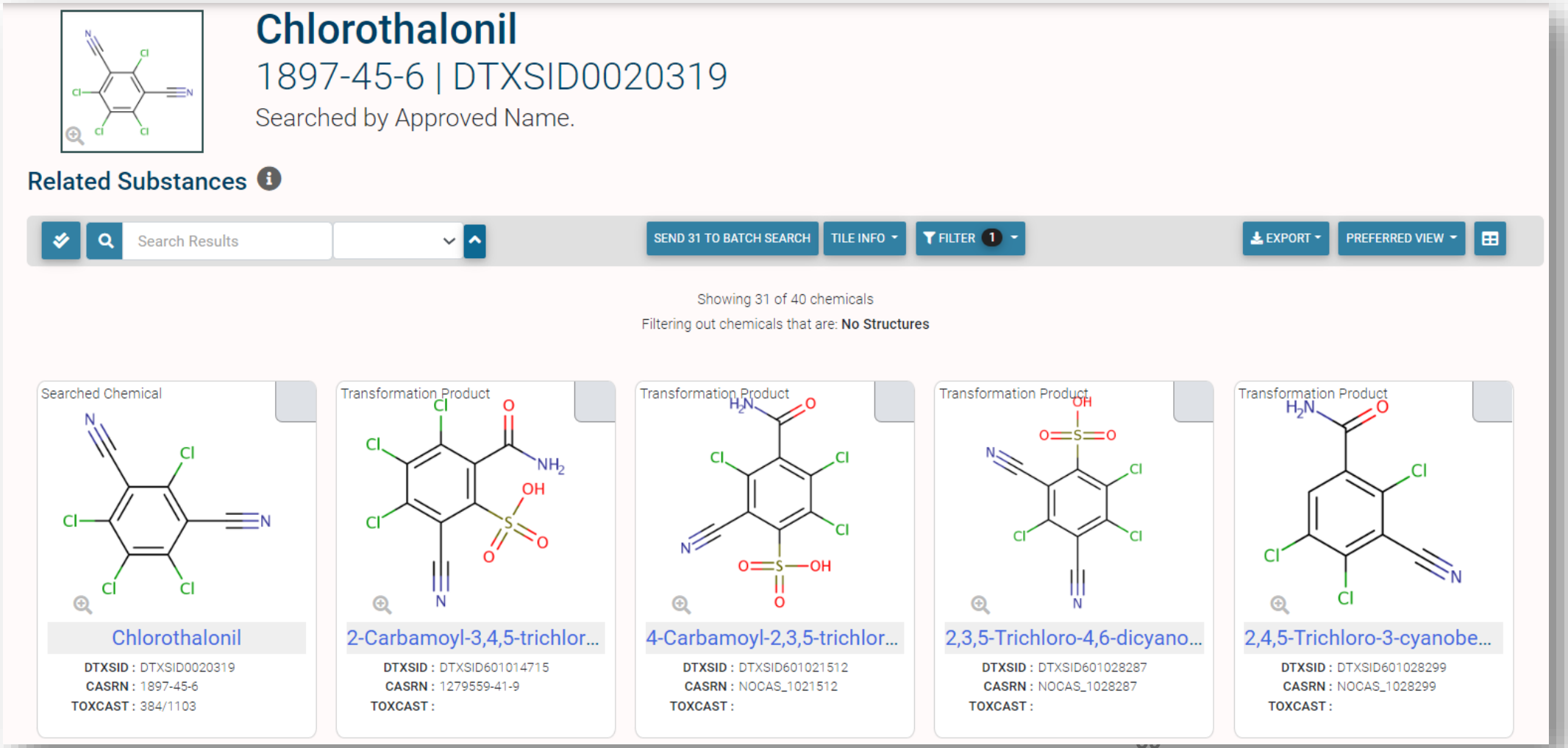


What's Next?

- Adding Thousands of Parent-Product mappings from the Dashboard



Supporting Analytical Chemistry

1) Non-Targeted Analysis

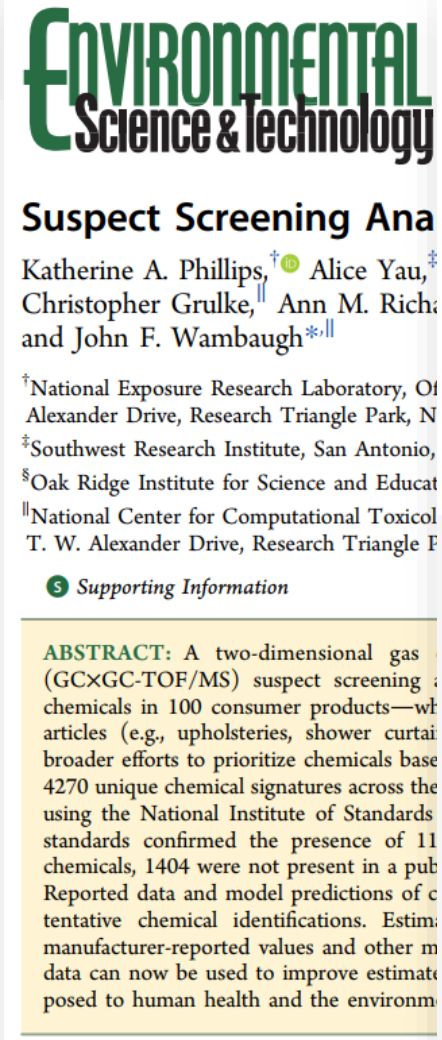
2) Open Spectral Data

3) Analytical Methods

(Work in Progress)

Chemical Identification and Exposure

EPA United States Environmental Protection Agency



ENVIRONMENTAL Science & Technology

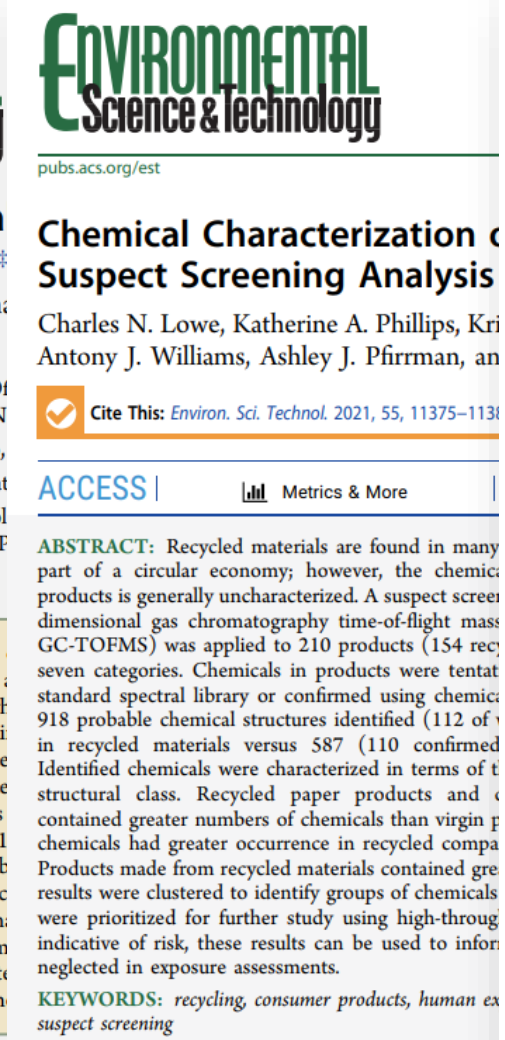
Suspect Screening Ana

Katherine A. Phillips,[†] Alice Yau,[‡] Christopher Grulke,[∥] Ann M. Richa and John F. Wambaugh*[,∥]

[†]National Exposure Research Laboratory, Of Alexander Drive, Research Triangle Park, N
[‡]Southwest Research Institute, San Antonio,
[§]Oak Ridge Institute for Science and Educat
[∥]National Center for Computational Toxicol T. W. Alexander Drive, Research Triangle P

Supporting Information

ABSTRACT: A two-dimensional gas (GC×GC-TOF/MS) suspect screening chemicals in 100 consumer products—wh articles (e.g., upholsteries, shower curtai broader efforts to prioritize chemicals base 4270 unique chemical signatures across the using the National Institute of Standards standards confirmed the presence of 11 chemicals, 1404 were not present in a pub Reported data and model predictions of c tentative chemical identifications. Estim manufacturer-reported values and other m data can now be used to improve estimate posed to human health and the environm



ENVIRONMENTAL Science & Technology

pubs.acs.org/est

Chemical Characterization c Suspect Screening Analysis

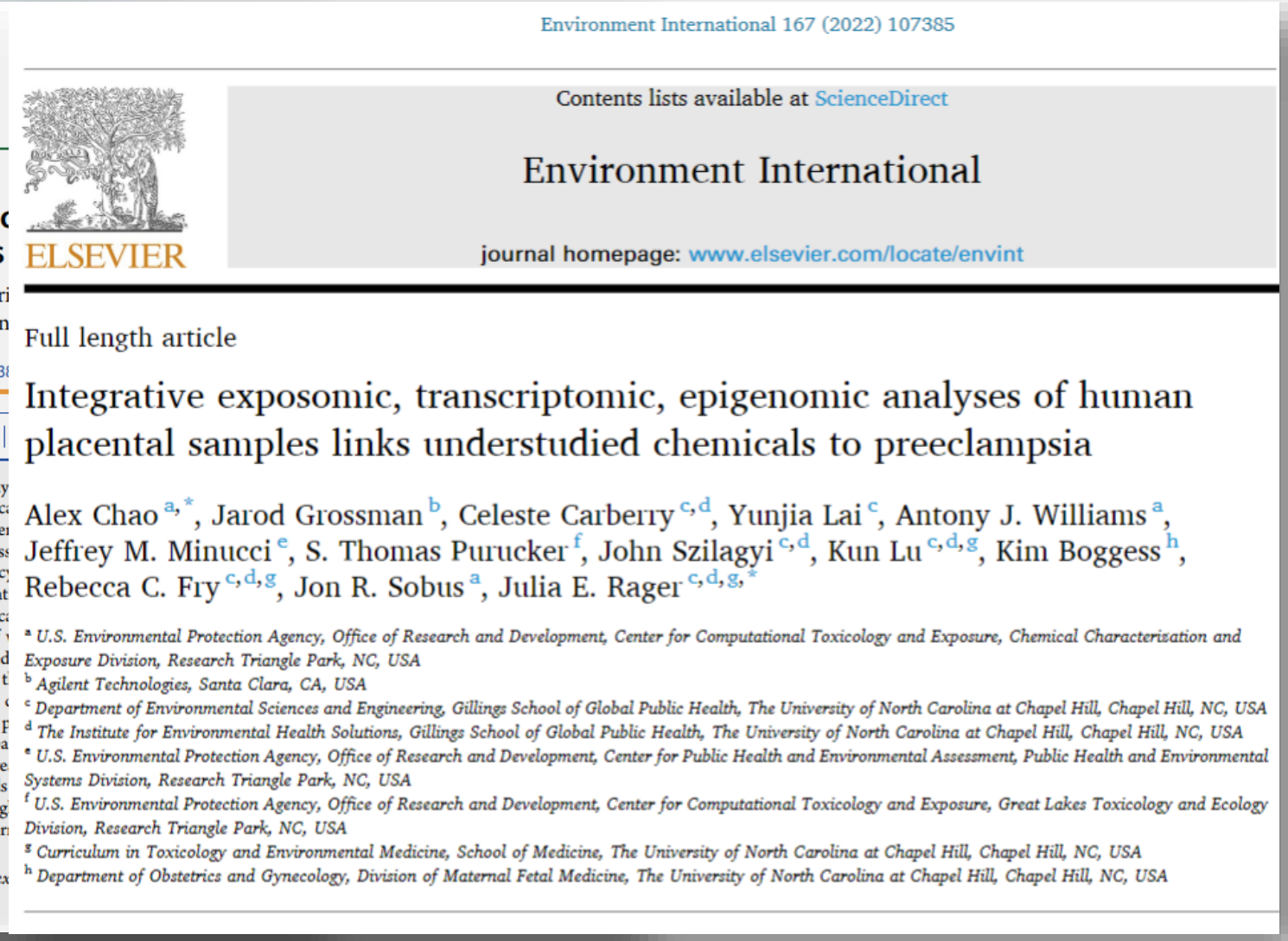
Charles N. Lowe, Katherine A. Phillips, Kri Antony J. Williams, Ashley J. Pfirrman, an

Cite This: *Environ. Sci. Technol.* 2021, 55, 11375–113

ACCESS | Metrics & More

ABSTRACT: Recycled materials are found in many part of a circular economy; however, the chemica products is generally uncharacterized. A suspect scree dimensional gas chromatography time-of-flight mass GC-TOFMS) was applied to 210 products (154 rec seven categories. Chemicals in products were tentat standard spectral library or confirmed using chemica 918 probable chemical structures identified (112 of in recycled materials versus 587 (110 confirmed Identified chemicals were characterized in terms of t structural class. Recycled paper products and contained greater numbers of chemicals than virgin p chemicals had greater occurrence in recycled compa Products made from recycled materials contained gre results were clustered to identify groups of chemicals were prioritized for further study using high-throug indicative of risk, these results can be used to infor neglected in exposure assessments.

KEYWORDS: *recycling, consumer products, human ex suspect screening*



Environment International 167 (2022) 107385

Contents lists available at ScienceDirect

Environment International

journal homepage: www.elsevier.com/locate/envint

ELSEVIER

Full length article

Integrative exposomic, transcriptomic, epigenomic analyses of human placental samples links understudied chemicals to preeclampsia

Alex Chao [a,*], Jarod Grossman [b], Celeste Carberry [c,d], Yunjia Lai [c], Antony J. Williams [a], Jeffrey M. Minucci [e], S. Thomas Purucker [f], John Szilagyi [c,d], Kun Lu [c,d,g], Kim Boggess [h], Rebecca C. Fry [c,d,g], Jon R. Sobus [a], Julia E. Rager [c,d,g,*]

[a] *U.S. Environmental Protection Agency, Office of Research and Development, Center for Computational Toxicology and Exposure, Chemical Characterization and Exposure Division, Research Triangle Park, NC, USA*
[b] *Agilent Technologies, Santa Clara, CA, USA*
[c] *Department of Environmental Sciences and Engineering, Gillings School of Global Public Health, The University of North Carolina at Chapel Hill, Chapel Hill, NC, USA*
[d] *The Institute for Environmental Health Solutions, Gillings School of Global Public Health, The University of North Carolina at Chapel Hill, Chapel Hill, NC, USA*
[e] *U.S. Environmental Protection Agency, Office of Research and Development, Center for Public Health and Environmental Assessment, Public Health and Environmental Systems Division, Research Triangle Park, NC, USA*
[f] *U.S. Environmental Protection Agency, Office of Research and Development, Center for Computational Toxicology and Exposure, Great Lakes Toxicology and Ecology Division, Research Triangle Park, NC, USA*
[g] *Curriculum in Toxicology and Environmental Medicine, School of Medicine, The University of North Carolina at Chapel Hill, Chapel Hill, NC, USA*
[h] *Department of Obstetrics and Gynecology, Division of Maternal Fetal Medicine, The University of North Carolina at Chapel Hill, Chapel Hill, NC, USA*

Rudimentary NTA Workflow

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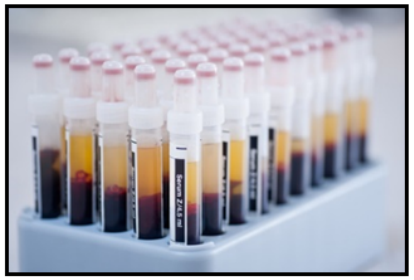
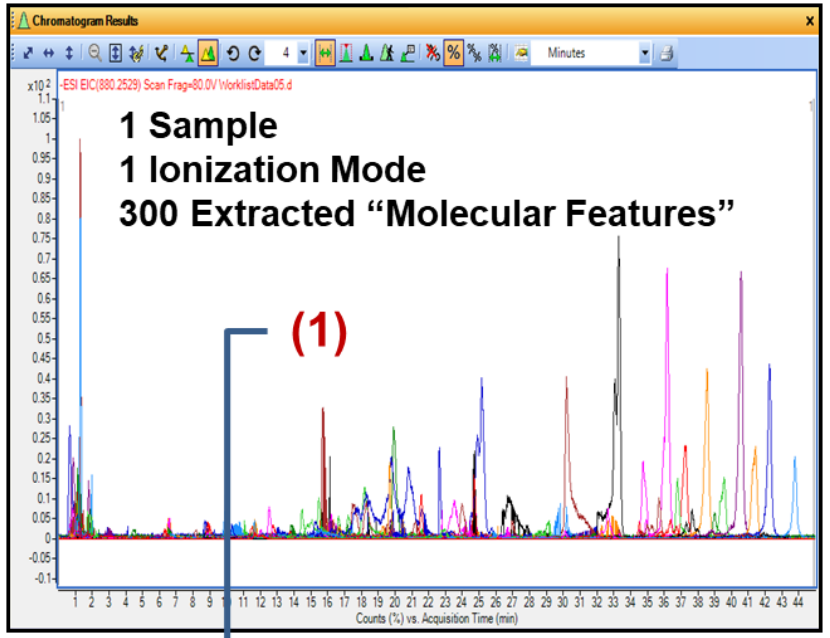
Samples



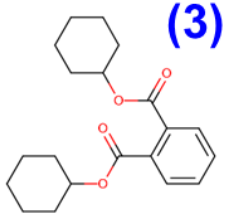
High-Resolution MS



1) Prioritize "molecular features"
2) Correctly assign formulas
3) Correctly assign structures
4) Predict chemical concentrations
5) Determine chemical sources

(2) $C_{20}H_{26}O_4$

(3)



(4) 12 µg/mL

(5)

Non-Targeted Analysis Informatics

EPA United States Environmental Protection Agency

Anal Bioanal Chem (2017) 409:1729–1735
DOI 10.1007/s00216-016-0139-z

CrossMark

RAPID COMMUNICATION

Identifying known unknowns using the US EPA's CompTox Chemistry Dashboard

Andrew D. McEachran[1] · Jon R. Sobus[2] · Antony J. Williams[3]

Environmental Toxicology and Chemistry—Volume 41, Number 5—pp. 1117–1130, 2022
Received: 28 June 2021 | Revised: 26 July 2021 | Accepted: 17 August 2021

Critical Perspectives

A Framework for Utilizing High-Resolution Mass Spectrometry and Nontargeted Analysis in Rapid Response and Emergency Situations

Allison L. Phillips,[a] Antony J. Williams,[b] Jon R. Sobus,[b] Elin M. Ulrich,[b] Jennifer Gundersen,[c] Christina Langlois-Miller,[d] and Seth R. Newton[b,*]

metabolites

MDPI

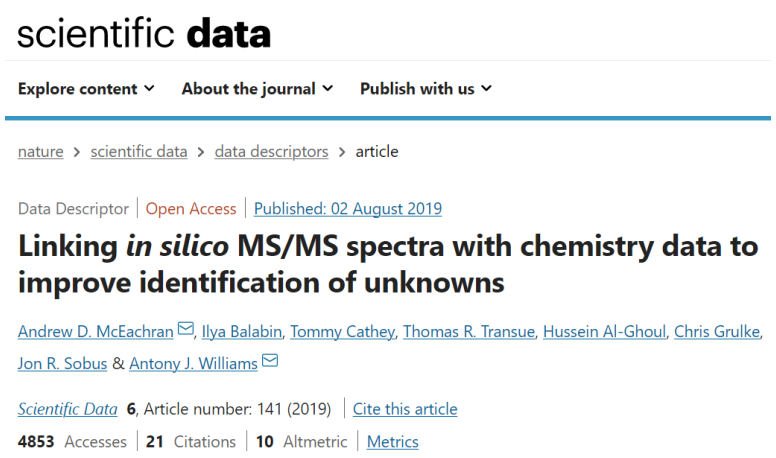
Article

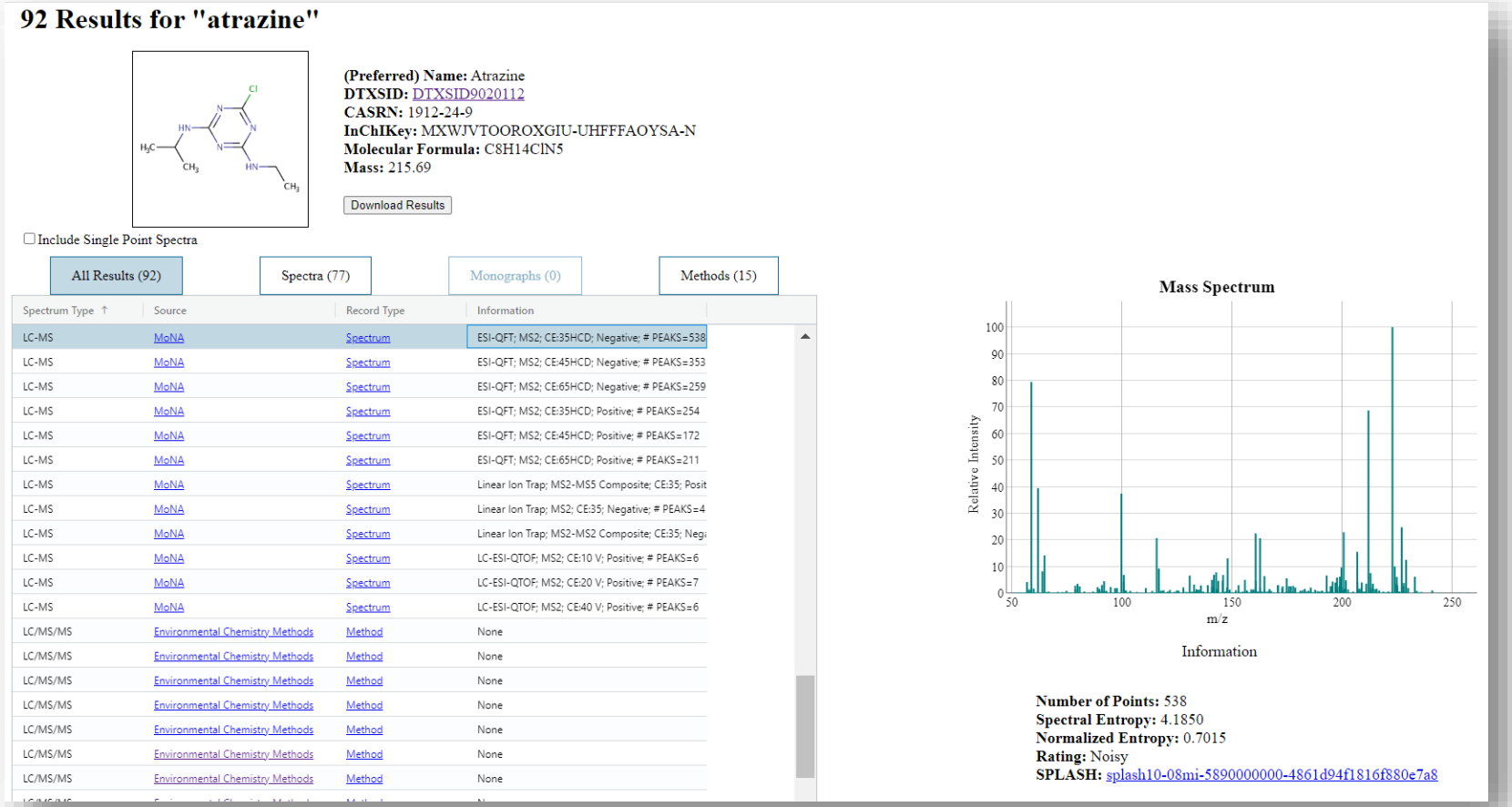
Revisiting Five Years of CASMI Contests with EPA Identification Tools

Andrew D. McEachran [1,*], Alex Chao [1], Hussein Al-Ghoul [1], Charles Lowe [2], Christopher Grulke [2], Jon R. Sobus [2] and Antony J. Williams [2,*]

The Next Phase
Assembling Public Domain Spectra

- Assemble data from MoNA, MassBank, internal EPA data
- Already have CFM-ID data for 1.2M chemicals





- Experimental searching

Integrated Methods Database

- Simple Vision: Find the best method(s) for a particular chemical

- Approach:
  - Aggregate MS method documents
  - Extract chemistry (mostly CASRN and Names)
  - Map CASRN and Names to **structures**
  - Build a searchable database of chemicals mapped to methods
    - Chemical identifier search
    - Structure/substructure and similarity search

Where are there methods?

- 900 method documents

Related Topics: Pesticide Analytical Methods

CONTACT US

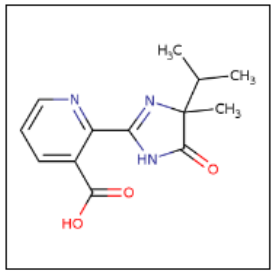
Environmental Chemistry Methods (ECM) Index – 0–9

0-9 | A | B | C | D | E | F | G | H | I | K | L | M | N | O | P | Q | R | S | T | V | Z

Analyte(s) by Pesticide	ECM MRID	Matrix	Method Date
1,2,4-triazole	49762553	Water	2/19/13
1,3-dichloropropene & 1,2-dichloropropane	44536511	Soil	3/27/98
1,3-dichloropropene & 1,2-dichloropropane	44536511	Water	3/27/98
1,3-dichloropropene Degradate 3-chloroallyl Alcohol	44536505	Water	12/12/97

Embedding old Method PDFs

Search Results for "Imazapyr"



(Preferred) Name: Imazapyr
DTXSID: DTXSID8034665
CASRN: 81334-34-1
InChIKey: CLQMBPJKHLGMQK-UHFFFAOYNA-N
Molecular Formula: C13H15N3O3
Mass: 261.281

Spectrum Type ↑	Source	Record Type	View
	Environmental Chemistry Methods	Method	PDF
	Environmental Chemistry Methods	Method	PDF
LC-MS+	MoNA	Spectrum	Spectrum
LC-MS+	MassBank EU	Spectrum	Spectrum
LC-MS+	MassBank EU	Spectrum	Spectrum
LC-MS+	MassBank EU	Spectrum	Spectrum
LC-MS+	MassBank EU	Spectrum	Spectrum
LC-MS+	MassBank EU	Spectrum	Spectrum

Imazapyr

MRID: 41891501
Date: 10/1/89
Matrix: Water
Registrant: American Cyanamide Co
Analysis: HPLC/UV
Limit of Quantitation: 5.0 µg/L

US EPA - ECM for Imazapyr ... 1 / 8 90%

41891501

CYANAMID C3197 CONFIDENTIAL
Page 5 of 22

SOP M1900
A. Khunachak/hm
09/05/89
Approved by:
J. M. Devine 09/05/89 Date

AMERICAN CYANAMID COMPANY
AGRICULTURAL RESEARCH DIVISION
CHEMICAL DEVELOPMENT
P. O. Box 400
Princeton, New Jersey 08540 USA

RECOMMENDED METHOD OF ANALYSIS

Imazapyr (CL 243,997): HPLC Method for the Determination of CL 243,997 Residues in Water

A. Principle

Residues of CL 243,997 are extracted from water by using a C18 solid phase extraction (SPE) cartridge. Additional cleanup and specificity are achieved by

Vendor Methods

United States Environmental Protection Agency

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Environmental Topics | Laws & Regulations | About EPA

Search Term [ ] Search

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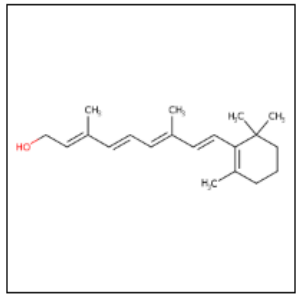
Search Results for "Retinol"



(Preferred) Name: Retinol
DTXSID: DTXSID3023556
CASRN: 68-26-8
InChIKey: FPIPGXGPPPQFEQ-OVSJKPMPSA-N
Molecular Formula: C20H30O
Mass: 286.459

Spectrum Type	Source	Record Type	View
GC-MS	Spectrabase	Spectrum	External Link
GC-MS	Spectrabase	Spectrum	External Link
GC-MS	Spectrabase	Spectrum	External Link
GC-MS	Spectrabase	Spectrum	External Link
GC-MS	Spectrabase	Spectrum	External Link
GC-MS	Spectrabase	Spectrum	External Link
GC-MS	Spectrabase	Spectrum	External Link
GC-MS	Spectrabase	Spectrum	External Link
LC-MS	Agilent	Method	PDF
LC-MS+	MoNA	Spectrum	Spectrum

Determination of Fat-Soluble Vitamins in Foods Using Agilent Chem Elut S Extraction with LC/DAD and LC/MS/MS Triple-Quadrupole

Author: Hui Zhao
Focus/Analyte: Reliable sample preparation and identification/quantitation in various food matrices
Synopsis: This application note describes a method for the determination of fat-soluble vitamins, including vitamin A (retinol), vitamin D3 (cholecalciferol), vitamin D2 (ergocalciferol), and vitamin E (α-tocopherol) in complex food matrices, including infant formula, egg, canned tuna, and mushroom. Samples were saponified as sample pretreatment, extracted using Agilent Chem Elut S (Supported Liquid Extraction (SLE)) 12 mL cartridges, and fat-soluble vitamins were then simultaneously identified and quantified by an Agilent 1290 Infinity II LC coupled to an Agilent diode array detector (DAD) and Agilent 6470 triple quadrupole LC/MS in series. Data were analyzed using Agilent MassHunter workstation software.

PDF Viewer | Compounds (grid) | Compounds (table)

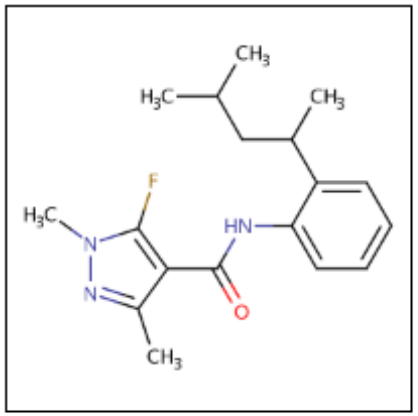
Determination of Fat-Solubl... 1 / 13 100%

Application Note
Food Testing & Agriculture

Agilent
Trusted Answers

Structure Tables/Tiles view

Search Results for "DTXSID9058107"



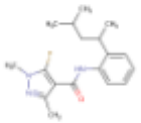
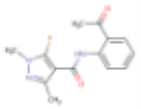
(Preferred) Name: Penflufen
DTXSID: DTXSID9058107
CASRN: 494793-67-8
InChIKey: GOFJDXZZHFNFLV-UHFFFAOYNA-N
Molecular Formula: C18H24FN3O
Mass: 317.408

Penflufen & Degradates

MRID: 48023715
Date: 1/8/10
Matrix: Water
Registrant: Bayer CropScience
Analysis: LC/MS/MS
Limit of Quantitation: 0.1 µg/L

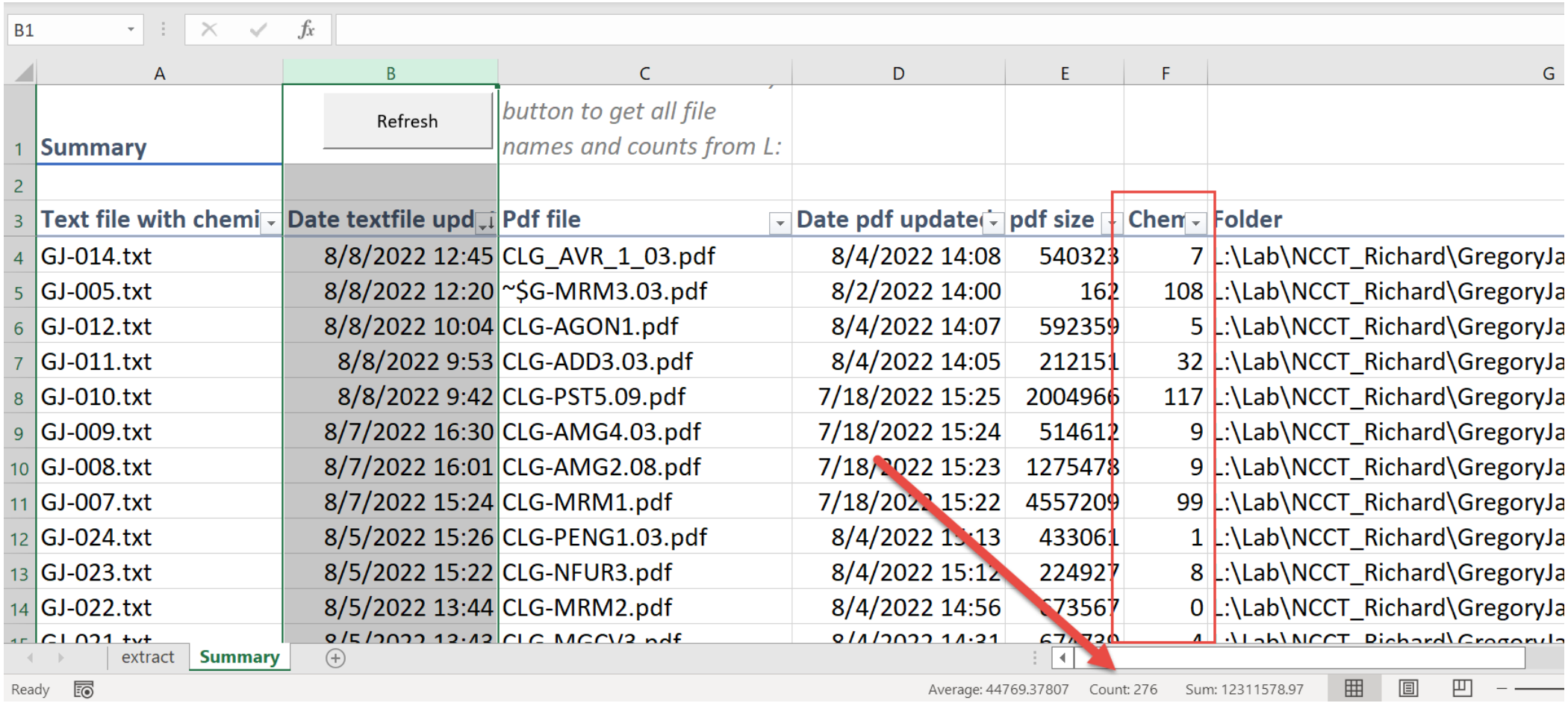
Spectrum Type ↑	Source	Record Type	Info...
LC/MS/MS	Environmental Chemistry Methods	Method (PDF)	
LC/MS/MS	Environmental Chemistry Methods	Method (PDF)	
LC/MS/MS	Environmental Chemistry Methods	Method (PDF)	
LC/MS/MS	Environmental Chemistry Methods	Method (PDF)	

PDF Viewer | Compounds (grid) | Compounds (table)

Structure	DTXSID	CASRN	Compound Name
	DTXSID9058107	494793-67-8	Penflufen
	DTXSID601024859	NOCAS_102485	N-(2-Acetylphenyl)-5-fluoro-1,3-dime

How many methods do we have?

- We have 2785 method documents to extract
- 40% have been extracted – ca. 25 documents per day



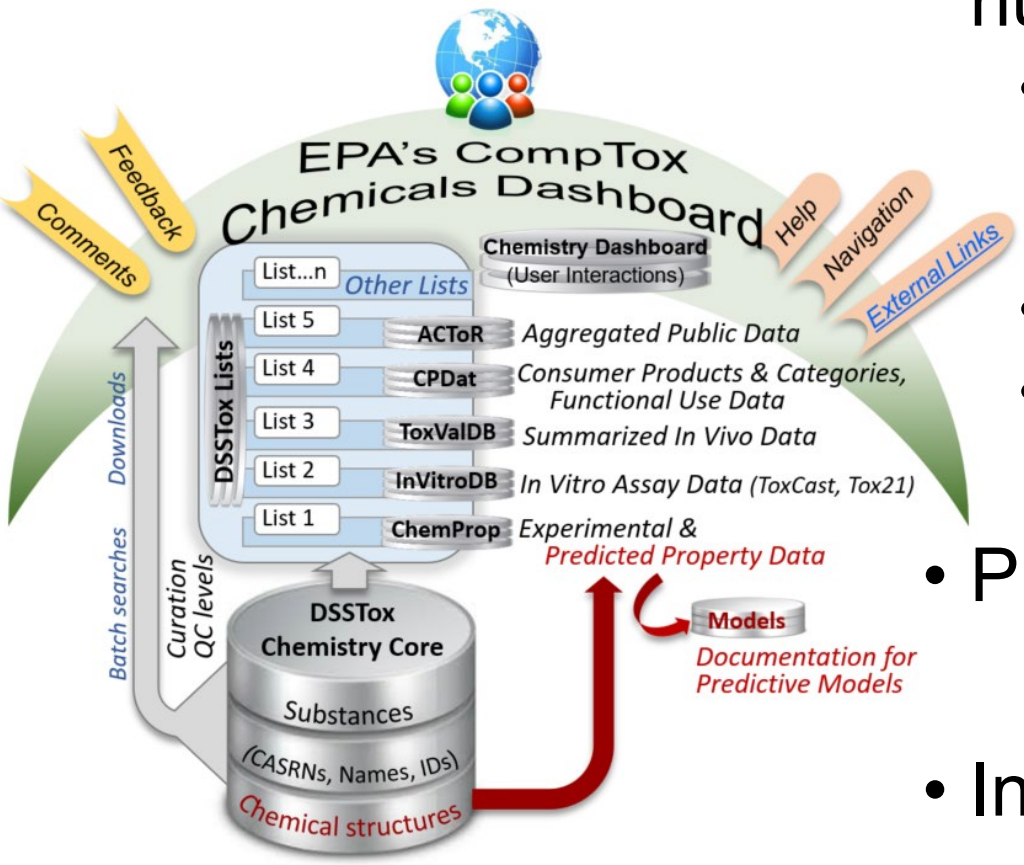
B1

	A	B	C	D	E	F	G
1	Summary	Refresh	button to get all file names and counts from L:				
2							
3	Text file with chemi	Date textfile upd	Pdf file	Date pdf update	pdf size	Chem	Folder
4	GJ-014.txt	8/8/2022 12:45	CLG_AVR_1_03.pdf	8/4/2022 14:08	540323	7	L:\Lab\NCCT_Richard\GregoryJa
5	GJ-005.txt	8/8/2022 12:20	~$G-MRM3.03.pdf	8/2/2022 14:00	162	108	L:\Lab\NCCT_Richard\GregoryJa
6	GJ-012.txt	8/8/2022 10:04	CLG-AGON1.pdf	8/4/2022 14:07	592359	5	L:\Lab\NCCT_Richard\GregoryJa
7	GJ-011.txt	8/8/2022 9:53	CLG-ADD3.03.pdf	8/4/2022 14:05	212151	32	L:\Lab\NCCT_Richard\GregoryJa
8	GJ-010.txt	8/8/2022 9:42	CLG-PST5.09.pdf	7/18/2022 15:25	2004966	117	L:\Lab\NCCT_Richard\GregoryJa
9	GJ-009.txt	8/7/2022 16:30	CLG-AMG4.03.pdf	7/18/2022 15:24	514612	9	L:\Lab\NCCT_Richard\GregoryJa
10	GJ-008.txt	8/7/2022 16:01	CLG-AMG2.08.pdf	7/18/2022 15:23	1275478	9	L:\Lab\NCCT_Richard\GregoryJa
11	GJ-007.txt	8/7/2022 15:24	CLG-MRM1.pdf	7/18/2022 15:22	4557209	99	L:\Lab\NCCT_Richard\GregoryJa
12	GJ-024.txt	8/5/2022 15:26	CLG-PENG1.03.pdf	8/4/2022 15:13	433061	1	L:\Lab\NCCT_Richard\GregoryJa
13	GJ-023.txt	8/5/2022 15:22	CLG-NFUR3.pdf	8/4/2022 15:12	224927	8	L:\Lab\NCCT_Richard\GregoryJa
14	GJ-022.txt	8/5/2022 13:44	CLG-MRM2.pdf	8/4/2022 14:56	573567	0	L:\Lab\NCCT_Richard\GregoryJa
15	GJ-021.txt	8/5/2022 13:43	CLG-MGCV3.pdf	8/4/2022 14:31	674739	4	L:\Lab\NCCT_Richard\GregoryJa

extract | Summary

Ready | Average: 44769.37807 | Count: 276 | Sum: 12311578.97

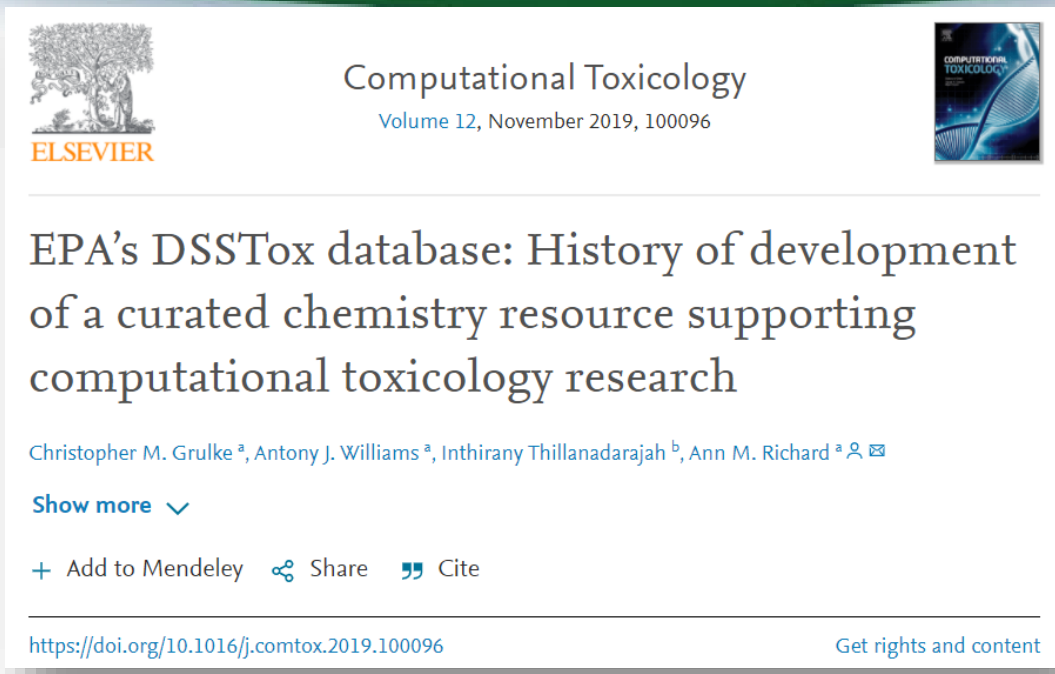
Summary and Conclusion



- CompTox Chemicals Dashboard - a central hub for environmental data
  - 1.2M chemical substances integrating property data, hazard data, exposure data, *in vitro* bioactivity data
  - Batch search for thousands of chemicals
  - Real-time property and toxicity predictions
- Proof-of-concept cheminformatics modules
- Informatics support for Non-Targeted Analysis
  - Open Spectral data
  - Analytical Methods database

Some Related Publications of Interest

EPA United States Environmental Protection Agency



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Computational Toxicology

Volume 12, November 2019, 100096

EPA's DSSTox database: History of development of a curated chemistry resource supporting computational toxicology research

Christopher M. Grulke [a], Antony J. Williams [a], Inthirany Thillanadarajah [b], Ann M. Richard [a]

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https://doi.org/10.1016/j.comtox.2019.100096

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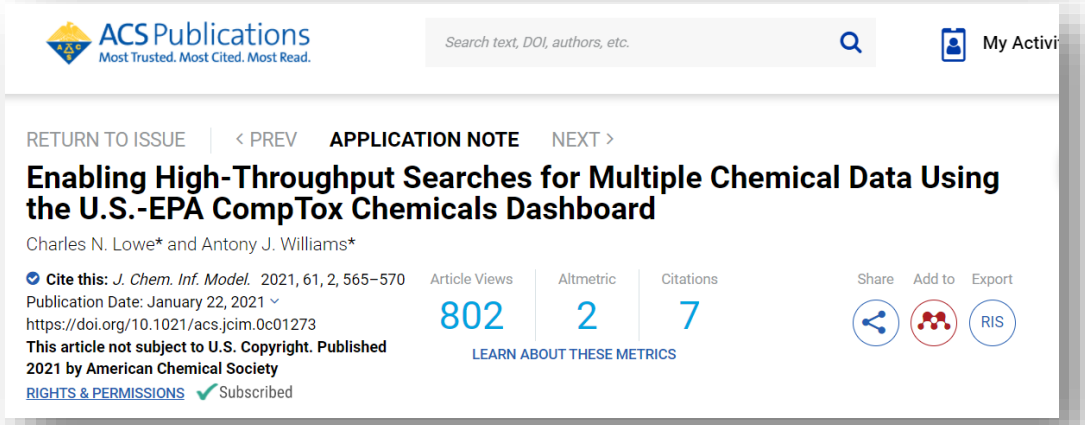

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Enabling High-Throughput Searches for Multiple Chemical Data Using the U.S.-EPA CompTox Chemicals Dashboard

Charles N. Lowe* and Antony J. Williams*

Cite this: *J. Chem. Inf. Model.* 2021, 61, 2, 565−570
Publication Date: January 22, 2021
https://doi.org/10.1021/acs.jcim.0c01273

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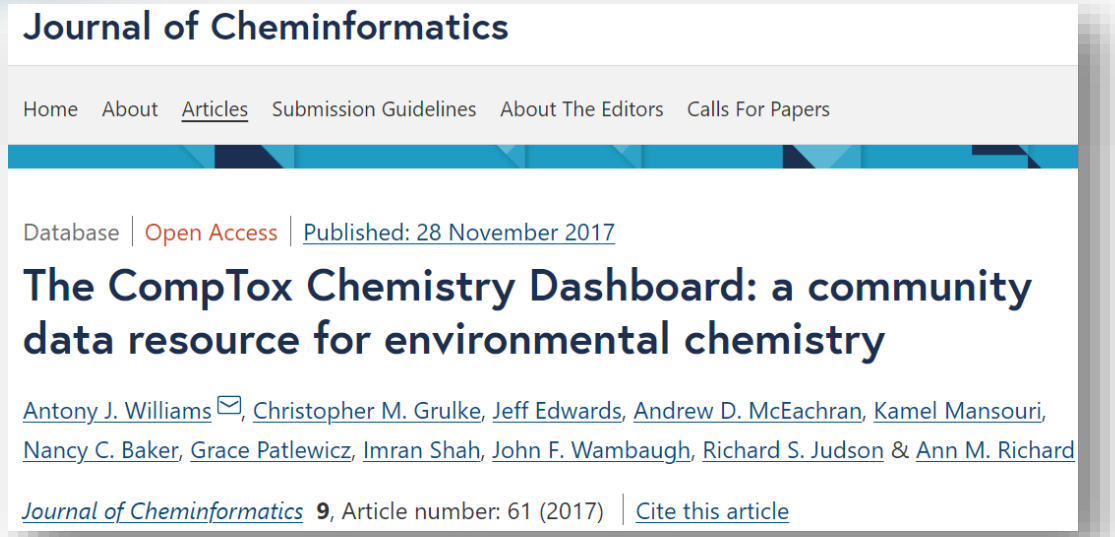

Journal of Cheminformatics

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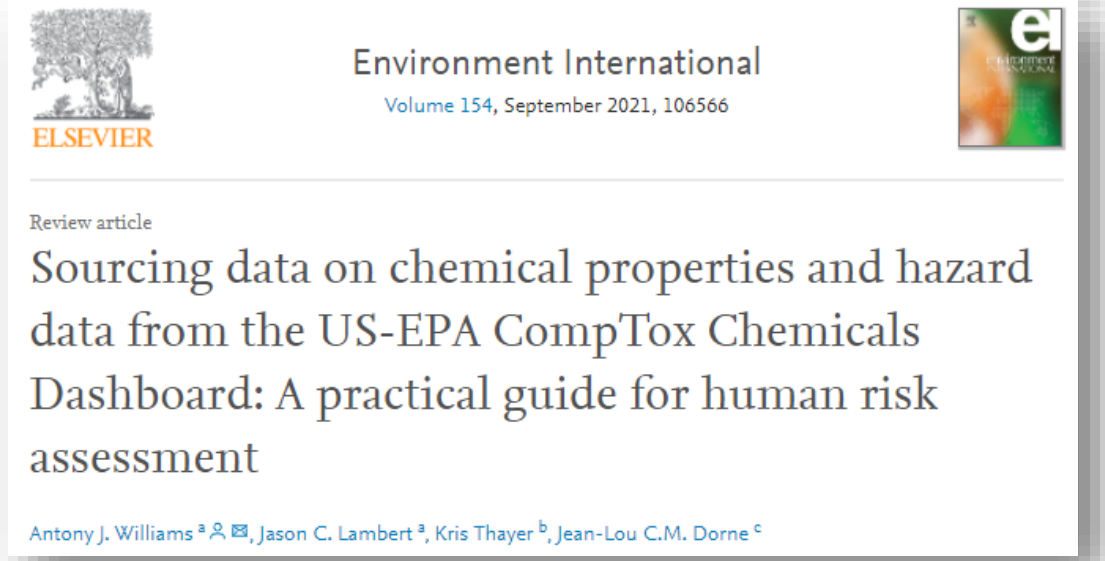
Database | Open Access | Published: 28 November 2017

The CompTox Chemistry Dashboard: a community data resource for environmental chemistry

Antony J. Williams, Christopher M. Grulke, Jeff Edwards, Andrew D. McEachran, Kamel Mansouri, Nancy C. Baker, Grace Patlewicz, Imran Shah, John F. Wambaugh, Richard S. Judson & Ann M. Richard

Journal of Cheminformatics **9**, Article number: 61 (2017) | Cite this article



ELSEVIER

Environment International

Volume 154, September 2021, 106566

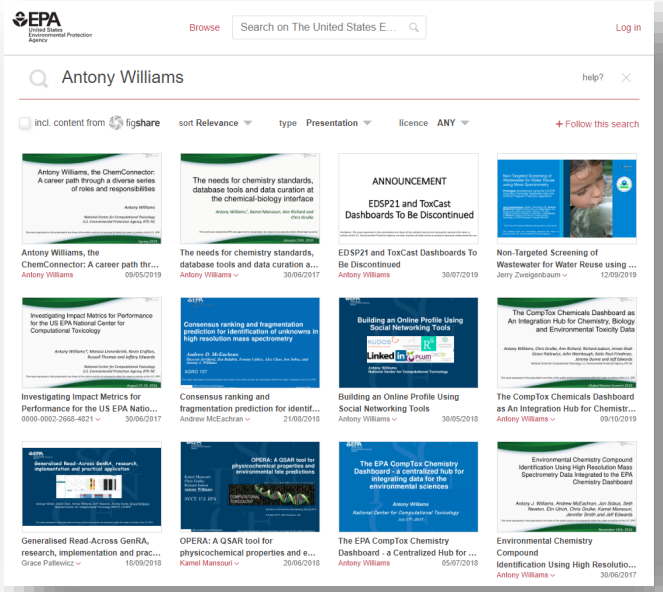
Review article

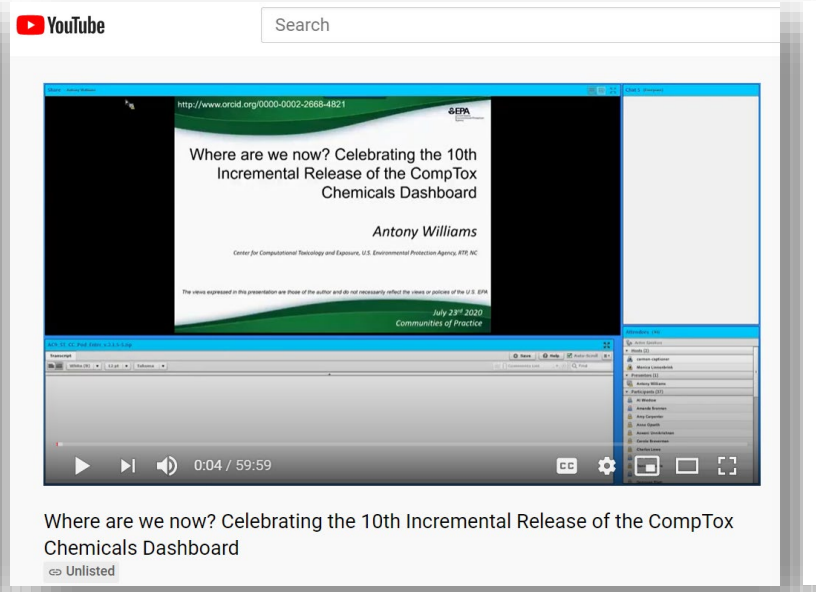
Sourcing data on chemical properties and hazard data from the US-EPA CompTox Chemicals Dashboard: A practical guide for human risk assessment

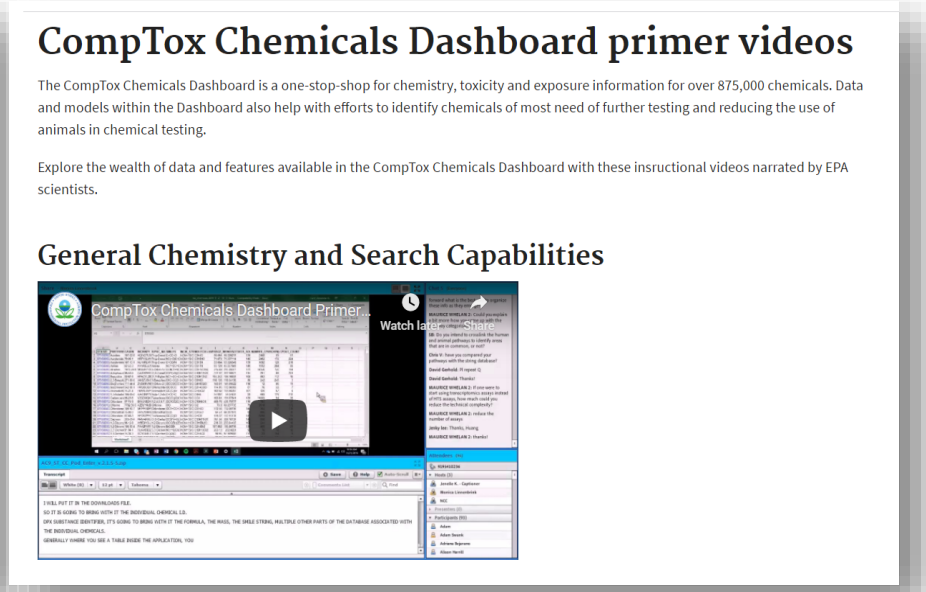
Antony J. Williams [a], Jason C. Lambert [a], Kris Thayer [b], Jean-Lou C.M. Dorne [c]

You want to know more…

- Lots of resources available
  - Presentations: https://tinyurl.com/w5hqs55
  - Communities of Practice Videos: https://rb.gy/qsbno1
  - Manual: https://rb.gy/4fgydc
  - Latest News: https://comptox.epa.gov/dashboard/news_info







Acknowledgments

- Contact:Williams.Antony@epa.gov
- Feedback and follow-up is welcomed! Your questions help
- If anyone wants a deep dive into any of the software applications feel free to contact me

EPA's Center for Computational Toxicology and Exposure