

CompTox Chemicals Dashboard

- Making Connections for You

Nisha S. Sipes, PhD

US EPA, Office of Research and Development, Center for Computational Toxicology and Exposure

SETAC, Pittsburgh, PA

8.05 – Software and Database Demonstrations

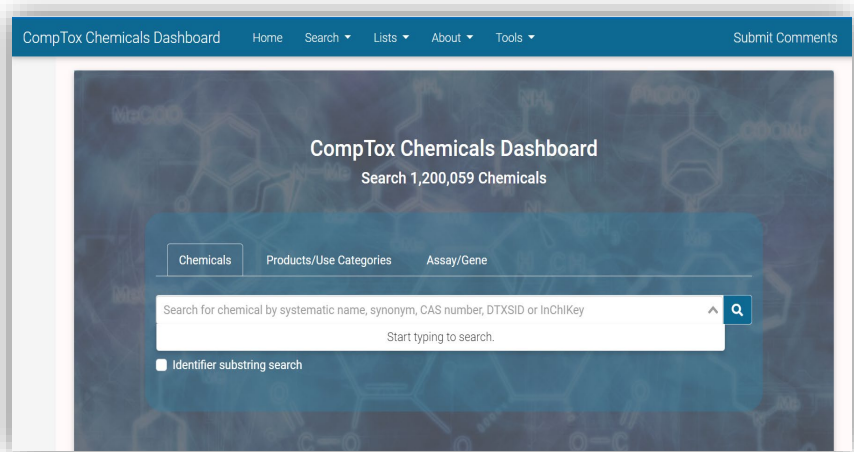
November 17, 2022

Sipes.Nisha@epa.gov

Sipes.Nisha@epa.gov

Easy access to data improves efficiency and ultimately accelerates chemical risk assessment

CompTox Chemicals Dashboard



<https://comptox.epa.gov/dashboard/>

- **Centralized location** for publicly available chemical toxicity data
 - **Chemical characterization** physchem properties, structure, synonym, chemical lists, related substances, similarity
 - **Hazard** safety classifications, human health and ecological data, *in vivo* animal data, biological targets (effect), dose-response characterization (dose)
 - **Exposure** use categories, functional use, biomonitoring, production, high throughput toxicokinetics
 - **Bioactivity** biological targets (effect), dose-response characterization (dose)
- Combination of existing legacy, and high throughput and predictive model data
- Supports EPA and partner decision making
 - e.g., Well-studied chemicals: data can be found in most areas
 - e.g., Data-poor substances: predictive data, similar compound and literature searches, in vitro data

Batch Search

- Several incl. chemical lists
- User defined

Links Out

[illegible]

File Home Insert Draw Formulas Data Review View Help Acrobat

Clipboard Font Alignment Number Styles Cells Editing Sensitivity

SEARCHED: CHEMICAL

	A	B	C	D	E	F	G	H	I	J	K	L	M	N	O	P
1	SEARCHED	ATC	CASRN	NAME	SOURCE	SU	SOUT	TXWAL	TXWAL	TXWAL	TXWAL	TXWAL	TXWAL	TXWAL	TXWAL	TXWAL
2	HMR1426	DTXSID9026376	7HMR1426	ToxRefDB EPA ORD	LEL	LEL	Point of L	LEL	<	315 315						
3	HMR1426	DTXSID9026376	7HMR1426	ToxRefDB EPA ORD	LEL	LEL	Point of L	LEL	<	623 502.5						
4	HMR1426	DTXSID9026376	7HMR1426	ToxRefDB EPA ORD	LOEL	LOEL	Point of L	LOEL	<	100 500						
5	HMR1426	DTXSID9026376	7HMR1426	ToxRefDB EPA ORD	LOEL	LOEL	Point of L	LOEL	<	315 315						
6	HMR1426	DTXSID9026376	7HMR1426	ToxRefDB EPA ORD	LOEL	LOEL	Point of L	LOEL	<	100 500						
7	HMR1426	DTXSID9026376	7HMR1426	ToxRefDB EPA ORD	LOEL	LOEL	Point of L	LOEL	<	315 315						
8	HMR1426	DTXSID9026376	7HMR1426	ToxRefDB EPA ORD	LOEL	LOEL	Point of L	LOEL	<	500 500						
9	HMR1426	DTXSID9026376	7HMR1426	ToxRefDB EPA ORD	LOEL	LOEL	Point of L	LOEL	<	1000 1000						
10	HMR1426	DTXSID9026376	7HMR1426	ToxRefDB EPA ORD	LOEL	LOEL	Point of L	LOEL	<	315 315						
11	HMR1426	DTXSID9026376	7HMR1426	ToxRefDB EPA ORD	LOEL	LOEL	Point of L	LOEL	<	500 500						
12	HMR1426	DTXSID9026376	7HMR1426	ToxRefDB EPA ORD	LOEL	LOEL	Point of L	LOEL	<	100 500						
13	HMR1426	DTXSID9026376	7HMR1426	ToxRefDB EPA ORD	LOEL	LOEL	Point of L	LOEL	<	1000 1000						
14	HMR1426	DTXSID9026376	7HMR1426	ToxRefDB EPA ORD	LOEL	LOEL	Point of L	LOEL	<	1600 1600						
15	HMR1426	DTXSID9026376	7HMR1426	ToxRefDB EPA ORD	NEL	NEL	Point of L	NEL	<	315 315						
16	HMR1426	DTXSID9026376	7HMR1426	ToxRefDB EPA ORD	NEL	NEL	Point of L	NEL	<	623 502.5						
17	HMR1426	DTXSID9026376	7HMR1426	ToxRefDB EPA ORD	NEL	NEL	Point of L	NEL	<	63 63						
18	HMR1426	DTXSID9026376	7HMR1426	ToxRefDB EPA ORD	NEL	NEL	Point of L	NEL	<	100 100						
19	HMR1426	DTXSID9026376	7HMR1426	ToxRefDB EPA ORD	NEL	NEL	Point of L	NEL	<	400 400						

Ready Accessibility Investigate

Display Settings

PubChem Bisphenol A (Compound)

18.1 BioAssay Results

An agency of the European Union

Sign In English (en)

ECHA EUROPEAN CHEMICALS AG

AOP-Wiki AOPs Key Events KE Relationships Prototypical Stressors Developers' Handbook Login Register

LEGISLATION

ECHA > Substance Information

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Sex Applicability

View history Discussion Snapshots API XML

This AOP is licensed under a Creative Commons Attribution 4.0 International License.

Aop: 33

Title

Kidney toxicity induced by activation of 5HT2C

Short name

Kidney toxicity induced by activation of 5HT2C

Graphical Representation

Click to download graphical representation template

Explore AOP in a Third Party Tool

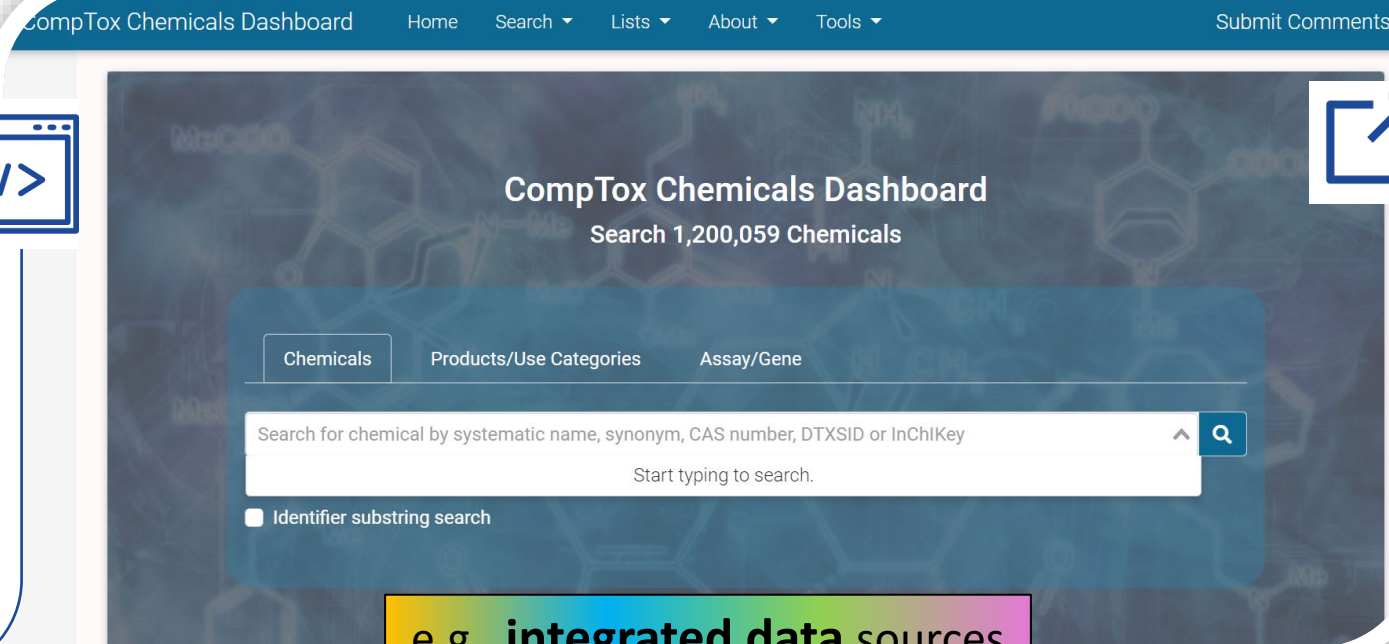
interoperability

e.g., embedded iframes

- ☐ EPA's Toxics Release Inventory
- ☐ Google Scholar
- ☐ PubChem links (e.g., Articles, Patents, Bioassays, GHS Classification)
- ☐ Integrated Risk Information System (IRIS)
- ☐ Provisional Peer-Reviewed Toxicity Value (PPRTV)



<https://comptox.epa.gov/dashboard/>



e.g., integrated data sources

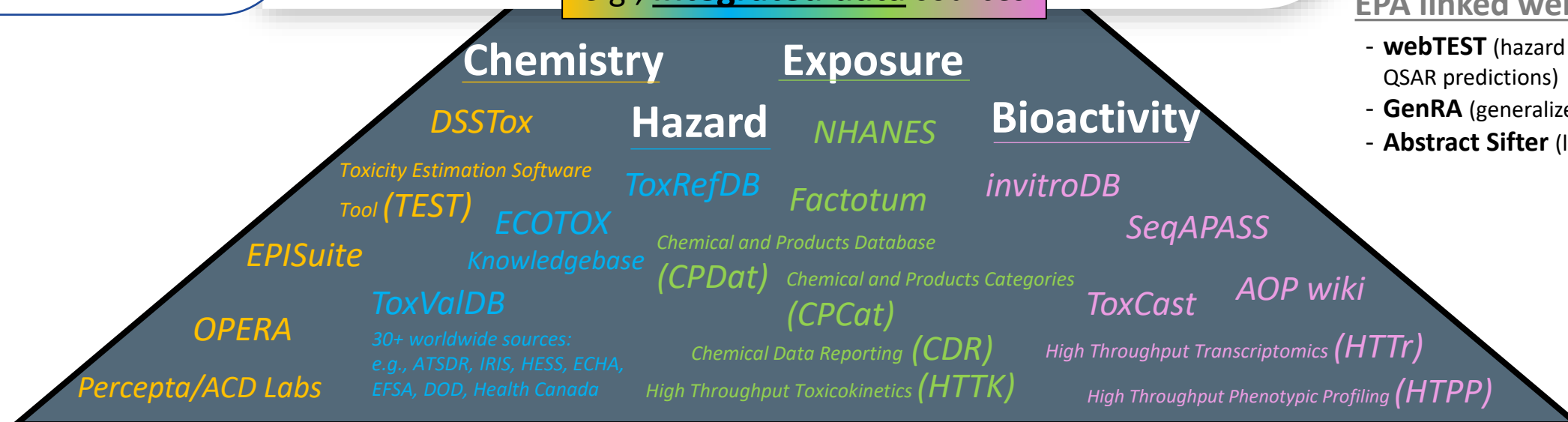
e.g., linked sources



- ☐ **General**
 - ECHA, MSDS, NIOSH, NIST, Wiki
- ☐ **Toxicology**
 - CalEPA, CTD, ECOTOX, AOP Wiki
- ☐ **Publications**
 - Google, IRIS, PubMed, Regulations.gov
- ☐ **Analytical**
 - MONA, NIST, PDB, Tox21 QC
- ☐ **Prediction**
 - NMDB, NMRShiftDB, LSERD

EPA linked webtools

- **webTEST** (hazard and physchem QSAR predictions)
- **GenRA** (generalized read-across)
- **Abstract Sifter** (literature search)



Acknowledgments



Efforts include many more than who are listed here

Many external collaborators provided data & links

Sipes.Nisha@epa.gov