

CompTox Chemicals Dashboard

- Making Connections for You

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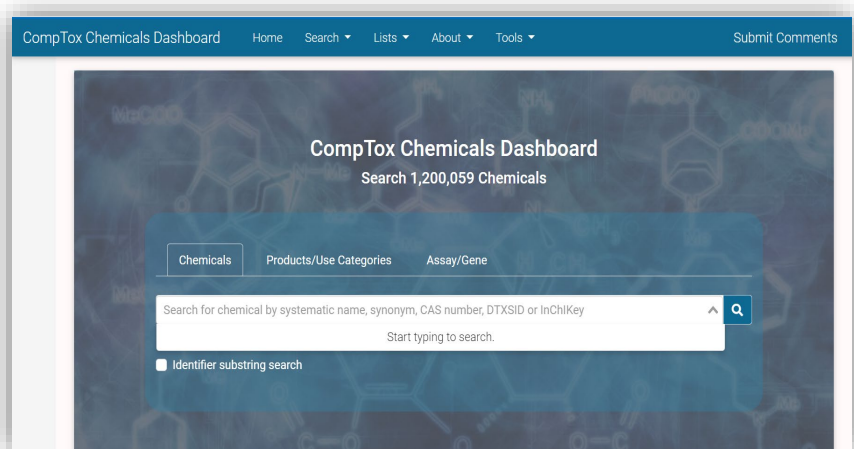
NEHA, New Orleans
EPA Tools Café

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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, 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][illegible]

PubChem Bisphenol A (Compound)

18.1 BioAssay Results

An agency of the European Union

Sign In English (en)


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

LEGISLATION


ECHA | Substance Information

ABOUT US
 Who we are
 The way we work

Table of Contents
 AOP Title
 Graphical Representation
 Abstract
 AOP Development Strategy
 Context
 Strategy
 Summary of the AOP
 Events
 Relationships Between Two Key Events
 Network View
 Prototypical Stressors
 Life Stage Applicability
 Taxonomic Applicability
 Sex Applicability

View history | Discussion | Snapshots

API | XML


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Aop: 33

Title

Kidney toxicity induced by activation of 5HT2C

Short name

Kidney toxicity induced by activation of 5HT2C

Graphical Representation

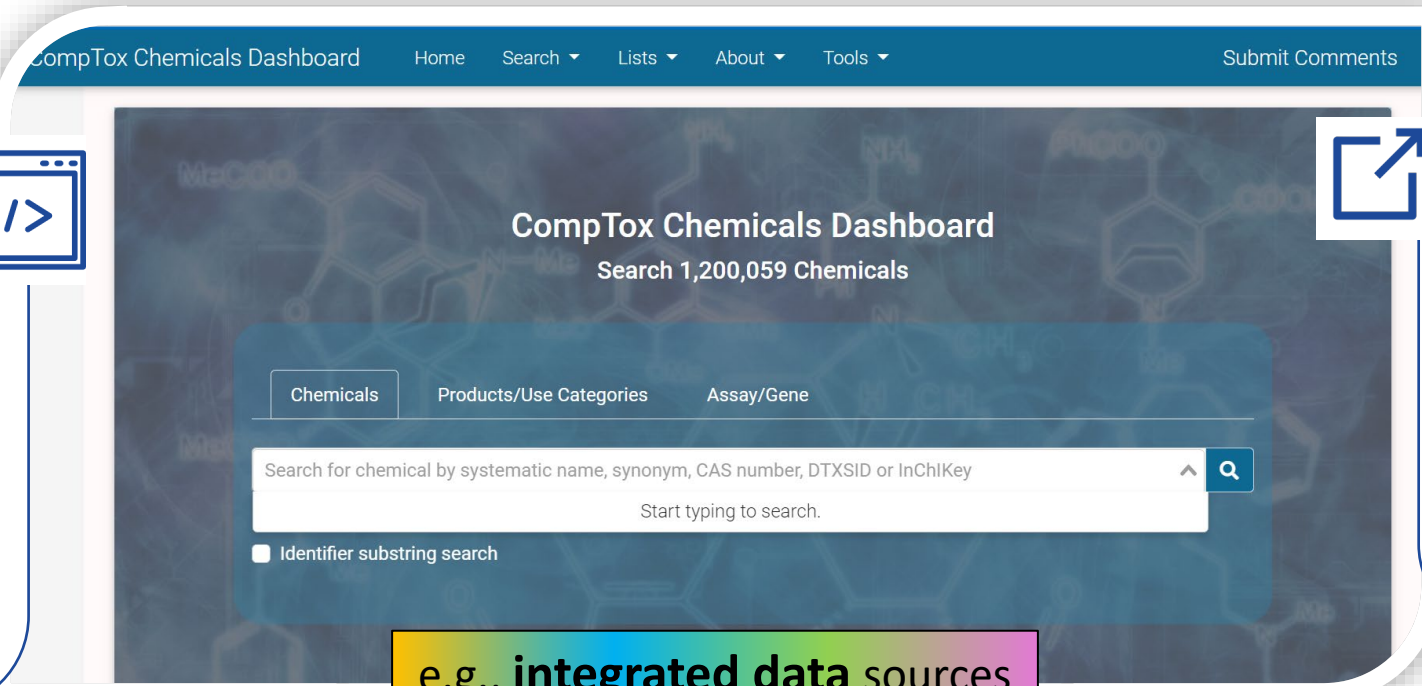
Click to download graphical representation template

Explore AOP in a Third Party Tool

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

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)



e.g., integrated data sources

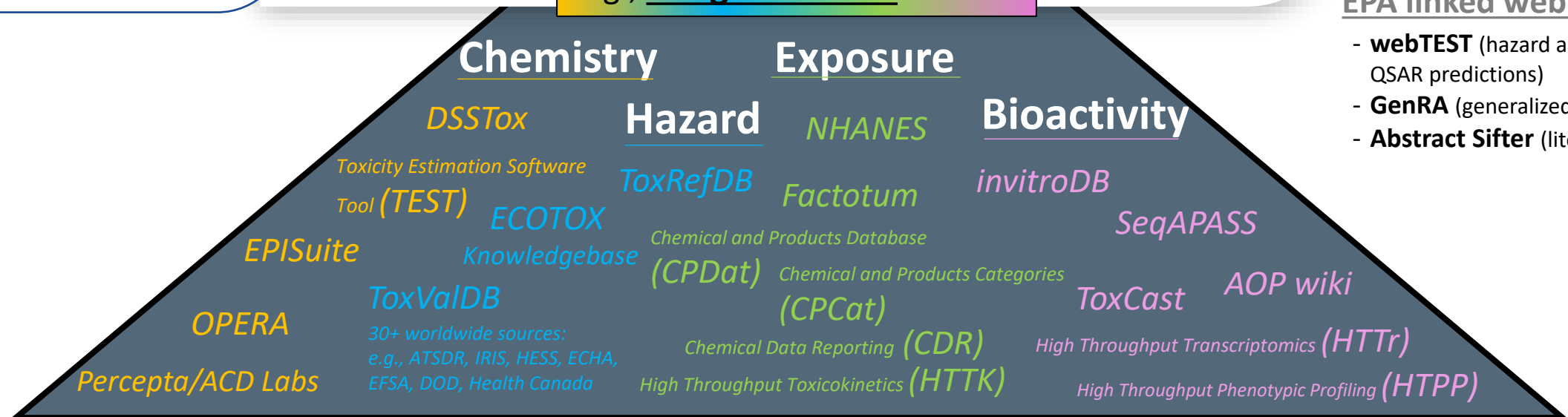
e.g., linked sources



- ☐ **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

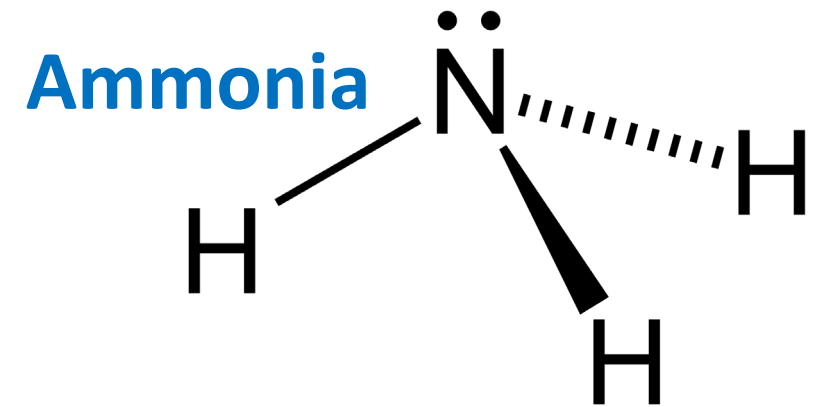
EPA linked webtools

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



Landfill Leachate

- **Leachate** - formed when rainwater filters through wastes placed in a landfill. When this liquid meets buried wastes, it leaches, or draws out, chemicals or constituents from those wastes.



Acknowledgments



Efforts include many more than who are shown here

Many external collaborators provided data & links

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EPA/ORD/Center for Computational Toxicology and Exposure