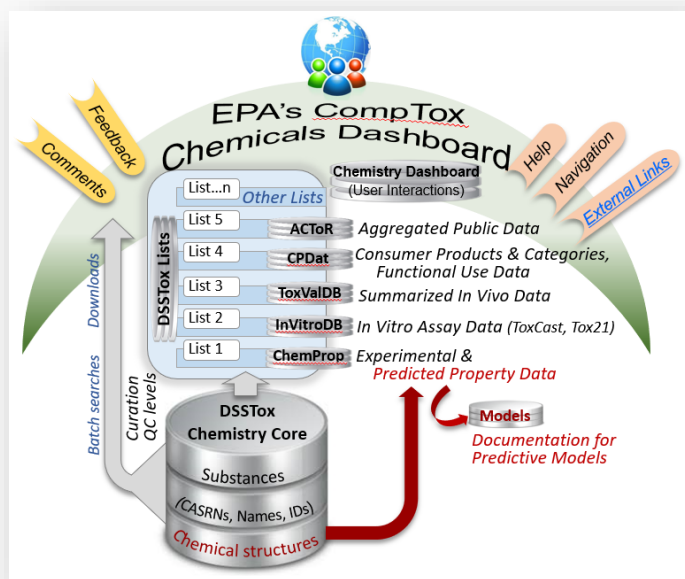


EPA CompTox Chemicals Dashboard as a Data Integration Hub for Environmental Chemistry Data



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The views expressed in this presentation are those of the author and do not necessarily reflect the views or policies of the U.S. EPA

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SETAC, Toronto, Canada*

- Freely accessible website and integration hub
 - Chemical substances – the majority with structures
 - Searchable by chemical, product use and gene
 - Experimental and predicted physicochemical property data
 - Experimental and predicted fate and transport data
 - Bioactivity data for the ToxCast/Tox21 project
 - Literature searches for chemicals using public resources
 - Links to other agency websites and public data resources
 - Batch searching for *thousands* of chemicals
 - Chemical lists of interest – pesticides, leachables, PFAS
 - **DOWNLOADABLE Open Data** for reuse and repurposing

A single application integrating...

875 Thousand Chemicals



Chemicals Product/Use Categories Assay/Gene

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

Identifier substring search

SEARCH

Home Advanced Search Batch Search Lists Predictions Downloads

BATCH SEARCH

Step Four: Select Data Output Format and Choose Data Fields to Download

Enter one identifier per line

Select Input Type(s)

- ☒ Identifiers
- ☐ Chemical Name(s)
- ☐ CASRN(s)
- ☐ InChIkey(s)
- ☐ DTXSID Substring(s)
- ☐ DDTSC Compound ID(s)
- ☐ InChIkey Substring(s)
- ☐ MS-Ready Formula(s)
- ☐ Exact Formula(s)
- ☐ Monoisotopic Mass(s)

Enter Identifiers to Search (searches should be limited to <5000 identifiers)

107-26-2
88-39-2
1402-55-6
33468-75-5
7784-40-9
1632-40-9
60332-96-5
2122-76-5
126833-17-8
7786-81-4

Display All Chemicals Download Chemical Data

Select Output Format:

Excel

Download

Customize Results

Select All

Select All in Lists

Chemical Identifiers

DTXSID

Chemical Name(s)

DTXSID

DTXSID

DTXSID

DTXSID

DTXSID

DTXSID

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Home Advanced Search Batch Search Lists Predictions Downloads

Bisphenol A

80-05-7 | DTXTSID7020182

Searched by Expert Validated Synonym.

Details Executive Summary Properties ENVI. RATE/TRANSPORT HAZARD

ACME EXPOSURE BIOACTIVITY GENRA (BETA) RELATED SUBSTANCES

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Chemical Activity Summary

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SIMILARITY

Searched with a similarity threshold of 0.8

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A data integration hub

LOTS of data!

- >875,000 chemicals curated over 20 years
- >700,000 toxicity data points from >30 sources
- Millions of synonyms and identifiers
- Tens of thousands of experimental data points
- Millions of QSAR prediction reports
- Millions of bioactivity data points for >4000 chemicals and hundreds of assay end points
- Searching of Pubmed's 29 million abstracts