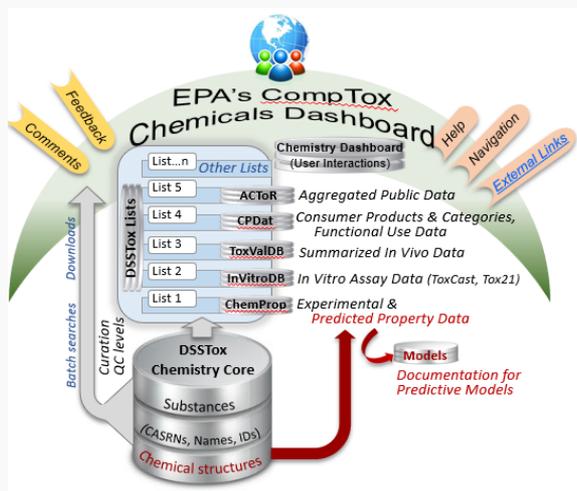


The EPA CompTox Chemicals Dashboard: An Integration Hub for Data Supporting Computational Toxicology

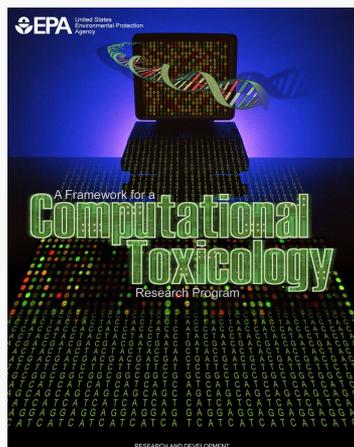


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*National Center for Computational Toxicology
U.S. Environmental Protection Agency, RTP, NC*

This work was reviewed by the U.S. EPA and approved for presentation but does not necessarily reflect official Agency policy.

US-EPA National Center for Computational Toxicology (NCCT)



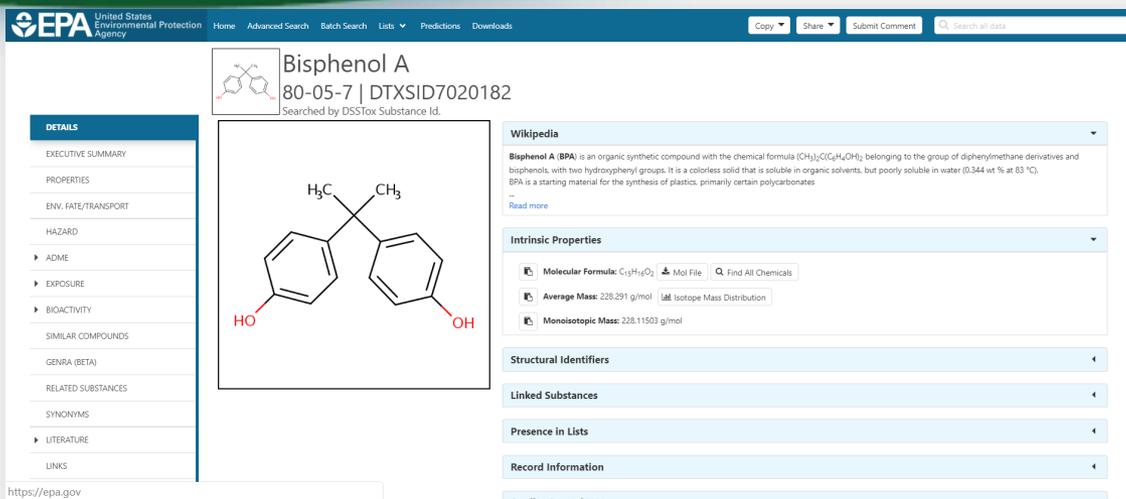
- National Center for Computational Toxicology established in 2005 to integrate:
 - High-throughput and high-content technologies
 - Modern molecular biology
 - Data mining and statistical modeling
 - Computational biology and chemistry
- Currently staffed by ~60 employees as part of EPA's Office of Research and Development
- Home of ToxCast & ExpoCast research efforts
- Key partner in U.S. Tox21 federal consortium

US-EPA National Center for Computational Toxicology (NCCT)

- Tens of thousands of chemicals in commerce and 100s more introduced every year
- Testing is expensive and slow with only a small fraction of chemicals fully evaluated for potential human health effects
- NCCT researchers integrate advances in biology, chemistry, and computer science to prioritize chemicals based on risk
- Underpinnings of our computational toxicology approaches
 - Data – high quality, curated data sourced from public resources and literature
 - Transparency – FAIR data available for download, reuse and repurposing
 - Prediction models – transparent, openly available (Github)

CompTox Chemicals Dashboard

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



The screenshot shows the EPA CompTox Chemicals Dashboard for Bisphenol A. The page header includes the EPA logo, navigation links (Home, Advanced Search, Batch Search, Lists, Predictions, Downloads), and utility buttons (Copy, Share, Submit Comment, Search all data). The main content area displays the chemical name "Bisphenol A" with its CAS number (80-05-7) and DTXSID (DTXSID7020182). A search filter "Searched by DSSTox Substance Id." is visible. A chemical structure diagram of Bisphenol A is shown, featuring two phenol rings connected by a central carbon atom bonded to two methyl groups (CH₃). The left sidebar contains a "DETAILS" menu with options like EXECUTIVE SUMMARY, PROPERTIES, ENV. FATE/TRANSPORT, HAZARD, ADME, EXPOSURE, BIOACTIVITY, SIMILAR COMPOUNDS, GENRA (BETA), RELATED SUBSTANCES, SYNONYMS, LITERATURE, and LINKS. The right sidebar provides information from Wikipedia, intrinsic properties (Molecular Formula: C₁₅H₁₆O₂, Average Mass: 228.291 g/mol, Monoisotopic Mass: 228.11503 g/mol), and expandable sections for Structural Identifiers, Linked Substances, Presence in Lists, and Record Information.

Publicly accessible website delivering access to:

- **>875,000** chemicals with **>25 million** property data points
- **>750,000** toxicity data points from 30 public resources and **>65,000** literature articles
- Millions of “Biological assay” data points for 1000s of chemicals
- Information about chemicals in consumer products
- Links to other agency websites and public data resources
- Integrated “literature” searches for **~30 million** abstracts

F indable A ccessible I nteroperable R eusable

EPA Comptox Chemicals Dashboard

General Information

The found...
scientists t...
access to a...
physicoche...
to their co...
such as the...



Homepage...
Developed...
Created in...
Taxonomic...

- Main page
- Community portal
- Project chat
- Create a new item
- Recent changes
- Random item
- Query Service
- Nearby
- Help
- Donate

Print/export

Download as PDF

Property

Discussion

Read

View history

Search Wikidata

DSSTOX substance identifier (P3117)

DSSTox substance identifier used in the Environmental Protection Agency CompTox Dashboard

DTXSID

In more languages [Configure](#)

Language	Label	Description	Also known as
English	DSSTOX substance identifier	DSSTox substance identifier used in the Environmental Protection Agency CompTox Dashboard	DTXSID
German	DSSTOX-Identifikator	No description defined	DTXSID
French	identifiant DSSTOX	identifiant DSSTox d'une substance utilisé par l'agence de protection de l'environnement américaine	DTXSID

Take Home Messages

- FAIR and Open Data is critical to building scientific data hubs for the community
- Transparency – in data and predictive models is the new approach to science and should be embraced
- Data QUALITY is key and community collaboration and crowdsourcing is critical to success
- Interoperability is enabled by the adoption of open standards – especially ontologies and taxonomies