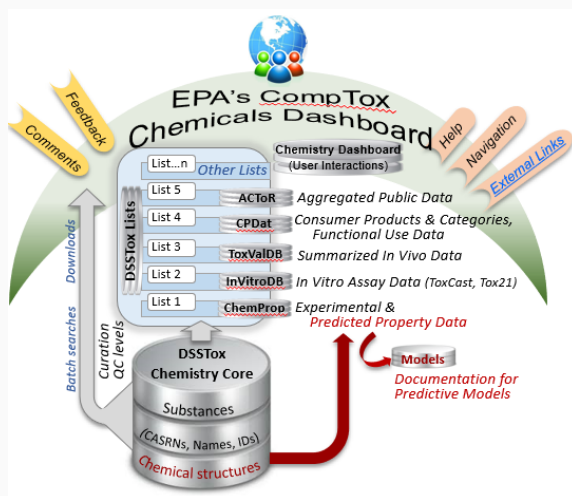


# The EPA CompTox Chemicals Dashboard: An Integration Hub for Data Supporting Computational Toxicology

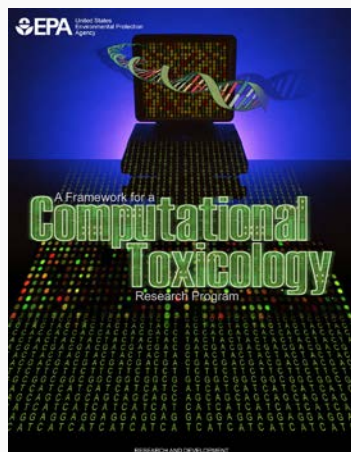


**Antony Williams**

*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)

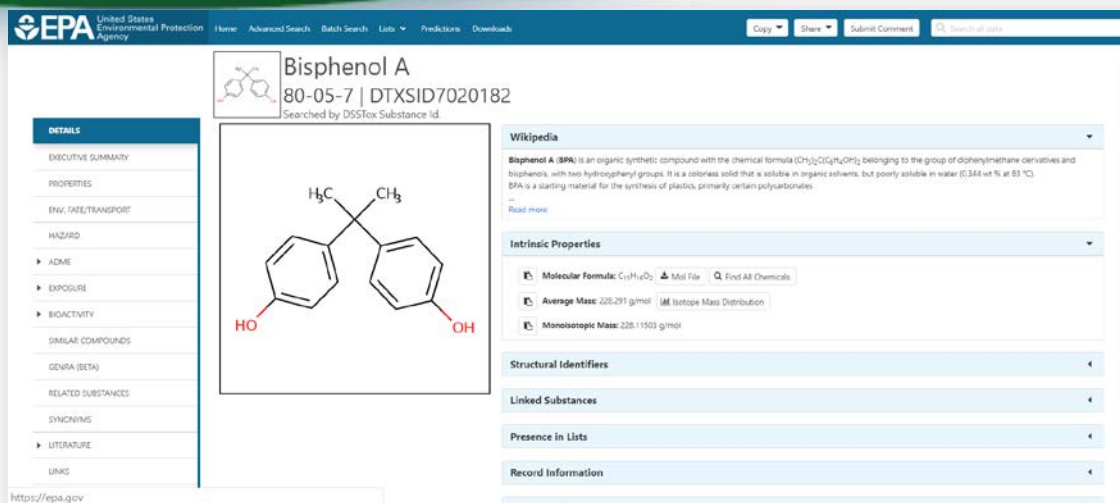


- National Center for Computational Toxicology established in 2005 to integrate:
  - High-throughput and high-content technologies
  - Modern molecular biology
  - Data mining and statistical modeling
  - Computational biology and chemistry
- Currently staffed by ~60 employees as part of EPA's Office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

- 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 and navigation links: Home, Advanced Search, Batch Search, Lists, Predictions, Downloads. The main content area displays the chemical name "Bisphenol A" with its CAS number "80-05-7" and DTXSID "DTXSID7020182". A search bar indicates it was searched by "DSSTox Substance Id". A chemical structure diagram shows two phenol rings connected by a central carbon atom bonded to two methyl groups (H3C and CH3). The left ring has a hydroxyl group (HO) at the para position, and the right ring has a hydroxyl group (OH) at the para position. The right sidebar contains a "Wikipedia" section with a brief description of Bisphenol A (BPA) as an organic synthetic compound with the chemical formula (C15H16O2) and its use in plastics. Below this are sections for "Intrinsic Properties" (Molecular Formula: C15H16O2, Average Mass: 228.291 g/mol, Monoisotopic Mass: 228.11503 g/mol), "Structural Identifiers", "Linked Substances", "Presence in Lists", and "Record Information". A left sidebar lists various detail categories like EXECUTIVE SUMMARY, PROPERTIES, ENV. FATE/TRANSPORT, HAZARD, ADMET, EXPOSURE, BIOACTIVITY, SIMILAR COMPOUNDS, GENRA (BETA), RELATED SUBSTANCES, SYNCING, LITERATURE, and LINKS.

## Publicly accessible website delivering access to:

- **>875,000** chemicals with **>25 million** property data points
- **>1 million** 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

## R 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

Scope and

Bioactivity

Print/export

Download as PDF

Property

Discussion

Read

View history

Search W

## 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