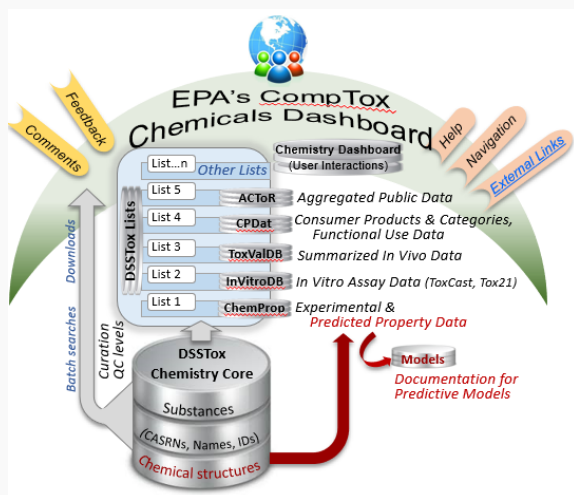


The EPA CompTox Chemicals Dashboard: An Integration Hub for Data Supporting Computational Toxicology



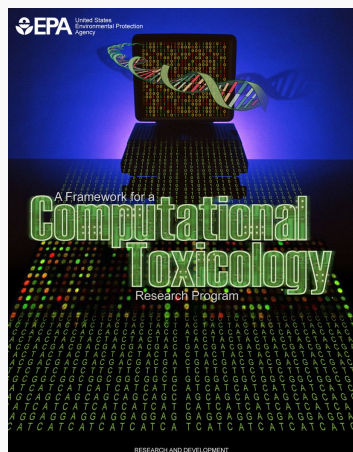
Antony Williams

*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.

June 13th 2019

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

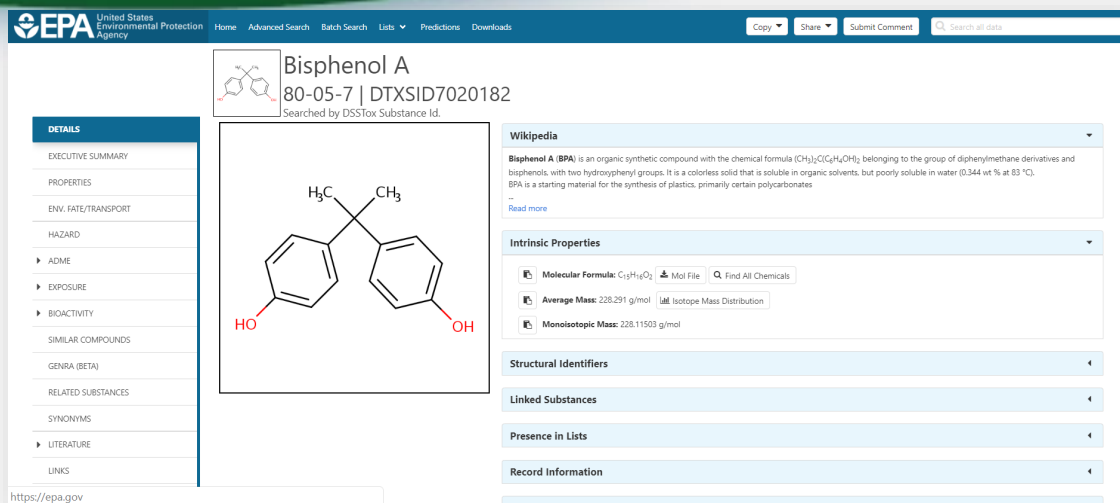
US-EPA National Center for Computational Toxicology (NCCT)



- 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>



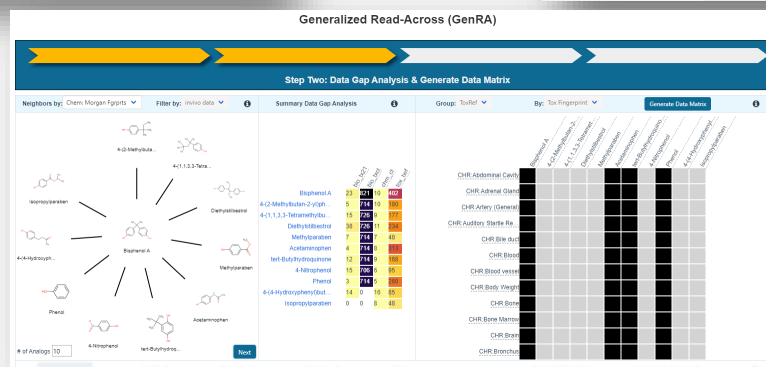
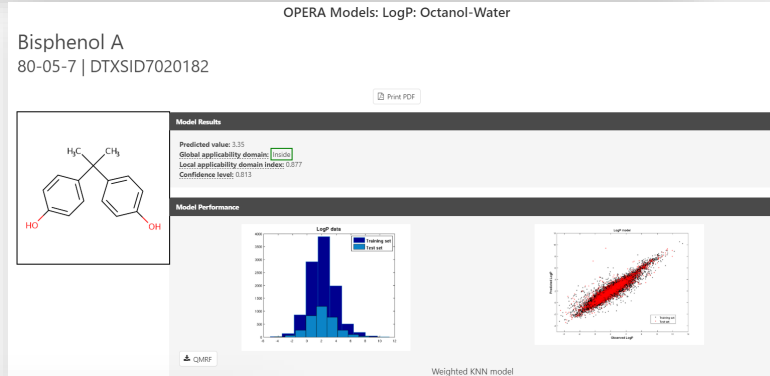
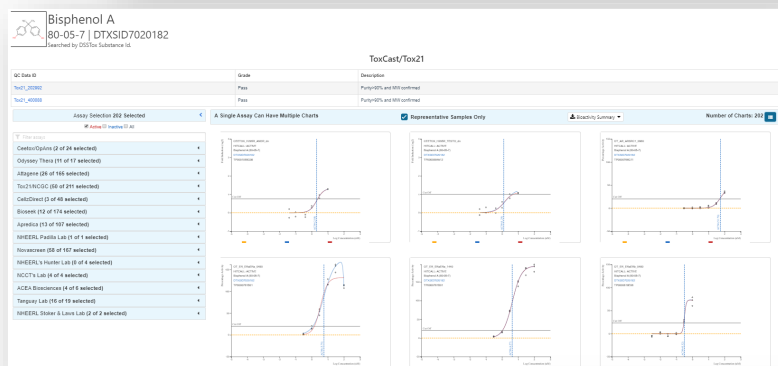
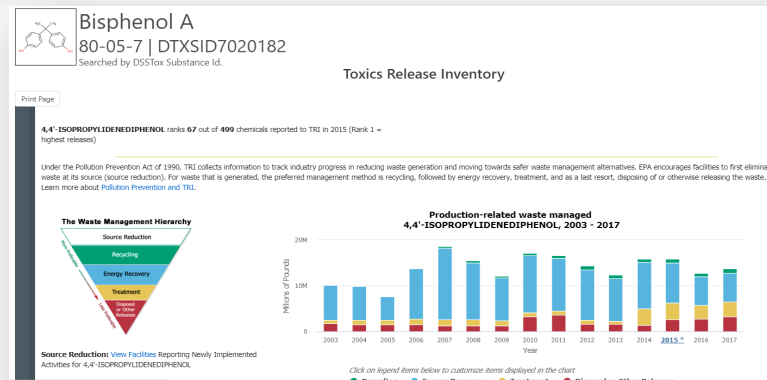
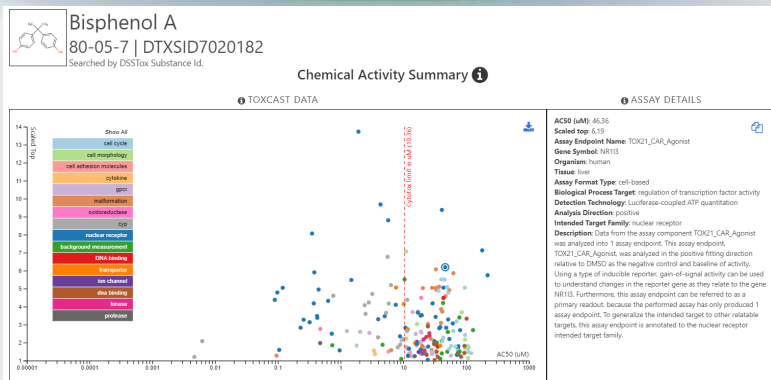
The screenshot shows the EPA CompTox Chemicals Dashboard for Bisphenol A. The header includes the EPA logo, navigation links (Home, Advanced Search, Batch Search, Lists, Predictions, Downloads), and user options (Copy, Share, Submit Comment, Search all data). The main content area displays the chemical name "Bisphenol A", its CAS number "80-05-7", and its DTXSID "DTXSID7020182". A chemical structure diagram of Bisphenol A is shown, featuring two phenol rings connected by a central carbon atom bonded to two methyl groups. The left sidebar contains a "DETAILS" menu with links to EXECUTIVE SUMMARY, PROPERTIES, ENV. FATE/TRANSPORT, HAZARD, ADME, EXPOSURE, BIOACTIVITY, SIMILAR COMPOUNDS, GENRA (BETA), RELATED SUBSTANCES, SYNONYMS, LITERATURE, and LINKS. The right sidebar provides a Wikipedia summary, intrinsic properties (Molecular Formula: $C_{15}H_{16}O_2$, 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

CompTox Chemicals Dashboard

Rich data content, Powerful Tools



FAIRsharing.org page

<https://fairsharing.org/FAIRsharing.tfj7gt>

F indable A ccessible I nteroperable R eusable

FAIRsharing.org
standards, databases, policies

Search all of FAIRsharing

Standards

Databases

Policies

Collections

Add/Claim Content

Stats

Log in or Register

R EPA Comptox Chemicals Dashboard

General Information

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



Homepage
Developed
Created in
Taxonomic

Not applicable

Scope and

Bioactivity

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 |

Substance Identifiers for Semantic Mapping

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