US-EPA CompTox Chemicals Dashboard: Bioactivity Data for Endocrine Assays

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Abstract

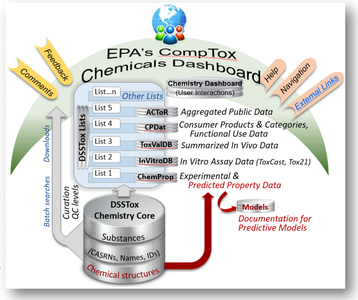
EPA's National Center for Computational Toxicology is developing automated workflows for curating large databases within the DSSTox project and for providing accurate linkages of data to chemical structures, exposure, and hazard data. The data are made available via the EPA's CompTox Chemicals Dashboard[1] (https://comptox.epa.gov/dashboard), a publicly accessible website providing access to data for ~875,000 chemical substances, the majority of these represented with chemical structures. The web application delivers a wide array of computed and measured physicochemical properties, *in vitro* high-throughput screening data and *in vivo* toxicity data, and linkages to a growing list of literature, toxicology, and analytical chemistry websites. The dashboard version 3:March 2019 release includes support for the *invitroDBv3.1* data release[2] and includes new functionality to interact with all ToxCast and Tox21 data with the intention of replacing the previously available EDSP21 and ToxCast dashboards. **The previous dashboards will be retired in summer 2019.**

Problem Definition and Goals

Problem: The support of multiple dashboards is inefficient and has required significant overhead. Improved efficiencies and functionality enhancements have resulted from migrating functionality in the EDSP21 and ToxCast dashboards to the CompTox Chemicals Dashboard. This migration was synchronized to the release of the *invitroDBv3.1* data expanding coverage of both the number of chemicals and assays available.

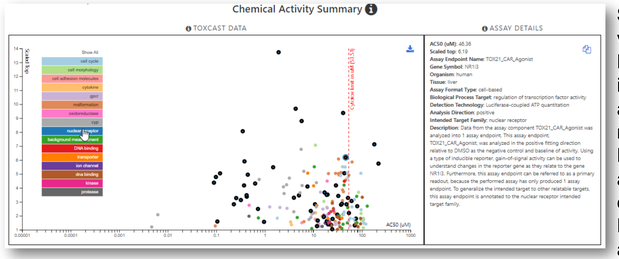
The CompTox Chemicals Dashboard

The CompTox Chemicals Dashboard provides access to data associated with **875k** chemical substances. Integrating data from a series of databases into a simple to use web-based interface, the dashboard provides access to experimental and predicted physicochemical properties and fate and transport data, *in vivo* hazard and exposure data. The dashboard provides real-time prediction for both property and toxicity endpoints, batch searching for thousands of chemicals and new approaches to navigate through bioactivity data. This includes a segregated list of the EDSP universe of chemicals and assays associated with the *invitroDBv3.1* release of data.



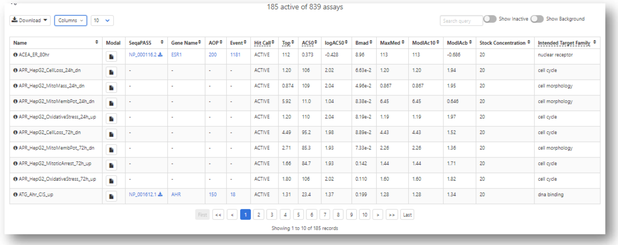
Navigating the EDSP Universe of Chemicals and Assays

The screenshots below illustrate navigation of bioactivity data associated with a single chemical, Bisphenol A. Version 3 of the dashboard includes all data associated with the *invitroDBv3.1* data release.



SUMMARY VIEW: A summary view of bioactivity data for Bisphenol A. Clicking on each individual data point displays the assay description and associated meta data in a summary form. More expansive details for each assay are available including citations, reagents and ToxCast Pipeline (tcpl) processing[3] analysis.

ASSAY HIT-CALL TABLE: A table of the hit calls for a chemical with details including the AC50 values, a subset of associated fit parameters and mappings to the AOP-Wiki. All data can be downloaded in Excel format for review and analysis.

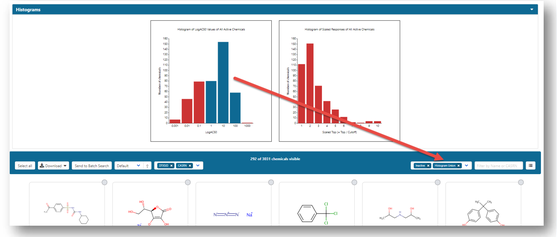


BIOACTIVITY CURVES: The ability to view only EDSP-related assays, or the entire suite of assays associated with Toxcast and Tox21, as shown, brings the previous dashboards together into a single application.

Navigating Lists of Chemicals and Assays

A simplified navigation of lists of chemicals and assays has been introduced into the latest release of the dashboard. The data associated with an assay endpoint allows for navigation of the associated set of chemicals with intuitive filtering.

Data can be downloaded to the desktop for further analysis (e.g. as Excel files) or passed to the integrated batch search to intersect with additional data of interest for the selected chemicals.



Related data and utilities

ToxCast data, including single concentration screening data and other supporting information, are available freely in invitrodb_v3.1, which is managed using tcpl v.2.0.1.
Download invitrodb_v3.1: https://www.epa.gov/chemical-research/exploring-toxcast-data-downloadable-data
Download the R package for the ToxCast Pipeline (tcpl v2.0.1) and
peruse the tcpl v2.0.1 vignettes that explain the package and invitrodb structure: https://cran.r-project.org/web/packages/tcpl/index.html (also available on Git and EPA FTP)

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References

1. Williams *et al.,* The CompTox Chemicals Dashboard, Journal of Cheminformatics, 2017, 9:61, https://doi.org/10.1186/s13321-017-0247-6
2. Downloadable invitrodbv3.1 data: https://www.epa.gov/chemical-research/exploring-toxcast-data-downloadable-data
3. tcpl version 2.0.1 available on CRAN https://cran.r-project.org/web/packages/tcpl/