

## Interactive Chemical Safety for Sustainability (iCSS) ToxCast Dashboard

### Overview

Thousands of chemicals are currently in use, and hundreds more are introduced every year. Because current chemical testing is expensive and time consuming, only a small fraction of chemicals have been thoroughly evaluated for potential human health effects.

Through its safer chemicals research, the U.S. Environmental Protection Agency (EPA) is developing ground-breaking approaches to change how chemicals are evaluated for potential health effects. EPA's ToxCast research effort uses automated chemical screening technologies (called "high-throughput screening assays") to expose living cells or isolated proteins to chemicals. The cells or proteins are then screened for changes in biological activity that may suggest potential toxic effects.

EPA's ToxCast effort contributes to the Toxicology in the 21st Century (Tox21) federal agency consortium. Through Tox21, the EPA, National Toxicology Program at the National Institute of Environmental Health Science, the National Institutes of Health's National Center for Advancing Translational Sciences, and the Food and Drug Administration are using robotic technology to screen tens of thousands of chemicals. These approaches have generated vast amounts of data on thousands of chemicals.

To access and visualize these data generated, EPA has developed online tools called interactive Chemical Safety for Sustainability Dashboards. One of these dashboards, the iCSS ToxCast Dashboard, helps users

The screenshot displays the iCSS ToxCast Dashboard interface. It features a navigation menu with options like 'Assays' and 'Chemicals'. The main content area is divided into several panels: a list of chemicals (e.g., Bisphenol A, Bisphenol B, Bisphenol F), a list of assays (e.g., ACEA\_147D\_80W\_Positive), and a detailed view of a chemical structure (Bisphenol A) with its SMILES string and various physicochemical properties. A table at the bottom shows 'Tox21 Chemical QC' results for different samples.

examine high-throughput assay data to inform chemical safety decisions. To date, the iCSS ToxCast Dashboard has data on over 9,000 chemicals and information on approximately 1000 assay endpoints.

Users of the iCSS ToxCast Dashboard can explore the data from a chemical or an assay viewpoint. Once the user selects the chemicals and assays of interest, they can then explore the biological activity for the chemical-assay combinations. Results from the selections are shown with tables, graphs, and charts that can be downloaded by the user.

### Chemical Viewpoint

Users can select chemicals of interest using a number of filters. Chemical data filters include Chemical Abstract Service Registry Number (CASRN), chemical name, chemical category, use category, and physicochemical properties such as the octanol-water partition coefficient (log P). For each chemical, the iCSS ToxCast

Dashboard summarizes chemical information.

- Chemical structure and data such as CASRN, simplified molecular input line entry system (SMILES), IUPAC International Chemical Identifier (InChI), chemical structures, chemical annotations, quality control information on the chemical tested, information on the chemical sample, and physicochemical properties.
- Chemical assay activity summaries and charts for the selected chemicals.
- Chemical Product Category (CPCAT) information listing product use category for the selected chemicals.
- Exposure estimations based on manufacture and use information for the chemicals selected.

### Assay Viewpoint

Users can select assays of interest using a number of filters. Assay

filters include gene symbol, intended target, assay name, tissue, and 'actives' only. For each assay, the iCSS ToxCast Dashboard summarizes assay information.

- Assay data including assay descriptions, reagents used, citations from scientific papers that conducted an analysis of the assay data, and descriptions of methods used to process the assay data.
- Assay summary charts that show summaries of the assay activity for all the chemicals screened in the selected assay and a list of chemicals tested in the selected assay.

## Biological Activity

The biological activity function of selected chemical and assay pairs is summarized in the iCSS ToxCast Dashboard. Examples of summary information include hit calls, AC50 (chemical concentration producing 50% of the maximum activity in the assay), statistical model used to fit the activity data, and a plot of biological activity. If a user selects multiple chemical and assay pairs, the biological activity for each pair is added to the summary charts, which are downloadable and interactive.

## Stakeholder Engagement

EPA actively engages stakeholders to solicit feedback in order to improve the iCSS Dashboard, and the underlying ToxCast data. These stakeholder engagement activities include EPA hosted workshops, webinars, demonstrations, videos, and trainings. Using input from these activities, EPA adds functionality and improves the utility of the iCSS ToxCast Dashboard.

## Related Data and Online Tools

We recommend using the iCSS ToxCast Dashboard to view and visualize the ToxCast data. If you are conducting an in-depth analysis of the data, we encourage you to download all of the data from the ToxCast data download page.

Another publicly available iCSS Dashboard is the iCSS Chemistry Dashboard. This new dashboard, acts as a public chemistry resource supporting improved predictive toxicology. A distinguishing feature of the iCSS Chemistry Dashboard is the mapping of curated physicochemical property data associated with chemical substances to their corresponding chemical structures. It also integrates chemistry linkages across other EPA dashboards and chemistry resources.

More information, go to:

### ToxCast

<http://epa.gov/ncct/toxcast/>

### iCSS Dashboard:

<http://actor.epa.gov/dashboard/>

### ToxCast Data:

<http://epa.gov/ncct/toxcast/data.html>

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