

CompTox Chemicals Dashboard

Overview

Under different federal statutes, EPA makes a broad range of decisions to protect public health and the environment from unintended consequences of using chemicals. Decisions about chemicals are also made by other Federal Agencies, State Environmental and Health Agencies, International Governmental Agencies and Industry. As examples, there are specific federal laws for pesticides, drinking water contaminants, commercial and industrial chemicals, chemicals found on contaminated sites and endocrine disrupting chemicals.

These laws give EPA the authority to: Gather health, safety and exposure data on chemicals; Require necessary testing; and Control human and environmental exposures. To help support this mission, EPA researchers are integrating available chemical information including chemistry, toxicity and exposure information into an online tool called the Computational Toxicology Chemicals (CompTox) Dashboard to help decision-makers and scientists quickly and efficiently evaluate chemicals.

The CompTox Chemicals Dashboard is a one-stop-shop for chemistry, toxicity and exposure information for almost 900,000 chemicals. Data and models within the CompTox Chemicals Dashboard also help with efforts to identify chemicals of most need of further testing and reduce the use of animals in chemical testing.

The Dashboard can be searched by chemical identifiers (e.g. Name and CASRN), consumer product categories (i.e. view chemicals found in certain product types), and assays/ genes associated with high-throughput screening data. Using high-throughput screening, living cells or proteins are exposed to chemicals and examined

for subsequent changes that suggest potential biological responses.

Users can also batch search for thousands of chemicals and view chemical lists organized by chemical categories of interest (e.g. PFAS), or assay/gene to view biological activity of interest (e.g. estrogen receptor binding which would be of interest to those evaluating chemicals for potential endocrine disruption). Data in the Dashboard can also be exported to a spreadsheet or .csv file for further analysis.

Chemistry Information

Within the Dashboard, users can access high-quality chemical structures experimental and predicted physicochemical properties, environmental fate and transport, and toxicity data, with links to relevant websites and applications. The chemical structures and chemistry information have been extensively curated and quality checked. These data are available in the

chemicals tab, providing valuable information for analytical scientists involved in structure identification.

Toxicology Information

The Dashboard includes chemical hazard data from both traditional laboratory animal studies and high-throughput screening. High-throughput screening evaluates thousands of chemicals rapidly for bioactivity, and is intended to limit the resources, including animals, needed for chemical testing. Biological activity data from high-throughput screening is generated by EPA's Toxicity Forecaster (ToxCast) research effort. ToxCast has evaluated thousands of chemicals in hundreds of high-throughput screening assays. The ToxCast data in the Dashboard provides information about the assays used to evaluate the chemicals, and response potency and efficacy. This data can

be used to evaluate and prioritize chemicals. Concentration response plots are also available for all ToxCast chemicals. These data can be found in the bioactivity tab.

Traditional toxicology data in the Dashboard is compiled from existing studies evaluating chemicals for human and ecological health effects. The human health section has effect level data for different study designs, including subchronic, chronic, reproductive, and developmental neurological toxicity.

The ecological health information includes lowest concentration of a chemical that produces an adverse effect for acute, chronic and reproductive toxicity. Included with this data is information about the study type, exposure route, what species was involved in the experiment, links to the source of the data and links to find detailed information about each study.

Exposure Information

The Dashboard also contains a variety of exposure information. There is information about how much of a chemical is produced, which chemicals are found in categories of consumer products (e.g. shampoo and paint), what the chemical is designed to do (e.g. fragrance and colorant), and how much of a chemical is released into the environment.

It also includes results from monitoring data and exposure predictions for chemicals lacking monitoring data. The monitoring data is from the Center for Disease Control's National Health and Nutrition Examination Survey. The survey collects blood and urine from a sample of the United States population to better the health and nutrition of the US population including gaining a better understanding of chemical exposure levels.

NHANES has monitoring data for hundreds of chemicals, but there are thousands of chemicals in the environment. To help close the data gap, EPA researchers have developed a rapid exposure prediction model called ExpoCast.

ExpoCast quickly looks at multiple routes of exposure and makes predictions using a combination of far-field and near-field models. The far-field models provide an exposure prediction for chemicals that are released into the environment through industrial releases, while near-field models provide a prediction for chemicals used in consumer and in-home products. These models are evaluated and continually refined as more data is gathered from sources such as consumer product use.

The Dashboard also contains measured, predicted and computed absorption, distribution, metabolism and excretion (ADME) data. The data is used to quantify the amount of chemicals entering, moving around, changing, and leaving the body. These data are available in the exposure tab.

Other Capabilities

Within the Dashboard, users can find similar compounds, related substances and synonyms for a given chemical. They can also use the drawing tool to draw new chemical structures and make real-time toxicity predictions based on what is known about existing chemicals with similar structures.

EPA researchers have also developed an automated read across tool called Generalized Read-Across (GenRA) and a beta version of it is integrated into the Dashboard. Read-across uses known information about the property of a chemical to make a prediction of the same property for another chemical that is "similar," but does not have the same amount of data available.

The goal of GenRA is to encode as many expert considerations used within current read-across approaches and automate grouping similar chemicals to help predict toxicity.

The Dashboard also has the capability to search existing scientific literature sources such as Google Scholar and PubMed, and reports from EPA's Provisional Peer Reviewed Toxicity Values (PPRTV) and the Integrated Risk Information System (IRIS).

The Dashboard data comes from a variety of sources including EPA's computational toxicology databases,

other EPA sources and public domain databases.

Expansion, curation, and verification of the Dashboard content is an ongoing process. We welcome the opportunity to integrate new data and resources into the dashboard. Users can share the Dashboard with others and contact us through the information below or use the comments tab within the Dashboard to identify data anomalies or provide suggestions.

More information, go to:

CompTox Chemicals Dashboard
<http://comptox.epa.gov/dashboard>

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