

Chemistry Dashboard

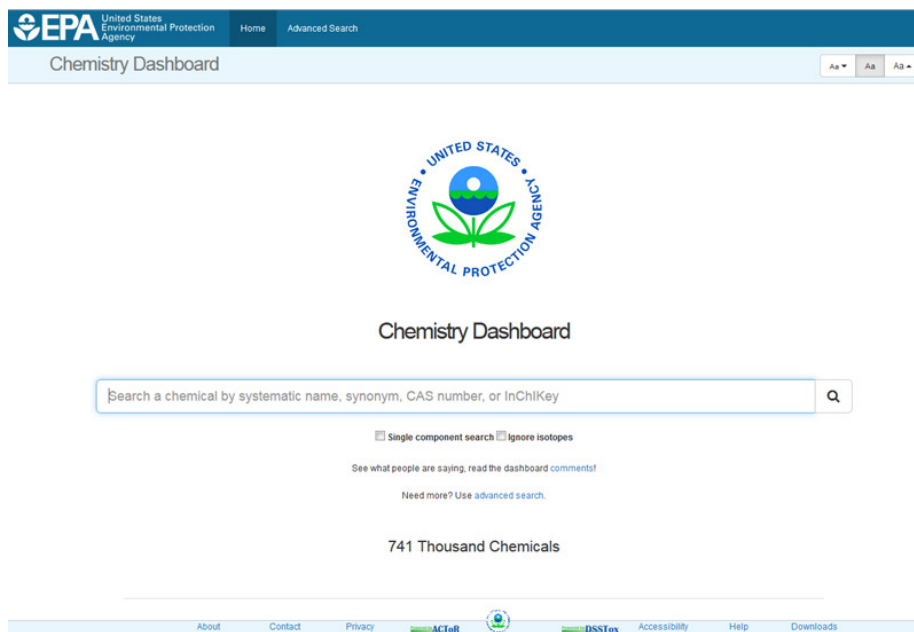
Overview

Thousands of chemicals are currently in use, and hundreds more are introduced into commerce every year. Due to the time and resource intensive nature of chemical safety testing, only a small fraction of chemicals have been thoroughly evaluated for potential human health effects. Through its computational toxicology research, the U.S. Environmental Protection Agency (EPA) is developing groundbreaking approaches to change how chemicals are evaluated for potential health effects.

The foundation of computational toxicology and chemical safety testing relies on high-quality chemical structures and physicochemical properties. Chemical structures and properties are used in computational models to predict a range of hazard, pharmacokinetic, and exposure-related endpoints that are necessary to understand potential health risks. The EPA has recently expanded and curated its chemical structure and physicochemical property database. The public can now access these data through the Chemistry Dashboard. The Chemistry Dashboard is part of a suite of dashboards to enable stakeholders to interact with a variety of safety-related data being collected and collated on the thousands of chemicals in use.

Chemistry Dashboard

The Chemistry Dashboard provides access to chemistry data for ~700,000 chemicals. The data is compiled from a variety of sources



including the EPA's computational toxicology research databases, other EPA sources, and public domain databases such as the National Center for Biotechnology Information's PubChem database. The database includes quality assurance flags that indicate the degree of curation and confidence associated with the data.

Within the Chemistry Dashboard, users can access chemical structures, experimental and predicted physicochemical and toxicity data, and additional links to relevant websites and applications. It maps curated physicochemical property data associated with chemical substances to their corresponding chemical structures. Millions of predicted physical-chemical properties developed using machine-learning modeling of highly curated datasets are also mapped to chemicals. These

data provide valuable information for analytical scientists involved in structure identification and can support targeted and non-targeted screening identification of environmental chemicals.

The Chemistry Dashboard includes search capabilities allowing the user to filter results by chemical name, mass or molecular formula, or by chemical identifiers including CAS Registry Numbers, systematic and common names, and InChIKeys. If data relevant to a search query is identified in the database, a detailed results page with associated information for the chemical is generated. In addition, the Chemistry Dashboard has a series of navigation tabs providing access to additional chemical information including Physical Properties, External Links to additional resources, Synonyms, Biological Activities, Articles, and Patents.

Stakeholder Feedback

Expansion, curation, and verification of the Chemistry Dashboard content is an ongoing process. We welcome the opportunity to integrate new data and resources into the dashboard. Please contact us using the contact information below or using the Comments tab within the Chemistry dashboard to identify data anomalies or provide suggestions.

Related Data and Online Tools

Another publicly available Dashboard is the ToxCast Dashboard. The ToxCast Dashboard provides access to data from automated chemical screening technologies, called "high-throughput screening assays," that expose living cells or isolated proteins to chemicals to determine potential biological activity. The ToxCast Dashboard helps users access and visualize the data generated from high-throughput screening data in order to help inform decisions related to potential chemical risks.

More information, go to:

Chemistry Dashboard<http://comptox.epa.gov/dashboard>

Contact:

National Center for Computational Toxicology

Antony Williams

Project Lead
williams.antony@epa.gov

Monica Linnenbrink

Communications Director
linnenbrink.monica@epa.gov

Main Office: 919·541·4219
www.epa.gov/comptox
109 T.W. Alexander Drive
Mailcode D143-02
Research Triangle Park, NC 27711



Recycled/Recyclable

Printed on paper that contains a minimum of 50% postconsumer fiber content processed chlorine free