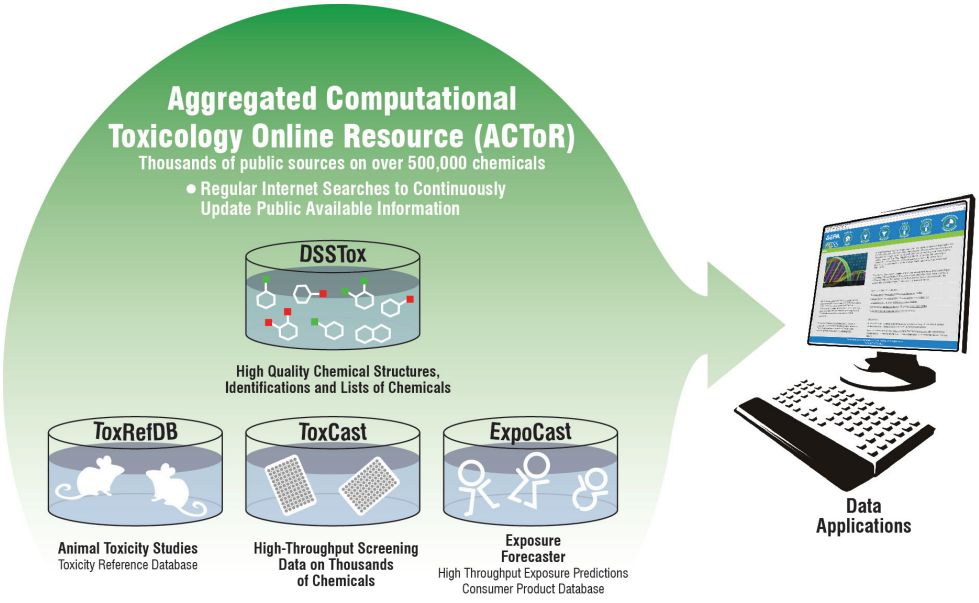
Chemical Toxicity Databases

CHEMICAL SAFETY RESEARCH: ONLINE DATA APPLICATIONS

Tens of thousands of chemicals are currently in commerce, and hundreds more are introduced every year. Since current chemical testing is expensive and time consuming, only a small fraction of chemicals have been fully evaluated for potential human health effects.

Through its computational toxicology research (CompTox), the U.S. Environmental Protection Agency (EPA) is working to figure out how to change the current approach used to evaluate the safety of chemicals. CompTox research integrates advances in biology, biotechnology, chemistry, and computer science to identify important biological processes that may be disrupted by certain chemicals and tracing those biological disruptions to a related dose and human exposure. The combined information helps prioritize chemicals based on potential human health risks. Using CompTox, thousands of chemicals can be evaluated for potential risk at a small cost in a very short amount of time.

Evaluating thousands of chemicals this way results in massive amounts of data. As part of EPA's commitment to share research in open and transparent ways, all of this data is publicly available for anyone to access and use. Chemical safety research data is made available through online applications called dashboards. The vision is that the dashboard, called the interactive Chemical Safety and Sustainability (iCSS) dashboard, will be the portal to access all EPA chemical safety research data and studies including:



- Rapid, automated (or in vitro high-throughput) chemical screening data generated by the EPA's Toxicity Forecaster (ToxCast) project and the federal Toxicity Testing in the 21st century (Tox21) collaboration.
- Aggregated public sources of chemical toxicity data.
- Animal toxicity studies.
- Chemical exposure data and prediction models.
- High quality chemical structures and annotations.

Currently, the iCSS dashboard provides a portal for users to search and query the ToxCast chemical screening data.

ToxCast & Tox21 Data

ToxCast 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. ToxCast has generated data on over 2,000 chemicals evaluated in over 700 high-throughput assays. Using the iCSS dashboard, users can select and view the chemicals and high-throughput screening data of interest. Providing ToxCast data through the dashboard helps external stakeholders evaluate this new data and determine ways it could be used to inform decision making. The EPA's Endocrine Disruption Screening Program has already started the scientific review process necessary for using ToxCast data to prioritize the thousands of chemicals that need to be tested for potential endocrine-related activity.

Long-term, the iCSS dashboard will be the online portal for all the chemical safety research data and studies. While EPA researchers are continually adding features to the dashboard, the following databases are publicly available at: www.epa.gov/research/mmtd/chemsafe.htm

Chemical Toxicity Databases

Aggregated Public Sources of Chemical Data

Aggregated Computational Toxicology Online Resource (AcTOR) is EPA's online aggregator of all the public sources of chemical toxicity data. ACToR aggregates data from over 1,000 public sources on over 500,000 chemicals and is searchable by chemical name, other identifiers and by chemical structure. It can be used to query a specific chemical and find all publicly available hazard, exposure and risk assessment data.

Toxicity Reference Database

The Toxicity Reference Database (ToxRefDB) contains approximately 30 years and $2 billion worth of animal studies. ToxRefDB allows scientists and the interested public to search and download thousands of animal toxicity testing results for hundreds of chemicals that were previously found only in paper documents. Currently, there are 474 chemicals in ToxRefDB, primarily the data rich pesticide active ingredients, but the number will continue to expand.

DSSTox

The Distributed Structure Searchable Toxicity (DSSTox) online resource provides high quality chemical structures and annotations in association with toxicity data. It helps to build a data foundation for improved structure-activity relationships and predictive toxicology. DSSTox publishes summarized chemical activity representations for structure-activity modeling and provides a structure browser. This tool also houses the chemical inventories for the ToxCast and Tox21 projects.

ExpoCastDB

The Exposure Forecaster Database (ExpoCastDB) is EPA's database for aggregating chemical exposure information and can be used to help with chemical exposure predictions. The database currently includes biomonitoring exposure data from three studies: the American Healthy Homes Survey, the First National Environmental Health Survey of Child Care Centers and the Children's Total Exposure to Persistent Pesticides and Other Persistent Organic Pollutants study. Data include the amounts of chemicals found in food, drinking water, air, dust indoor surfaces and urine.

The database will eventually include high-throughput exposure predictions for thousands of chemicals based on manufacture and use information. EPA researchers developed high-throughput exposure models to predict exposures for 1,763 chemicals using production volume, environmental fate and transport models, and a simple indicator of consumer product use. The model is being improved by adding more refined indoor and consumer use information since these are also large determinants of exposure. As these models are refined and more exposure data is collected, it will be added to ExpoCastDB.

Chemical and Product Categories

The Chemical and Product Categories database (CPCat) catalogs the use of over 40,000 chemicals and their presence in different consumer products. The chemical use information is compiled from multiple sources while product information is gathered from publicly available Material Safety Data Sheets (MSDS). EPA researchers are evaluating the possibility of expanding the database with additional product and use information.

Collaboration Opportunities

CompTox actively engages a wide-range of partners including EPA regions and program offices, industry, academia, trade associations, other federal agencies, state and local government agencies and non-governmental organizations to help make this new chemical information understandable and useable for decisions made about chemicals.

CompTox has workshops, webinars, and training to inform partners and to ask for partner feedback about how to improve CompTox research. CompTox hosts monthly Communities of Practice webinars and anyone with an interest in CompTox research can participate. CompTox also partners with hundreds of outside organizations to collaborate on research and it funds academic centers working on various aspects of computational toxicology through EPA's Science to Achieve Results (STAR) program. In addition, CompTox hosts visiting scientists, doctoral students and post-doctoral fellows collaborating on computational research.

For more information:

ToxCast:
http://epa.gov/ncct/toxcast/
ACToR:
http://actor.epa.gov/actor
ToxRefDB:
http://actor.epa.gov/toxrefdb
CSS Dashboards:
http://actor.epa.gov/actor/faces/CSSDashboardLaunch.jsp

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