Chemical Toxicity Databases

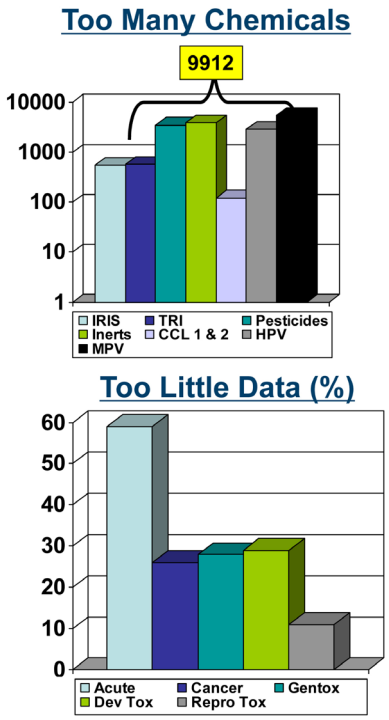
U.S. EPA's PUBLICLY AVAILABLE CHEMICAL TOXICITY DATABASES

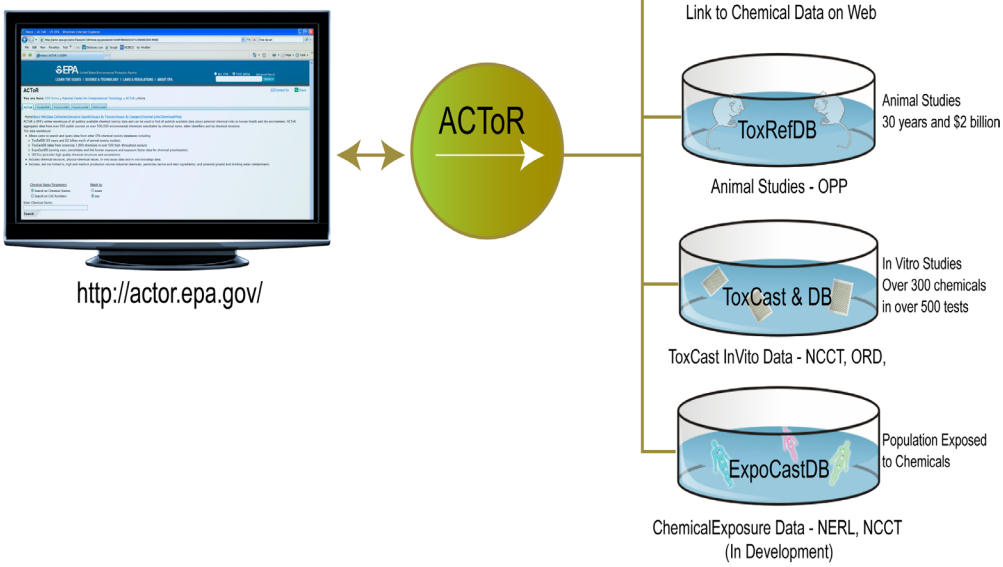
Tens of thousands of chemicals are currently in commerce, and hundreds more are introduced every year. Because current chemical testing is expensive and time consuming, only a small fraction of chemicals have been assessed adequately for potential risk.

The U.S. Environmental Protection Agency is working to change the current approach to chemical toxicity risk assessment through its Computational Toxicology Research Program (CompTox). The program uses innovative research that integrates advances in molecular biology, chemistry, and computer science to more effectively and efficiently rank chemicals based on potential risks. Using CompTox methods and tools, a large number of chemicals can be screened for risks at a small cost in a very short amount of time.

CompTox has a package of decision-support tools that provide information about chemical risk, hazard and exposure. Many of these tools are publically available.

ACToR (Aggregated Computational Toxicology Online Resource) is EPA's online warehouse of all publicly available chemical toxicity data and can be used to find data about potential chemical risks to human health and the environment. ACToR aggregates data from over 650 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query a specific chemical and find all available public hazard, exposure and risk assessment data as well as previously unpublished studies related to cancer, reproductive and developmental toxicity.





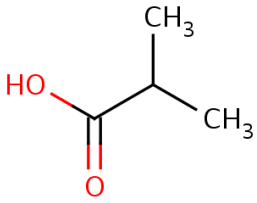
ACToR allows users to search and query data from other EPA chemical toxicity databases including: **ToxRefDB** (30 years and $2 billion worth of animal toxicity studies), **DSSTox** (provides high quality chemical structures and annotations), **ToxCastDB** (data from screening ToxCast chemicals in over 500 high-throughput assays) and **ExpoCastDB** consolidates human exposure data from observational studies that have collected chemical measurements from homes and child care centers.

ToxRefDB allows scientists and the interested public to search and download thousands of animal toxicity testing results on hundreds of chemicals that were previously found only in paper documents.

ToxRefDB contains animal toxicity information that when combined with other sources of information, such as exposure and metabolism,

Chemical Toxicity Databases

form the basis for pesticide risk assessments.



The DSSTox database provides a public forum for publishing downloadable, structure-searchable, standardized chemical structure files associated with toxicity data developed from available structure-viewing freeware and open-source programming tools. It delivers a simple, easy-to-use structure-searching capability through the chemical inventory of published DSSTox data files.

Using ToxCastDB, scientists and others who are interested can access data resulting from another EPA chemical screening tool called ToxCast™. ToxCast™ is a multi-year, multi-million dollar effort that uses advanced science tools to help efficiently understand biological processes impacted by chemicals that may lead to adverse health effects.

ToxCast™ currently includes 500 fast, automated chemical screening tests that are currently assessing 1,000 environmental chemicals.

ToxCastDB provides access to all ToxCast data. Users can search and download data for all ToxCast chemicals, assays, genes, pathways and endpoints. The database allows for associations and biologically driven data mining. It also provides links to available animal data through ToxRefDB.

ExpoCastDB users can obtain summary statistics of exposure data and download datasets. Exposure data currently available online come from three EPA 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. EPA will continue to add internal and external chemical exposure data and advanced user interface features to ExpoCastDB.

ACToR allows users to take advantage of this linkage to find and download these results.

Collaboration Opportunities

The CompTox Research Program partners and collaborates with EPA regions and program offices, industry, academia, trade associations, other federal agencies, state and local government agencies and non-governmental organizations with an interest in revolutionizing the current approach to assessing chemical toxicity risk to humans and the environment. Collaboration opportunities include a Communities of Practice group and different types of agreements that facilitate the sharing of research data and studies.

The CompTox program goal is to provide fast, automated tests for screening and assessing chemical exposure, hazard and risk. Housed within EPA's Office of Research and Development, CompTox is composed of three main elements. The largest component is the National Center for Computational Toxicology (NCCT), which was established in 2005 to coordinate research on chemical screening and prioritization, informatics and systems modeling.

The second element consists of research in EPA's National Health and Environmental Effects Research Laboratory (NHEERL) and National Exposure Research Laboratory (NERL). The final components are the academic centers working on various aspects of computational toxicology funded by EPA's Science to Achieve Results (STAR) program.

Other CompTox decision support tools and research projects include ExpoCast, Virtual Liver, Virtual Embryo, ToxPi and Tox21.

For more information:

ToxRefDB:
http://actor.epa.gov/toxrefdb
ToxCastDB:
http://actor.epa.gov/actor/faces/ToxMiner/Home.jsp
ExpoCastDB:
http://actor.epa.gov/actor/faces/ExpoCast/Home.jsp
DSSTox:
http://epa.gov/ncct/dsstox/

Contact:

National Center for Computational Toxicology

David Dix
Deputy Director
dix.david@epa.gov

Monica Linnenbrink
Public Affairs Specialist
linnenbrink.monica@epa.gov

Main Office: 919·541·4219
www.epa.gov/comptox
109 T.W. Alexander Drive (B-205-01)
Research Triangle Park, NC 27711