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Science in ACTION

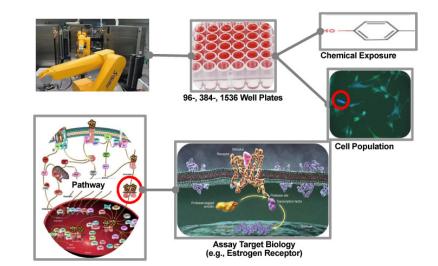
Toxicity Forecaster (ToxCast[™])

SCREENING CHEMICALS TO PREDICT TOXICITY FASTER AND BETTER

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 effectively for risks at a small cost in a very short amount of time.

One developed chemical screening tool is the Toxicity Forecaster (ToxCast[™]). ToxĆast[™] is a multi-year effort that was launched in 2007 to develop a cost-effective approach for prioritizing the thousands of chemicals that need toxicity testing. ToxCast uses advanced science tools to help understand how human body processes are impacted by exposure to chemicals and to determine which exposures are most likely to lead to adverse health effects. ToxCast is being developed in phases. The first phase appropriately called "Proof of Concept" was completed in 2009 and it profiled over 300 researched chemicals (primarily pesticides) in



ToxCast Chemical Screening

over 500 state-of-the-art tests called high-throughput screening assays. The chemicals screened in phase one already had extensive toxicity testing results from traditional chemical tests, mostly animal tests. Having both the ToxCast and animal testing results allows EPA to compare results and determine if both screening processes make similar predictions. Phase two is screening 700 additional chemicals from a broad range of sources including drugs, "green" chemicals, chemicals in cosmetics and other consumer products.

A large contributor to ToxCast[™] is the Tox21 collaboration. Tox21 pools chemical research, data and screening tools from multiple federal agencies including the Food and Drug Administration (FDA), National Toxicology Program/ National Institute of Environmental Health Science and National Human Genome Research Institute/ NIH Chemical Genomics Center to provide additional chemical safety information.

As ToxCast screens more chemicals, EPA will be able to determine which combinations of high-throughput assays are best used as indicators for different types of potential toxicity that can lead to health effects such as chronic diseases or reproductive problems.

Using EPA's online Aggregated Computational Toxicology data warehouse, scientists and others who are interested can search and find all available toxicity testing data including results from ToxCast which can be found in the ToxCast database (ToxCastDB).

ACToR aggregates chemical research data from over 500 public sources on over 500,000 chemicals and links to ToxRefDB which stores the thousands of animal toxicity studies on hundreds of chemicals.

ToxCastDB allows users to search and download data for all ToxCast

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Toxicity Forecaster (ToxCast[™])

chemicals, assays, genes, pathways and endpoints. It allows for associations and biologically driven data mining.

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 tools and research projects include DSSTox, ExpoCast, Virtual Liver, Virtual Embryo, and ToxPi. For more information:

ToxCast: http://epa.gov/ncct/toxcast/ ToxCastDB: http://actor.epa.gov/actor/faces/ ToxMiner/Home.jsp ACTOR: http://actor.epa.gov/actor ToxRefDB: http://actor.epa.gov/toxrefdb

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