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Virtual Tissues Research Project

ADVANCED COMPUTER SIMULATED MODELS OF LIVER & EMBRYO USED TO PREDICT CHEMICAL TOXICITY

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.

It is difficult to conduct research to predict how human health will be impacted long-term by exposure to chemicals. EPA's Virtual Liver and Embryo projects are researching how to use advanced computer models to simulate how chemicals may affect these systems. The traditional method of exploring how chemicals affect humans is done using controlled tests on pregnant laboratory animals. While these practices provide valuable information, they can be both costly and slow. Reliance on them is one reason the pace of testing has not kept up with the development of commercial chemicals, leaving significant data gaps.

Since the liver frequently shows the earliest signs of injury, the Virtual Liver (v-Liver™) project is researching how to simulate liver function that can be used to help predict the effects of chemicals in humans. The idea is to have a cell-based model that works to simulate chemical actions in the liver in order to estimate how much of a chemical it takes to lead to health-related effects, such as liver disease and cancer.

Currently, v-Liver is using a selection of every day chemical contaminants with known human health effects to develop proof that it can be used to predict the potential for chemicals to cause diseases. It organizes evidence about biological networks to clarify the toxic effects of new chemicals (mechanism of action).

v-Liver plans to use fast, automated chemical screening data from EPA's Toxicity Forecaster (ToxCast™) and other chemical data to simulate how chemicals could cause liver toxicity.

ToxCast™ 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™ currently includes 500 fast, automated chemical screens called high-throughput assays that are assessing 1,000 chemicals.

Other computer simulated models being developed are the Virtual Embryo (v-Embryo™) models. v-Embryo models will provide insights into how pregnant mother's exposures to chemicals in the environment might affect prenatal development. The development of an embryo, from conception to birth, includes a highly coordinated sequence of cellular behaviors and interactions. While that process goes perfectly the vast majority of the time, at least three percent of babies are born each year with some observable malformation or developmental condition that may permanently shape the life of the child.

The Virtual Tissues team includes an interdisciplinary team of toxicologists, computer engineers, programmers, bioinformaticians, biologists, mathematicians, and other experts. The team aims to use a selection of everyday chemicals with known health effects in animals to develop methods to use vast collections of data, biological knowledgebases and high-tech computer modeling to build computer-based virtual models.

The Virtual Tissue research project works with EPA scientists and outside partners, including contractors, academia, industry, and other governmental agencies.

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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, ACTor, ToxRefDB and ToxPi.

For more information:

Virtual Liver:
www.epa.gov/ncct/virtual_liver
Virtual Embryo:
www.epa.gov/ncct/v-Embryo

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