

Abstract for invited presentation at Dalton College, GA to the Alliance for Innovation & Sustainability, April 20, 2017.

U.S. EPA's Computational Toxicology Program: Innovation Powered by Chemistry

It is estimated that tens of thousands of commercial and industrial chemicals are present in the environment, and many thousands more are produced through environmental degradation and biotransformation. Traditional animal toxicity studies are slow, expensive, and increasingly controversial, both in terms of animal use and relevance to humans. As a result, toxicity data and exposure estimates are lacking for the vast majority of chemicals that enter commerce and the environment through human activity. The ToxCast program within EPA's National Center for Computational Toxicology, and a related multi-federal agency Tox21 program, are spearheading the use of modern high-throughput chemical screening methods and innovative computational modeling approaches to fill data gaps and better prioritize research and testing resources. These research programs, which are accompanied by full public release of data, models, and web-access tools, are effectively transforming toxicology practice in the 21st century. Chemistry and cheminformatics, in turn, are the twin engines powering ToxCast, Tox21 and the full range of computational toxicology modeling projects within EPA. This talk will provide a broad overview of EPA's CompTox program, with particular focus on the pivotal role that chemistry and cheminformatics are playing in the generation, interpretation, and dissemination of data. *This abstract does not necessarily reflect U.S. EPA policy.*