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Abstract No. 4

Title:
The EPA Comptox Chemistry Dashboard: A Web-Based Data Integration Hub for Environmental Chemistry and Toxicology Data

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The U.S. Environmental Protection Agency (EPA) Computational Toxicology Program integrate advances in biology, chemistry, exposure and computer science to help prioritize chemicals for further research based on potential human health risks. This work involves computational and data driven approaches that integrate chemistry, exposure and biological data. As an outcome of these efforts the National Center for Computational Toxicology (NCCT) has measured, assembled and delivered an enormous quantity and diversity of data for the environmental sciences including high-throughput in vitro screening data, legacy in vivo animal data, consumer use and production information, exposure models and chemical structure databases with associated properties. A series of software applications and databases have been produced over the past decade to deliver these data, but recent developments have focused on the development of a new software architecture that assembles the resources into a single platform. Our web application, the CompTox Chemistry Dashboard provides access to data associated with ~750,000 chemical substances. These data include experimental and predicted physicochemical property data, bioassay screening data associated with the ToxCast program, product and functional use information and a myriad of related data of value to environmental scientists.

The dashboard provides chemical-based searching based on chemical names, synonyms and CAS Registry Numbers. Flexible search capabilities allow for chemical identification based on non-targeted analysis studies using mass spectrometry. Chemical identification using both mass and formula-based searching utilizes rank-ordering of results via functional use statistics, thereby providing a solution to help prioritize chemicals for further review when detected in environmental media.

This presentation will provide an overview of the dashboard, its capabilities for delivering data to the environmental chemistry community and how the architecture provides a foundation for the development of additional applications to support chemical risk assessment. This abstract does not reflect U.S. EPA policy.