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Invited oral presentation to: Division of Chemical Information (CINF) Session entitled "Chemical Text Mining & Public Molecular Databases", co-chaired by Alex Tropsha and Antony Williams

U.S. EPA computational toxicology programs: Central role of chemical-annotation efforts and molecular databases

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EPA's National Center for Computational Toxicology is engaged in high-profile research efforts to improve the ability to more efficiently and effectively prioritize and screen thousands of environmental chemicals for potential toxicity. A central component of these efforts involves the construction and integration of top-level chemically indexed, structure-searchable databases of historical toxicology data, including: 1) high quality structure-annotated toxicity data files from public resources (DSSTox); 2) a relational database of detailed toxicology studies from EPA regulatory programs (ToxRef DB); and 3) a publicly available relational database broadly spanning chemical data resources pertaining to environmental toxicology on the Internet (ACToR). Challenges of chemical structure annotation and indexing of public resources broadly pertaining to environmental toxicology will be described, highlighting DSSTox, ACToR, and recent efforts to annotate and publish chemical (treatment)-experiment index files for the primary public microarray database repositories, GEO and ArrayExpress. *This abstract does not necessarily reflect EPA policy.*

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