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New Toxico-Cheminformatics & Computational Toxicology Initiatives at EPA

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EPA's National Center for Computational Toxicology is building capabilities to support a new paradigm for toxicity screening and prediction. The DSSTox project is improving public access to quality structure-annotated chemical toxicity information in less summarized forms than traditionally employed in SAR modeling, and in ways that facilitate data-mining, and data read-across. The DSSTox Structure-Browser provides structure searchability across all published DSSTox toxicity-related inventory, and is enabling linkages between previously isolated toxicity data resources. As of early March 2008, the public DSSTox inventory has been integrated into PubChem, allowing a user to take full advantage of PubChem structure-activity and bioassay clustering features. The most recent DSSTox version of the Carcinogenic Potency Database file (CPDBAS) illustrates ways in which various summary definitions of carcinogenic activity can be employed in modeling and data mining. Phase I of the ToxCast™ project is generating high-throughput screening data from several hundred biochemical and cell-based assays for a set of 320 chemicals, mostly pesticide actives, with rich toxicology profiles. Incorporating and expanding traditional SAR concepts into this new high-throughput and data-rich world pose conceptual and practical challenges, but also holds great promise for improving predictive capabilities.
This work was reviewed by EPA and approved for publication, but does not necessarily reflect EPA policy.