

A Developmental Toxicity Database to Support Computational Toxicology; A Collaborative Project for Data Sharing and Harmonization

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Developmental toxicity is one of the most important non-cancer endpoints for both environmental and human health. Despite the fact that numerous developmental studies are being conducted, as required for regulatory decisions, there are not yet sufficient data available to develop robust computational methods. The SAR team at the Food and Drug Administration's (FDA) Center for Food Safety and Applied Nutrition (CFSAN) has been involved in developing ToxML (a toxicity database schema) and toxicity databases. In the Environmental Protection Agency (EPA), a database team at the National Center for Computational Toxicology implemented ToxRefDB with its data model inspired by ToxML. The new initiative at FDA CFSAN to build an institutional knowledge-base, the CERES (Chemical Evaluation and Risk Estimation System) project, has imposed the need to generate another database model for the Center's regulation data. The prospect of creating yet another toxicity data model was a real concern; hence, as part of the CERES project, an experiment has been conducted at FDA CFSAN to adopt EPA's ToxRefDB data entry tool to capture diverse effects from FDA's approved drugs. In further collaboration with National Institute of Child Health and Human Development (NICHD, NIH), we now have captured developmental data on 80 additional drugs at dose-response level. By incorporating pharmaceuticals data into the current agrochemical domain, both the chemical space and biological profiles are expanded. This experiment also assisted our database modeling while expanding and harmonizing the controlled vocabulary. It is our further goal to merge the data with previously prepared developmental toxicity databases to support computational method development. This poster will present comparisons of developmental toxicity data models, profiles of distinct and common effects, and the chemical domains in both ToxRefDB and CERES. *This abstract does not necessarily reflect U.S. EPA policy.*