Appendix A, Part 4: CSS Models, databases, and tools

Below are models, databases, and tools affiliated with the CSS program, and having undergone significant updates in 2019 or 2020.

The CompTox Chemicals Dashboard is a publicly available web-based application to provide access to chemistry, toxicity and exposure information for ~900,000 chemicals. The data and predictive models within the Dashboard support the Agency's efforts to identify chemicals that are most in need of further testing with the intention of reducing the use of animals in research and in keeping with the mission of the agency. In addition, *in silico* models facilitate the prediction of hazard properties of chemicals for which *in vivo* data are not available. *Last updated July 2020*

The Chemicals and Products Database (CPDat) is an integrated family of exposure databases, linking data across multiple different exposure data streams. The database includes qualitative and quantitative product specific, general use, functional use, and multimedia monitoring measurements for over 29,391 unique chemical structures. The data is available through the CompTox Chemicals Dashboard.

Last updated January 2021

The Chemical Transformation Simulator (CTS) is a web-based tool for predicting environmental and biological transformation pathways and physicochemical properties of organic chemicals.

Last updated August 2020

The ECOTOXicology knowledgebase (ECOTOX) is a comprehensive, publicly available knowledgebase providing single chemical environmental toxicity data. ECOTOX integrates three previously independent databases – AQUIRE, PHYTOTOX, and TERRETOX – into a unique system which includes toxicity data derived predominately from the peer-reviewed literature, for aquatic life, terrestrial plants, and terrestrial wildlife, respectively.

Last updated December 2020

httk: The R package 'httk,' available on CRAN, provides generic models and chemical-specific data for simulation and statistical analysis of chemical high throughput toxicokinetics, as described by Pearce at al.

Last updated September 2020

toxEval: The R package 'toxEval,' available on CRAN, is a data analysis package for estimating potential biological effects from chemical concentrations in environmental samples. Included are a set of functions to analyze, visualize, and organize measured concentration data as it relates to user-selected chemical-biological interaction benchmark data such as water quality criteria.

Last updated October 2020

The Sequence Alignment to Predict Across Species Susceptibility (SeqAPASS) is an online screening tool that allows researchers and regulators to extrapolate toxicity information across species. SeqAPASS extrapolates from data rich model organisms (e.g. humans, mice, rats, and zebrafish) to thousands of other non-target species to evaluate their specific potential chemical susceptibility.

Last updated November 2020

The Species Sensitivity Distribution (SSD) Toolbox is a common tool used for setting safe limits on chemical concentrations in surface waters. The SSD toolbox has aggregated a variety of algorithms to support users in fitting, summarizing, visualizing and interpreting SSDs to assist with this process.

Last updated November 2020

The Standardized Emission and Waste Inventories (StEWI) is a collection of Python modules that provide processed US EPA emission and waste generation inventory data in standard tabular formats.

Last updated December 2020

The Stochastic Human Exposure and Dose Simulation: High-Throughput (SHEDS-HT) model is a screening model for estimating human exposure to a thousands of chemicals in a rapid and cost efficient manner. The model is stochastic, and cross-sectional (producing exposure estimates for a single 24-hr period for each individual in the target population).

Last updated August 2019