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Title:
Real-time prediction of Physicochemical and Toxicological Endpoints Using the Web-based CompTox Chemistry Dashboard

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Abstract: The EPA CompTox Chemistry Dashboard developed by the National Center for Computational Toxicology (NCCT) provides access to data for ~750,000 chemical substances. The data include experimental and predicted data for physicochemical, environmental fate and transport and toxicological endpoints. Predicted data have been harvested from open data sources as well as generated using available online web services (for example EPI Suite), our EPA-NCCT OPERA models and using the EPA Toxicity Estimation Software Tool (T.E.S.T). Both OPERA and T.E.S.T utilize QSAR (Quantitative Structure Activity Relationship) models based on 2D molecular descriptors. While this offers access to a rich aggregation of data these are limited to pre-predicted data and limited to the chemicals included on the dashboard. This presentation will provide an overview of our efforts to provide real-time prediction (for single chemicals or chemical sets), using publicly available web services and our own open prediction models from the EPA. These models provide the community access to predictions for physicochemical, fate and transport and toxicological endpoints that can be used for the purpose of hazard, risk and exposure assessment and to support read - across applications. This abstract does not reflect U.S. EPA policy.