New developments in delivering public access to data from the National Center for Computational Toxicology at the EPA

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Abstract: Researchers at EPA's National Center for Computational Toxicology integrate advances in biology, chemistry, and computer science to examine the toxicity of chemicals and help prioritize chemicals for further research based on potential human health risks. The goal of this research program is to quickly evaluate thousands of chemicals, but at a much reduced cost and shorter time frame relative to traditional approaches. The data generated by the Center includes characterization of thousands of chemicals across hundreds of high-throughput screening assays, consumer use and production information, pharmacokinetic properties, literature data, physical-chemical properties as well as the predictive computational modeling of toxicity and exposure. We have developed a number of databases and applications to deliver the data to the public, academic community, industry stakeholders, and regulators. This presentation will provide an overview of our work to develop an architecture that integrates diverse large-scale data from the chemical and biological domains, our approaches to disseminate these data, and the delivery of models supporting predictive computational toxicology. In particular, this presentation will review our new CompTox Chemistry Dashboard and the developing architecture to support real-time property and toxicity endpoint prediction. *This abstract does not reflect U.S. EPA policy.*