American Chemical Society Fall meeting, Aug. 21-25, Philadelphia, Penn.

TOXI session: **Computational Chemistry & Toxicology in Chemical Discovery & Assessment (QSARs)-Oral**

Session Outline: Testing chemicals for performance/efficacy, toxicologic effects, and environmental fate is expensive and time consuming. Decisions to conduct such studies often involve cost/benefit evaluations leading to limitations on the data that can be developed. In addition, environmental professionals in recent years have been trying to reduce the numbers of test animals used in toxicologic studies, for ethical and cost reasons. Elucidating the toxicologic mechanism by which a chemical acts with experimental data can be difficult, expensive, and ultimately, equivocal. Finally, scientists often have to predict risks based on little or no data on chemicals and their metabolites in the context of the environmental statutes Toxic Substances Control Act (TSCA) and Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA). The goal of computational chemistry and toxicology is to meet these needs, at least partially. This general approach can involve the use of quantum chemistry to model toxicologic initiating events at the molecular level. Quantitative structure activity relationships (QSARs) can be used to predict environmental fate and adverse effects of a chemical. Thus the purpose of this symposium is to present papers on accomplishments and challenges in this field. A related goal is to consider where this prediction methodology will be in five to ten years.

Abstract Title: Delivering The Benefits of Chemical-Biological Integration in Computational Toxicology at the EPA

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Abstract: Researchers at the 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 intention of this research program is to quickly evaluate thousands of chemicals for potential risk but with much reduced cost relative to historical approaches. This work involves computational and data driven approaches including high-throughput screening, modeling, text-mining and the integration of chemistry, exposure and biological data. We have developed a number of databases and applications that are delivering on the vision of developing a deeper understanding of chemicals and their effects on exposure and biological processes that are supporting a large community of scientists in their research efforts. This presentation will provide an overview of our work to bring together diverse large scale data from the chemical and biological domains, our approaches to integrate and disseminate these data, and the delivery of models supporting computational toxicology. *This abstract does not reflect U.S. EPA policy.*