Chemoinformatic and Bioinformatic Challenges at the US Environmental Protection Agency. Robert Kavlock, National Center for Computational Toxicology, Office of Research and Development, US Environmental Protection Agency, Research Triangle Park, NC

The US EPA is faced with a number of challenges in establishing priorities for screening and testing of agents and for improving the efficiency and effectiveness of the processes by which the risk of chemicals to human and environmental health are assessed. Traditionally, the hazards and risks of chemicals has been approached chemical by chemical, but with the numbers of chemicals needing scrutiny now vastly outstripping the capacity to evaluate them by conventional tests, new approaches are being eagerly sought by the regulatory offices within EPA such as the pesticide program, the toxic substances program, and the drinking water program. Recent advances in molecular biology and chemistry, coupled with increasingly powerful computational tools provide opportunities to introduce new thinking into these problems. To help accelerate the use of new approaches in its mission, the EPA initiated a computational toxicology program (see www.epa.gov/comptox) and established the National Center for Computational Toxicology (NCCT) to carry out supporting research. This presentation will provide an overview of both the scientific program and the regulatory activities related to computational toxicology. To build the foundation for the transition to new approaches to hazard and risk assessment, a number of research projects are underway that are (1) helping to build improved linkages between the steps in the "source to outcome paradigm" (the processes by which a chemical is released into the environment, is transported and modified, comes in contact with an organism, travels to the site of potential toxicity and induces an adverse health); (2) improving information technology and utilizing multiplexed high throughput screening techniques to fingerprint the biological activity of chemicals, and (3) developing computational tools that reduce the uncertainties in the extrapolation of data across the dose-response range, across species, and across chemicals. On the regulatory side, cross Agency workgroups have been examining where genomic type data is likely to be first used by the EPA, how the data will be accepted, analyzed, interpreted and stored. The union of computational chemistry tools and advances in molecular biology, combined with informatic approaches offers the possibility to address many critical needs of protecting human health and the environment in a coordinated, efficient manner. This is an abstract of a proposed presentation, and does not necessarily reflect Agency policy.