Computational Toxicology: New Approaches to Improve Environmental Health Protection

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The mission of the U.S. Environmental Protection Agency is to safeguard public health and the environment from harmful effects that may be caused by exposure to pollutants in the air, water, soil, and food. Protecting human health and the environment carries with it the challenge of assessing the risk that is posed by tens of thousands of chemicals. The large number of chemicals that the Agency must evaluate and the many different legal statutes that regulate chemicals have traditionally made it impossible for the Agency to evaluate every chemical with the most rigorous testing strategies. Instead, standard toxicity tests have been limited to only a small number of chemicals. Today, however, the young field of computational biology offers the possibility that, with advances in computational biology's subdisciplines (e.g., genomics, proteomics, metabonomics and bioinformatics), scientists may have the ability to develop a more detailed understanding of the risks posed by a much larger number of chemicals. The application of the tools of computational biology to assess the risk chemicals pose to human health and the environment is termed *Computational Toxicology*. EPA defines computational toxicology as the application of mathematical and computer models to predict adverse effects and to better understand the mechanism(s) through which a given chemical induces harm. Three strategic objectives of the computational toxicology initiative are to: (1) improve understanding of the linkages in the continuum between the source of a chemical in the environment and adverse outcomes; (2) provide predictive models for screening and testing; and (3) improve quantitative risk assessment. Three research projects will used to illustrate the computational toxicology approach. The first employs the use of physiologically based pharmacokinetic models to understand chemical deposition across life stages, the second entails construction of predictive fingerprints of chemical toxicity through the use of high throughput bioassays; and the third involves development of a computational model of the liver. The outputs of these projects offer the potential to significantly improve the current processes of hazard and risk assessment. This is an abstract of a proposed presentation and does not necessarily represent EPA policy.