Abstract submitted for International Science Forum on Computational Toxicology
RTP, NC May 21-23, 2007

Computational Toxicology – Where is the Data?

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One goal of the field of Computational Toxicology is to predict chemical toxicity by combining computer models with biological and toxicological data. To achieve this goal, there is a need for large amounts of diverse, high quality, curated data that is easily accessible by modelers. Individual data sets are available from a variety of sources including academic groups, government agencies such as the EPA and NIH and companies. One problem is that much of this data is text-based, rather than being quantitative and tabular, and therefore ready for use by modelers and statisticians. This talk will briefly describe the state of the data world for computational toxicology and one approach to improve the situation, called ACToR (Aggregated Computational Toxicology Resource). ACToR will serve as a repository for a variety of types of quantitative chemical, biological and toxicological data that can be used for predictive modeling of chemical toxicology. ACToR is comprised of several independent databases, tied together through links to a common database of chemical structures and properties. The main databases cover biochemical (HTS) and cell-based assays, detailed *in vivo* toxicology data (ToxRefDB), experimental design information, genomics (mainly microarray) data, and reference information on genes and pathways. The system is collecting information from multiple sources both within and external to the EPA. Users will be able to access data through the web, initially on the EPA Intranet. The first use of ACToR will be to provide a repository and context for data from the ToxCast program, whose goal is to use in vitro biochemical and genomics assays to prioritize environmental chemicals for further testing.