Computational Toxicology at the US EPA

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Computational toxicology is the application of mathematical and computer models to help assess chemical hazards and risks to human health and the environment. Supported by advances in informatics, high-throughput screening (HTS) technologies, and systems biology, EPA is developing robust and flexible computational tools that can be applied to the thousands of chemicals in commerce, and contaminant mixtures found in America's air, water, and hazardous-waste sites. The ORD Computational Toxicology Research Program (CTRP) is composed of three main elements. The largest component is the National Center for Computational Toxicology (NCCT), which was established in 2005 to coordinate research on chemical screening and prioritization, informatics, and systems modeling. The second element consists of related activities in the National Health and Environmental Effects Research Laboratory (NHEERL) and the National Exposure Research Laboratory (NERL). The third and final component consists of academic centers working on various aspects of computational toxicology and funded by the EPA Science to Achieve Results (STAR) program. Key intramural projects of the CTRP include digitizing legacy toxicity testing information toxicity reference database (ToxRefDB), predicting toxicity (ToxCast™) and exposure (ExpoCast™), and creating virtual liver (v-Liver™) and virtual embryo (v-Embryo™) systems models. The models and underlying data are being made publicly available through the Aggregated Computational Toxicology Resource (ACToR), the Distributed Structure-Searchable Toxicity (DSSTox) Database Network, and other EPA websites. The CTRP will be a critical component in next generation risk assessments utilizing quantitative high-throughput data and providing a much higher capacity for assessing chemical toxicity than is currently available. *This is an abstract of a proposed presentation.*