TERATOLOGY SOCIETY
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ILSI HESI Workshop: Redesigning the Embryo-Fetal Developmental Toxicity Study: Evolution or Revolution? (Invited Talk)

In vitro data and *in silico* models for computational toxicology. Knudsen Thomas B. USEPA, National Center for Computational Toxicology, Research Triangle Park, NC.

The challenge of assessing the potential developmental health risks for the tens of thousands of environmental chemicals is beyond the capacity for resource-intensive animal protocols. Large data streams coming from high-throughput (HTS) and high-content (HCS) profiling of biological activities, coupled with machine-learning algorithms, literature-mining tools, and systems modeling, is a newer paradigm to toxicity testing in the 21st century (TT21). Newer resources are available to measure molecular components of cellular and tissue-level phenomena in great depth and detail. HTS/HCS data now in-hand (ToxCast/Tox21), 'evolution' implies the advancement of best practices and computational approaches to assemble the individual pieces into an integrative model that: scales to the human exposure universe; incorporates extant knowledge of human embryology; and deals probabilistically with spatiotemporal dynamics in a morphogenetic series of events. With the advent of computational approaches and computer models fit for that purpose, 'revolution' implies their continued refinement and cohesion to satisfy the fundamental principles of teratology: chemical structure, dosimetry, initiating mechanism(s), genetic susceptibility, stage specificity, and bioavailability. This presentation will provide examples of how *in vitro* data and *in silico* models can be integrated with biological knowledge to simulate how embryos might react to diverse exposure scenarios. [This abstract does not reflect US EPA policy].