

*In silico* dynamic models for developmental toxicity

Thomas Knudsen, PhD

National Center for Computational Toxicology, US EPA, Research Triangle Park, NC

Computer modeling and simulation of complex dynamical systems can provide a virtual framework for translating biomolecular lesions into critical phenomena underlying developmental processes and toxicities. *In silico* cell agent-based models (ABMs) may be executed to simulate how biomolecular lesions from *in vitro* HTS datasets (ToxCast) might propagate through a morphogenetic series of events to yield an adverse effect based on current theory as to molecular pathways and cellular processes that drive human embryology and development. The concept of testing a 'virtual embryo' will be demonstrated utilizing case studies tying the *in vitro* data and *in silico* models to fundamental principles of teratogenesis. *This work does not reflect EPA policy.*