Chemical Exploration: Providing Biological Context for NAMs

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New approach methodologies (NAMs) use in vitro and in silico models to predict toxicity based on a chemical's bioactivity and molecular properties. The National Toxicity Program (NTP) Interagency Center for the Evaluation of Alternative Toxicological Methods' (NICEATM) Integrated Chemical Environment (ICE) provides easy access to data and tools needed to explore and contextualize chemical bioactivity profiles. ICE Search provides summary-level information, curated reference data, and bioactivity details for chemicals and mixtures. Bioactivity can be further examined using the Curve Surfer tool to explore concentration-response relationships of curated high-throughput assays. ICE's IVIVE tool allows users to translate in vitro bioactivity profiles to estimated equivalent in vivo doses for different exposure routes. The new physiologically based pharmacokinetics (PBPK) tool predicts tissue-level concentrations resulting from in vivo doses. A new ICE feature allows users to explore ICE's database of >800,000 chemicals through a SMILES similarity search, providing information on target chemicals and those with similar structures. These similar chemicals can then be piped into any ICE tools, expanding available information. Additionally, ICE links to the NTP's Chemical Effects in Biological Systems and the U.S. Environmental Protection Agency's Chemical and Products Database, expanding ICE's capacity to examine and compare chemicals based on physicochemical properties, bioactivity, and product use categories. This presentation will use case studies to provide an overview of the tools and features available in ICE for chemical analyses and comparisons. This project was funded in whole or in part with federal funds from the NIEHS, NIH under Contract No. HHSN273201500010C.