NICEATM Computational Tools and Resources Supporting Alternative Test Method Development and Evaluation

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The NTP Interagency Center for the Evaluation of Alternative Toxicological Methods (NICEATM) provides computational tools and resources developed in partnership with federal agencies, industry, and academia to support creation and evaluation of alternatives to animal use for chemical safety testing. This presentation highlights two resources that make data and computational tools more accessible to our stakeholders. The Open Structure-activity/property Relationship App (OPERA) provides QSAR models to predict properties often needed in modeling. OPERA also includes consensus models built using global collaborative crowdsourcing approaches for toxicity endpoints such as estrogen and androgen receptor pathway activity and acute oral systemic toxicity (LD50) and hazard categories. The Integrated Chemical Environment (ICE) is an online database that provides users access to in vivo, in vitro, and in silico data for a range of toxicity endpoints, including curated Tox21 high-throughput screening data for >9,000 chemicals and OPERA predictions for >800,000 chemicals. The ICE web-based in vitro to in vivo extrapolation tool allows users to translate in vitro bioactivity concentrations to predicted exposures and compare those with doses from in vivo studies. A chemical characterization tool allows users to view and compare predicted chemical properties, using principal component analysis and interactive plots. ICE also provides curated lists of reference chemicals with known effects along with their supporting data. Features of both tools and example use cases in the context of chemical evaluations will be presented. This project was funded in whole or in part with federal funds from the NIEHS, NIH under Contract No. HHSN273201500010C.