

User-friendly Toxicology Tools from ICE Workflows

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Developing and evaluating new approaches to chemical safety testing require quality data and supporting information such as chemical properties and key modeling parameters. These activities also require tools that can put assay data into the appropriate biological context and determine whether a given dataset is appropriate for evaluating a method of interest. To address these needs, the NTP Interagency Center for the Evaluation of Alternative Toxicological Methods (NICEATM) developed the Integrated Chemical Environment (ICE) to house high-quality, curated in vivo data along with in vitro and in silico values for a range of endpoints. In this presentation, we announce the launch of ICE Workflows, which support chemical characterization, assist in data analysis and model building, and enable direct comparisons between in vitro assay data and relevant in vivo endpoints. ICE Workflows are a series of interactive tools that allow users to use ICE data to characterize the chemical space covered by their chemical lists, perform basic machine learning functionality, and generate in vitro to in vivo extrapolation predictions. Leveraging the ICE ontology, users can easily identify assays and data points within ICE that are relevant to their toxicological outcome of interest. This facilitates exploration of data and hypothesis generation for users without a strong background in computational toxicology. Future functionalities to be added will also be discussed, including input of user-supplied data. ICE was funded with U.S. federal funds from the NIEHS/NIH/HHS under Contract HHSN273201500010C.