Facilitating Chemical Evaluation and Data Exploration with the Integrated Chemical Environment

S. Bell*, J. Phillips**, X. Chang*, R. Rai*, A. Karmaus*, F. Hermes*, K. Mansouri*, D. Allen*, W. Casey***, N. Kleinstreuer***

ILS, Research Triangle Park, NC, USA

**Sciome LLC, Research Triangle Park, NC, USA*

***NIH/NIEHS/DNTP/NICEATM, Research Triangle Park, NC, USA*

Currently, toxicity testing utilizes a complex suite of approaches to understand the interactions between test substance and target organism. Traditionally, such evaluations have relied upon results from in vivo models; new approaches can now integrate in vitro testing, ex vivo testing, in silico predictions and computational tools to inform the decision process. These approaches require readily available, well-characterized data that is relevant to the toxicity under investigation. Launched in 2017, the Integrated Chemical Environment (ICE) is the source for curated and toxicologically relevant data from the NTP Interagency Center for the Evaluation of Alternative Test Methods (NICEATM) and federal agency stakeholders and partners. To better support the needs of method developers and risk assessors, ICE updates have included new features aimed at making data exploration easier. In this presentation, we describe changes to the search function and other computational tools targeted to toxicologists and risk assessors who may not have ready access to computational toxicology resources. Key among the updates is the expanded in vitro to in vivo extrapolation (IVIVE) tool that allows users to access some of EPA's httk models using the ICE web interface. A simple case study will show how to retrieve Tox21 data relevant to in vivo endpoints and apply IVIVE workflows and other ICE tools. The case study will emphasize the applicability of ICE for a practical use case, demonstrate ease of use, and provide suggestions for data interpretation. ICE was supported with federal funds from the NIEHS, NIH under Contract No. HHSN273201500010C.