

Facilitating NAM-Based Chemical Assessments with the Integrated Chemical Environment

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The National Toxicology Program's Integrated Chemical Environment (ICE, <https://ice.ntp.niehs.nih.gov/>) provides highly curated data and computational tools to facilitate the exploration, characterization, and interpretation of chemicals use, exposure, and hazard. ICE data and tools are frequently updated to address evolving stakeholder needs. The latest release introduced new datasets, chemical lists, and features that further enhance the capabilities of ICE tools. ICE users can now obtain population-level exposure predictions from the U.S. Environmental Protection Agency's SEEM3 prediction model through the ICE Search tool and the ICE REST API. Exposure estimates can also be compared to the equivalent administered doses predicted by the ICE In Vitro to In Vivo Extrapolation (IVIVE) tool. To support evaluation of new approach methodologies (NAMs) for developmental toxicity, the ICE Physiologically Based Pharmacokinetic (PBPK) and IVIVE tools now include a gestational model from the EPA's htk package (v2.2.2). The release also revised the ICE Chemical Characterization tool, implementing updates to curated chemical product use categories and adding reported and predicted functional use categories. The ICE Search tool now houses a beta Query Summary results tab, which provides summary visualizations to help users contextualize and interactively explore the data based on their specific needs. The presentation will detail these features and demonstrate how ICE can provide user-friendly solutions to navigating complex data and tools as well as contribute to establishing confidence in applying NAMs for chemical assessments. This project was funded with federal funds from the NIEHS, NIH under Contract No. HHSN273201500010C.