The Integrated Chemical Environment (ICE): Advancing Data Availability and Computational Tool Accessibility for the Development, Evaluation, and Application of New Approach Methods

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This presentation describes recent updates to the NTP Interagency Center for the Evaluation of Alternative Toxicological Methods' (NICEATM) Integrated Chemical Environment (ICE, https://ice.ntp.niehs.nih.gov/) and demonstrates the utility of this database and web-based application. ICE is an open-access, user-friendly platform that provides curated toxicologically relevant data and interactive tools to support chemical assessments. Since its inception, ICE has provided reliable and robust data and computational resources in support of advancing new approach methodologies (NAMs) and addressing evolving stakeholder needs. Recent ICE releases (4.0.2 in March 2024 and 4.1 in August 2024) introduced features that enhance data exploration and interpretation capabilities. The Search tool now has a new interface and data visualizations, offering a more intuitive user experience. Users can take advantage of new Chemical Quick Lists across ICE tools to easily identify and evaluate data, including for PFAS chemicals). The curated high throughput screening (cHTS) data curation pipeline now includes flags for potential technological interference based on interactions between chemicals and assay technology. Additionally, cHTS assay annotations have been updated with OBO Foundry-controlled terms to encompass a broader range of biological and toxicological processes. The new cHTS flags and annotations were added to the Curve Surfer tool, which also incorporates activity concentration at cut-off overlay functionality for more focused analysis of concentration-response curves. Finally, users can now access the concentration-response information using the ICE REST API. This project was federally funded by the NIEHS under Contract No. HHSN273201500010C.