

## ICE Data and Tools to Advance NAMs

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The Integrated Chemical Environment (ICE, <https://ice.ntp.niehs.nih.gov/>) provides highly curated toxicologically relevant data and analytical tools for data interpretation and exploration. ICE has made significant contributions to advancing NAMs, with data and tools being continuously updated to address evolving stakeholder needs. ICE version 4.0, released in March 2023, is a major update. ICE users can now obtain general population-level exposure predictions from EPA's SEEM3 model across multiple scenarios through the ICE Search tool and the ICE Search 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 better support development of new methods for developmental toxicity, ICE v.4.0 adds a new gestational model from the EPA's htk package to its Physiologically Based Pharmacokinetic (PBPK) and IVIVE tools. The ICE curated high-throughput screening (cHTS) dataset has been updated with the latest ToxCast and Tox21 data, providing in vitro data to use in bioactivity assessments and computational toxicology workflows. Several new warning flags for autofluorescence interference have been added into the curation workflow. Updates to the underlying chemical use data in the ICE Chemical Characterization tool have also been implemented, with reported and predicted functional use categories now available in addition to consumer use data. The presentation will include case studies to demonstrate how ICE can facilitate building confidence in NAM use for chemical assessments. Project was funded by NIEHS under Contract No. HHSN273201500010C.