

NICEATM Abstract: SOT 2021 Annual Meeting

Providing Context for Chemical Effects Through Bioactivity and Consumer Use

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New approach methodologies (NAMs) use in vitro and in silico models to predict toxicity based on a chemical's bioactivity and molecular properties. Ideally, NAMs are developed and evaluated using well-characterized reference chemicals with defined activity against toxicity endpoints of interest. Structure-based information for chemicals is needed to properly define the domain of applicability for the NAM and to compare chemicals proposed for testing to reference chemicals used to develop and evaluate the NAM. The National Toxicity Program Interagency Center for the Evaluation of Alternative Toxicological Methods (NICEATM) developed the Integrated Chemical Environment (ICE) Chemical Characterization tool to fill this need by allowing users to examine and compare chemicals' structural and chemical properties, bioactivity, and functional use. Recent ICE tool updates allow users to compare these properties to better characterize their chemicals of interest drawn from the ICE chemical database of over 800,000 chemicals. Principal component analysis plots allow users to easily generate visual comparisons based on structural and physicochemical properties between groups of chemicals and to examine which properties drive the separation of chemicals within the space described by the principal components. ICE users can also determine if there are differences in bioactivity that distinguish their chemicals of interest. Additionally, information from the U.S. Environmental Protection Agency's Chemical and Products Database has recently been added to ICE, allowing users to explore functional use categories and see how those relate to the available bioactivity data. This presentation will demonstrate the data users can obtain from the ICE Chemical Characterization tool with an emphasis on the new bioactivity and consumer product features. This project was funded with federal funds from the NIEHS and NIH under Contract No. HHSN273201500010C.