Presentation Abstracts and Background Materials

SCIENTIFIC ADVISORY COMMITTEE ON ALTERNATIVE TOXICOLOGICAL METHODS

Session IV: Computational Resources
Thursday, September 22, 2022

Update on NICEATM Computational Resources

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There is a need for integration and more efficient use of existing data, both from traditional in vivo and new approach methodologies (NAMs). The Integrated Chemical Environment (ICE; https://ice.ntp.niehs.nih.gov/), developed by the National Toxicology Program Interagency Center for the Evaluation of Alternative Methods (NICEATM), is a free online suite that houses curated toxicity and physicochemical property data. Moreover, it provides user-friendly tools to analyze and visualize chemical data including in vitro to in vivo extrapolation, physiologically based pharmacokinetic modeling, and quantitative structure-activity relationship predictions for more than 800,000 chemicals. ICE operates with data that are findable, accessible, interoperable, and reusable (FAIR), an important feature to advance toxicology and establish confidence in NAMs. ICE is constantly evolving to incorporate new tools, improve accessibility and interpretability of data.

Major points

- The importance of FAIR principles to enhance toxicology.
- Demonstration of ICE tools.
- Latest updates and future ideas for ICE.

Background

- An Integrated Chemical Environment to Support 21st-Century Toxicology
- An Integrated Chemical Environment with Tools for Chemical Safety Testing
- Application of New Approach Methodologies: ICE Tools to Support Chemical Evaluations
- Application of an Accessible Interface for Pharmacokinetic Modeling and In Vitro to In Vivo Extrapolation