Utilizing ICE Tools to Expand Chemical Knowledge: Chemical Quest

Jaleh Abedini[1*], Bethany Cook[1], Eric McAfee[2], Jason Phillips[2], Shannon Bell[1], John Rooney[1], David Allen[1], Warren M. Casey[3], and Nicole Kleinstreuer[3]

[1]ILS, Research Triangle Park, NC, USA; [2]Sciome, RTP, NC, USA;
[3]NIH/NIEHS/DNTP/NICEATM, Research Triangle Park, NC, USA

*Presenting author

The National Toxicology Program's Integrated Chemical Environment (ICE) provides easy access to data and tools to explore and contextualize chemical bioactivity. The interactive computational tools in ICE allow users to characterize, analyze, and predict bioactivity for their chemicals of interest. ICE Search provides summary-level information, curated reference data, and bioactivity details for chemicals and mixtures. However, developing an overall picture of potential bioactivity for a chemical can be a difficult challenge if there are limited data available for the chemical. ICE Chemical Quest allows users to explore ICE's database of over 800,000 chemicals through SMILES or 2D renderings, providing information on target chemicals and those with similar structures. Query results are ranked based on the similarity of the fingerprints of the query chemicals with chemicals in the ICE database. ICE returns drawings of all returned structures so the user can evaluate the appropriateness of the output list. These similar chemicals can then be entered into any ICE tool, including the Physiologically Based Pharmacokinetics and In Vitro to In Vivo Extrapolation tools, expanding available information and enhancing queries. This presentation includes case studies to provide an overview of the resources available in ICE for chemical analyses and comparisons. This project was funded with federal funds from the NIEHS, NIH under Contract No. HHSN273201500010C.