Chemical Exploration: Identifying Bioactivity with the Use of Structural Features

B Cook[1*], J Abedini[1], S Bell[1], E McAfee[2], J Phillips[2], D Allen[1], N. Kleinstreuer[3]

[1]*ILS, Research Triangle Park, NC, USA*

[2]*Sciome, RTP, NC, USA*

[3]*NIH/NIEHS/DNTP/NICEATM, Research Triangle Park, NC, USA*

New approach methodologies (NAMs) such as in vitro and in silico technologies facilitate chemical assessments without the use of animals. NAMs are often developed and/or validated using chemicals selected to address a specific set of regulatory or research needs, and as a result may have limited diversity in terms of chemical properties. For users without an extensive chemistry background, it can be difficult to assess how new chemicals proposed for testing in a NAM compare to a set of chemicals used in the NAM's validation. To assist in the development, interpretation, and implementation of NAMs, the National Toxicology Program maintains the Integrated Chemical Environment (ICE), an interactive web-based platform that contains tools and data in support of chemical safety assessment. ICE allows users to explore information on their chemicals of interest and those with similar structures. The Chemical Characterization tool in ICE allows for easy comparisons between two chemical lists by providing a variety of data visualization options. Visualizations based on structure and physicochemical properties are available for >800,000 chemicals in the ICE chemical database. Clustering based on bioactivity is available for a subset of these chemicals. The data that users obtain from ICE can be compared to information found from outside data resources to provide a comprehensive assessment of the chemicals of interest. This presentation will use case studies to provide an overview of the tools and features available in ICE for chemical comparisons. This project funded with federal funds from NIEHS, NIH under Contract No. HHSN273201500010C.