

Structure identification by Mass Spectrometry Non-Targeted Analysis using the US EPA's CompTox Chemistry Dashboard

Antony J. Williams, Andrew D. McEachran, Chris Grulke, Seth Newton, Kristin Isaacs, Katherine Phillips, Nancy Baker and Jon Sobus

Identification of unknowns in mass spectrometry based non-targeted analyses (NTA) requires the integration of complementary pieces of data to arrive at a confident, consensus structure. Researchers use chemical reference databases, spectral matching, fragment prediction tools, retention time prediction tools, and a variety of other data to arrive at tentative, probable, and confirmed, if possible, identifications. With the diverse, robust data contained within the US EPA's CompTox Chemistry Dashboard (<https://comptox.epa.gov>), the goal of this research is to identify and implement a harmonized identification tool and workflow using previously generated chemistry data. Data has been compiled from product use, functional use prediction models, environmental media occurrence prediction models, and PubMed references, among other sources. We will report on our development of a visualization tool whereby users can visualize the relative contribution of identification-based metrics on a list of candidate structures and observe the greatest likelihood of occurrence. These data and visualization tools support NTA identification via the Dashboard and demonstrate an open, accessible tool for all users of HRMS data. *This abstract does not necessarily represent the views or policies of the U.S. Environmental Protection Agency.*