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CHEMISTRY

The EPA iCSS Chemistry Dashboard to Support Compound Identification Using High Resolution Mass Spectrometry Data

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There is a growing need for rapid chemical screening and prioritization to inform regulatory decision-making on thousands of chemicals in the environment. We have previously used high-resolution mass spectrometry to examine household vacuum dust samples using liquid chromatography time-of-flight mass spectrometry (LC-TOF/MS). Using a combination of exact mass, isotope distribution, and isotope spacing, molecular features were matched with a list of chemical formulas from the EPA's Distributed Structure-Searchable Toxicity (DSSTox) database. This has further developed our understanding of how openly available chemical databases, together with the appropriate searches, could be used for the purpose of compound identification. We report here on the utility of the EPA's iCSS Chemistry Dashboard for the purpose of compound identification using searches against a database of over 720,000 chemicals. We also examine the benefits of QSAR prediction for the purpose of retention time prediction to allow for alignment of both chromatographic and mass spectral properties. *This abstract does not reflect U.S. EPA policy.*

The EPA iCSS Chemistry Dashboard to Support Compound Identification Using High Resolut\nion Mass Spectrometry Data from **US Environmental Protection Agency (EPA)**

THis work is relevant to the article: "Linking high resolution mass spectrometry data with exposure and toxicity forecasts to advance high-throughput environmental monitoring" DOI: http://dx.doi.org/10.1016/j.envint.2015.12.008