American Chemical Society Fall meeting, Aug. 21-25, Philadelphia, Penn.

ANYL session: **Emerging Mass Spectrometry Trends in Support of Agricultural Research & Development**

Session Outline "Advances in instrumentation have been one of the most important drivers in the way we conduct agricultural research and development. Newer mass spectrometer instrumentation has provided better analyte selectivity, better sensitivity, and higher sample throughput. Instruments incorporating accurate mass and high mass resolution capabilities will significantly impact how studies are analyzed. As instrument costs have dropped, these instruments are now more available to laboratories in industry, CROs, and academia. Laboratories are incorporating accurate mass technology into all aspects of agricultural R&D ranging from product discovery and development, product registration, and monitoring of food and environmental samples.**"**

Associated Abstract Title: Structure Identification Using High Resolution Mass Spectrometry Data and the EPA's Chemistry Dashboard

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Abstract: The iCSS Chemistry Dashboard is a publicly accessible dashboard provided by the National Center for Computation Toxicology at the US-EPA. It serves a number of purposes, including providing a chemistry database underpinning many of our public-facing projects (e.g. ToxCast and ExpoCast). The available data and searches provide a valuable path to structure identification using mass spectrometry as the source data. With an underlying database of over 720,000 chemicals, the dashboard has already been used to assist in identifying chemicals present in house dust. However, it can also be applied to many other purposes, e.g., the identification of agrochemicals in waste streams. This presentation will provide a review of the EPA's platform and underlying algorithms used for the purpose of compound identification using high-resolution mass spectrometry data. We will also discuss progress towards a high-throughput non-targeted analysis platform for use by the mass spectrometry community. *This abstract does not reflect U.S. EPA policy.*