

## Abstracts for ACS Spring Meeting

### Environmental Chemistry Division: **Presentation**

Session- “Identification and screening of emerging organic contaminants in the environment by accurate mass high resolution mass spectrometry”

Title: Using the US EPA’s CompTox Dashboard to support identification and screening of emerging organic contaminants in the environment

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The US EPA’s iCSS CompTox Dashboard is a curated, publicly accessible resource provided by the National Center for Computational Toxicology (<https://comptox.epa.gov>). The Dashboard provides support for toxicology and risk assessment within and external to the EPA (including ToxCast, ExpoCast, and CPCat, among others). In addition to these data, the underlying database of ~720,000 chemicals allows for tentative identification of chemical features for mass-spectrometry non-targeted analysis (NTA). Our approach includes a series of mass spectrometry specific searches that identify hypothetical molecular ions in complex mixtures and perform rank prioritization of search hit lists to help identify “known-unknowns”. We demonstrate that the availability of data regarding chemical functional use is valuable in assisting in the identification of structure candidates. This presentation will provide examples of using the Dashboard in the identification of unknown chemical features observed in a variety of environmental matrices including dust and wastewater. We will also present on batch-based searching to speed up mass-spectrometric data analyses of environmental samples. *This abstract does not necessarily represent the views or policies of the U.S. Environmental Protection Agency.*