

Unveiling the Unseen: Nontargeted Analysis for Discovering Novel Contaminants in Environmental Monitoring

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Traditional environmental monitoring relies on targeted analysis, focusing on specific contaminants with known health or ecological risks. But what about the unknown threats? This is where nontargeted analysis (NTA) steps in.

Advancements in technology in mass spectrometry and computer technology, including large data volume analysis, enable NTA in actual environmental pollution investigation and monitoring projects. This presentation will focus on the implementation of comprehensive two-dimensional gas chromatography coupled to time-of-flight mass spectrometry for NTA and the NTA implications on the discovery of novel contaminants in environments.

We have developed two approaches: 1) Strategy for the discovery of novel halogenated organic compounds because of their persistence and bioaccumulation in environments and 2) Broad contaminant suspect screening analysis.

The greatest obstacle of NTA is data processing due to the large volume because each sample's instrument run generates several thousand chromatographic features. For isolating halogenated organic compounds, we developed a filter using the R program based on isotope ratios of halogenation and loss of halogens in mass spectra. With the filter, the NTA data volume was substantially reduced, which enabled the discovery of novel or previously unknown/understudied halogenated organic contaminants in the Southern California Bight marine environment. Hundreds of halogenated organic compounds were identified in wildlife and sediment, leading to the discovery of a larger suite of DDT-related compounds.

For general contaminant screening, regardless of halogenation, we employed group comparison to isolate contaminants of interest. Hierarchical cluster analysis is a valuable tool for analyzing the detected chromatographic features. This is followed by compound identification through mass spectral similarity searches against a reference database. Criteria for mass spectral similarity were established and tested through confirmation with authentic standards. Following tentative compound identification, it's crucial to understand their potential environmental impact for prioritization. This involves determining the criteria we should consider and how to obtain relevant information for the hundreds of chemicals identified based on these criteria. In this presentation, I will share the case study for contaminant screening in transborder water runoff from Tijuana, Mexico to the border in San Diego, California, USA.