Enabling State Adoption of Non-Targeted Analysis (NTA) to Address Pressing Public Health Needs: Maryland, Minnesota, and California Leading the Way

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United States Environmental Protection Agency, Office of Research and Development

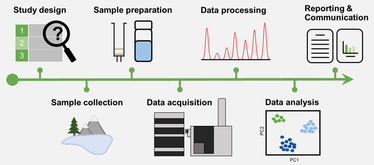
The use of high-resolution mass spectrometry (HRMS) with a new analytical technique, **Non-Targeted Analysis (NTA)**, allows for identification of contaminants of emerging concern without *a priori* knowledge/selection.

Scan to learn more about the U.S. EPA's use of NTA

SCAN ME

NTA workflows paving the way

While NTA workflows are similar to those used for traditional targeted analysis, NTA data processing and data analysis steps are more intensive, requiring multiple steps to translate chemical features into annotations with proposed or confirmed chemical structures.



PFAS NTA ROAR Project

Regional-Office of Research and Development Applied Research (ROAR)

Objective: To build capacity and empower states to access high-resolution mass spectrometry NTA knowledge and tools to independently apply NTA in their management of PFAS and other contaminants of emerging concern (CECs)

Region 3 & Maryland

Background: Large-scale drinking water surveillance program to understand presence of PFAS in finished drinking water- recently expanded to wastewaters, biosolids, fish & crabs

Motivation: To identify the presence of any additional PFAS and to understand their potential source(s) & fate(s)

Study: Approximately 50 drinking water samples collected in relation to an industrial release

Implementation barriers: Need for workflows and spectral libraries to generate high-confidence identifications of PFAS

Maryland DEPARTMENT OF HEALTH

Region 5 & Minnesota

Background: Ongoing surveillance of surface and groundwater contamination in relation to two known point sources

Motivation: To identify the presence of any additional PFAS and to understand their fate and transport behaviors

Study: Approximately 20 samples of surface and groundwater samples collected from upstream, at, and downstream of each point source for NTA

Implementation barriers: Need for tools and statistical modeling resources to support identification of probable PFAS

MINNESOTA POLLUTION CONTROL AGENCY

DEPARTMENT OF HEALTH

Region 9 & California

Background: Pilot study to compare and understand utility of various analytical techniques for PFAS, including NTA

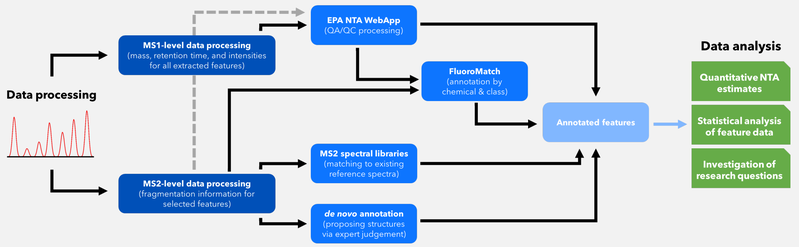
Motivation: To use combinations of analytical techniques to elucidate patterns and trends in the content of PFAS in drinking water to support investigations on sources and treatment technologies

Study: Approximately 4,000 drinking water supply wells to be sampled including ~1,000 to be analyzed with NTA

Implementation barriers: Need for study design that considers a multi-technique, multi-year data collection and analysis protocol

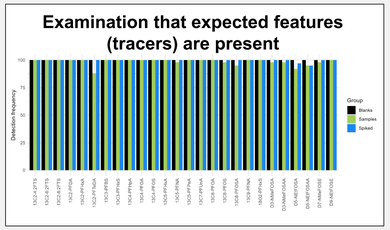
CALIFORNIA Water Boards

ROAR Data Processing & Analysis Steps

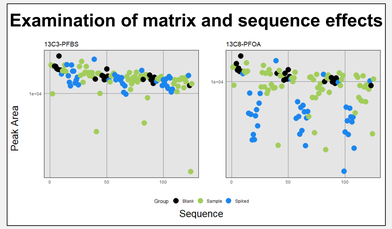


MS1-level data processing
(mass, retention time, and intensities for all extracted features)

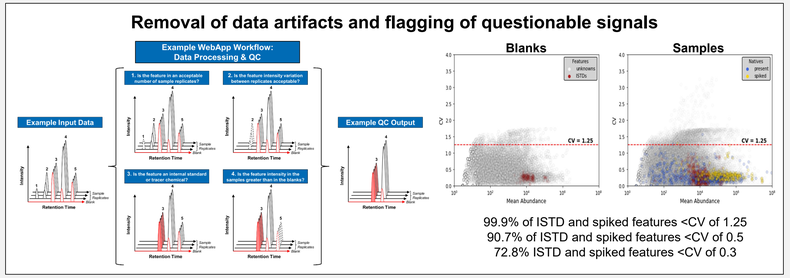
Examination that expected features (tracers) are present



Examination of matrix and sequence effects



Removal of data artifacts and flagging of questionable signals

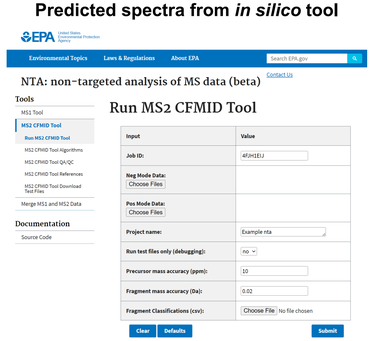


99.9% of ISTD and spiked features <CV of 1.25
90.7% of ISTD and spiked features <CV of 0.5
72.8% ISTD and spiked features <CV of 0.3

MS2-level data processing
(fragmentation information for selected features)

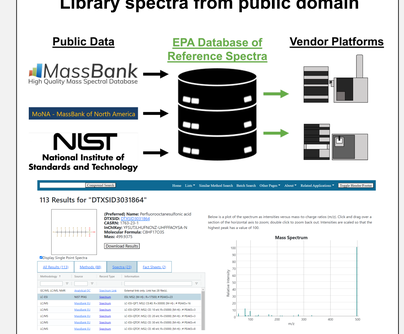
- The translation of MS2-level data into annotated identifications involves utilization of spectral libraries and *de novo* structural elucidation
- Vendors create purchasable spectral libraries for use on their platforms (e.g., *Sciex Fluorochemical Library*)
- Libraries can also draw upon in-house data, public data, and *in silico* predictions

Predicted spectra from *in silico* tool



Matching against predicted spectra for more than 1 million substances

Library spectra from public domain



Matching against real spectra for hundreds of known PFAS

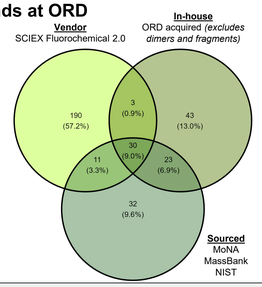
Collected spectra from PFAS compounds at ORD

Data acquisition for PFAS compounds available at ORD to support spectral library generation:

- 250-500 ng/mL solutions of standards and chemical samples in methanol
- Acquisition performed on three instruments (SCIEX QTOF, Agilent QTOF, Thermo Orbitrap)

Final in-house library includes 131 spectra

- 32 spectra from dimers/fragments
- 99 spectra from "true" compounds
  - 78 native, 21 isotopically-labeled compounds



United States Environmental Protection Agency

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