PFAS Signature®
Advanced Analytics Tool

Source Discrimination and Establishing Background Using HRMS Analysis

Per- and polyfluoroalkyl substances (PFAS) are a large class of chemicals widely used for many commercial and industrial applications, including aqueous film forming foams (AFFF), metal plating, plastic molds, photographic films, semiconductors and textile manufacturing. Many of these substances end up in the wastewater treatment plants (WWTPs) and landfills, which means these facilities also serve as potential sources of PFAS.

By understanding the specific signature of these analytes in different matrices, we can deduce information about their sources. This chemical forensic approach is not possible using the targeted analysis alone.

PFAS groundwater and soil contamination at impacted sites often cover large areas and may include co-mingled sources. There is a significant need to understand the source attribution and delineations to determine the fate and transport of these chemicals. In addition, at many of these sites, it has become a critical need for source tracking and differentiation of AFFF sources from non-AFFF sources.

Our Solution

The Battelle-developed PFAS Signature® advanced analytical tool offers PFAS source differentiation and tracking using high-resolution mass spectrometry (HRMS) techniques, in combination with PFAS targeted analysis and advanced statistical analysis.

The identification of sources of contamination is based on:
• Chemical signature
• Isomeric profiles
• Manufacturing
• Age of release
• Fate and transport
• Transformation products

Source Differentiation

Battelle has built a mass spectral PFAS source library based on PFAS targeted analysis and HRMS analysis of different known PFAS sources that can be applied to a site investigation to understand the source attribution of the substances. The developed library is used to compare and differentiate PFAS composition and trends seen in field-derived samples during a site investigation.

Our PFAS Signature® tool was applied to the environmental samples collected from different source scenarios. The results show clear delineation of different sources (Figure 1).

Database of Source Specific Signature Library

- AFFF Formulations
- AFFF-Impacted Sites (Multiple Matrices)
- Commercial Products
- Metal Plating

- Waste Sector
  - Landfill Leachates
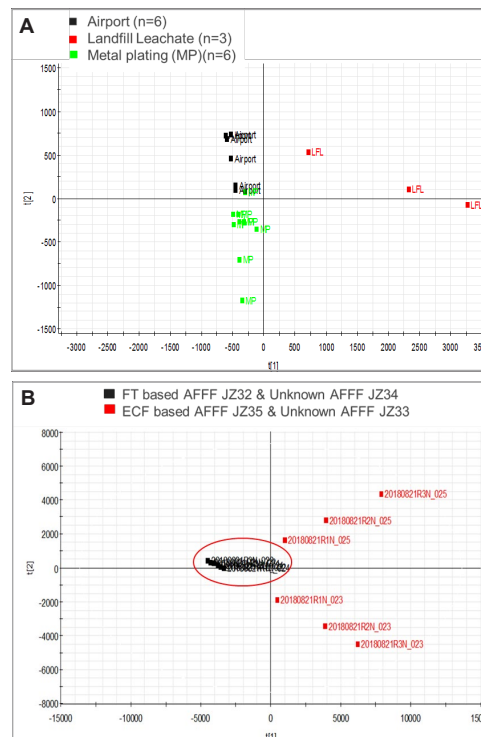 - Municipal WWTP
  - Paper Mill related WWTP
  - Compost

Figure 1. Example of PFAS Signature® Chemical Forensics results showing samples collected from (A) different environmental sources, and (B) AFFFs from known and unknown manufacturing sources.

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Source Tracking

Another application of our PFAS Signature® tool is in a higher-level source discrimination screening. It considers additional lines of evidence that screen for non-PFAS indicator chemicals, such as: pharmaceutical and personal care products, pesticides, and more, useful to identify non-AFFF sources. An example showing the differentiation of AFFF and non-AFFF sources is shown in Figure 2. The cluster of non-AFFF related samples collected from different locations clearly differentiates from the AFFF-impacted environmental samples collected from different sites. The non-AFFF samples shows sources of WWTP related and the landfill leachate samples collected from different parts of United States.
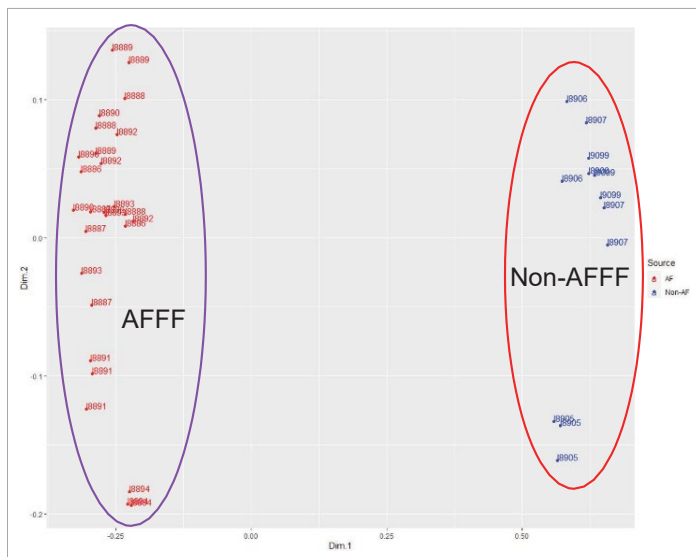

Figure 2. Multi-dimensional scaling plot showing clear differentiation of AFFF and non-AFFF sources. Plot shows HRMS PFAS data collected from different sources of non-AFFF and AFFF-impacted samples.

Establishing Background

From EPA Guidance EPA 540-R-01-003, background samples are needed for comparison of site and background concentrations for making risk management decisions concerning appropriate remedial actions. In addition to the PFAS targeted analysis quantitative data, semi-quantitative data generated from PFAS suspect screening analysis can also assist in establishing background levels of broader list of PFAS. Suspect screening analysis can help fill gaps in the available data (certain chemicals were excluded from the sample analyses). Applying multivariate analysis, background concentrations can be compared to site-specific concentrations.

Suspect Screening Library for up to 600 PFAS

- Identifies chemicals that would not have been identified by the targeted analysis
- Supports development of the conceptual site model to validate assumptions
- Identifies contributing sources that are not the 'known' or expected source(s)

Results

The information obtained from multiple lines of evidence is investigated to understand the PFAS sources and compare them. PFAS Signature® assesses how the unknown sample compares to the trained library to understand the similarities and differences between the unknown and known sources (Figure 3).

The following multiple lines of evidence are assessed to differentiate the sources:

- Targeted analysis
- High resolution mass spectral analysis
- Statistical analysis
- Fate and transport
- Transformation Products
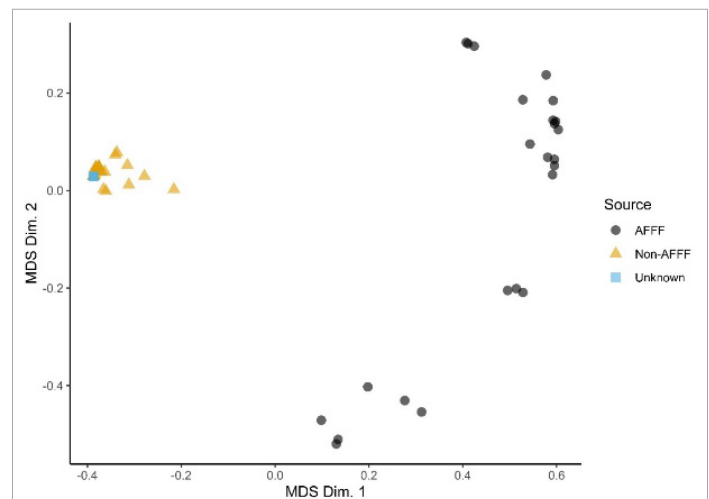- Screens for non-PFAS indicator chemicals

Figure 3. PFAS Signature® Analysis showing visualization of unknown sample compared to the known source samples.

Application of Battelle's PFAS Signature® approach, which is a combination of advanced HRMS tool and statistical analysis, shows great promise in understanding the source delineations and categorizations that are not possible using only targeted PFAS analysis by LC-MS/MS methods.

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It can be done