Food and Environmental

SCIEX
The Power of Precision

Screening for Legacy and Novel PFASs Using SCIEX Fluoros Library 2.0

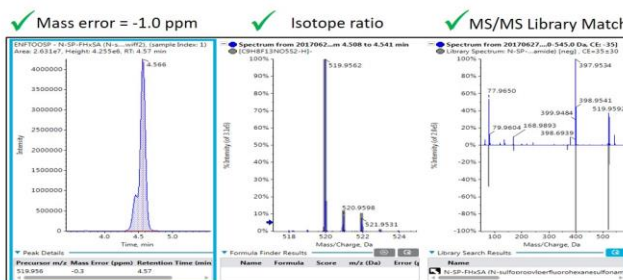**Enhanced Coverage of Per- and Poly- fluorinated (PFAS) Contaminants in Environmental Samples**

Karl A. Oetjen[1], Craig M. Butt[2], Katherine C. Hyland[1]
[1]SCIEX, Redwood City, CA, USA [2]SCIEX, Framingham, MA, USA

What: Currently there are more than 3000 Per- and Poly-fluorinated substance (PFAS) products that were or are available on the global market. Changing regulations and concern for human environmental impact make detection and identification of PFAS a high priority for many environmental testing laboratories. Many of these products may be not well understood or well characterized, and analytical grade standards are often unavailable, limiting the comprehensibility of targeted methods. Therefore, many laboratories have included suspect screening workflows in their routine analysis. Suspect screening allows laboratories to search against a spectral library or database of characterized compounds without the need of authentic standards, saving time and allowing for a more comprehensive characterization of environmental samples.
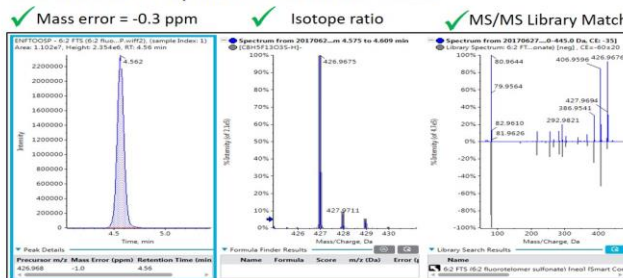
How: To provide complete characterization of PFAS contaminants in impacted water and soil, samples can be analyzed by using a *data independent acquisition* strategy (SWATH® Acquisition). This approach ensures potential compounds of interest are not missed, and provides a narrow precursor ion range. Combining this data acquisition strategy with the **SCIEX Fluoros Library 2.0** allows for the comprehensive characterization of environmental samples. This verified library contains MSMS spectra for over 250 PFAS compounds covering negative, positive, and zwitterionic compound classes. While this library was built specifically for the X500R, it is also compatible with SCIEX TripleTOF® and QTRAP® systems. Users can mine this spectral library to identify suspect chemicals based on the measured exact mass, isotope, and fragmentation patterns quickly and efficiently, providing greater confidence when making identifications.

Figure 1. Enhanced Coverage using SCIEX Fluoros Library 2.0. a.) 6:2 fluorotelomer sulfonate (6:2 FTS) a legacy PFAS and b.) N-SP-FHxSA a novel PFAS were identified in a sample of aqueous film forming foam (AFFF) impacted groundwater. The sample was analyzed using SWATH Acquisition on the SCIEX X500R QTOF System and the acquired data searched against the SCIEX Fluoros Library 2.0 using SCIEX OS Software for data processing.