

Developing compound-specific isotope analysis methods for per- and polyfluoroalkyl substances with Orbitrap mass spectrometry

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Per- and polyfluoroalkyl substances (PFAS) are anthropogenic contaminants widely used in various fields, highly persistent in environments, and cause public health concerns. Identifying their sources, transformation pathways, and fate is crucial to fully understand the PFAS behavior in environments. Here we present a new approach to quantify compound-specific isotopic analysis for various PFAS compounds using dual-inlet Orbitrap mass spectrometry. We selected perfluorobutane sulfonamide (FBSA, $C_4F_9NH_2SO_2$) as a model PFAS compound for quantifying major isotopologues ($\delta^{13}C$, $\delta^{15}N$, $\delta^{18}O$, and $\delta^{34}S$) using Electrospray Quadrupole-Orbitrap Mass Spectrometry (Orbitrap MS). We found $\delta^{34}S$ is the most reliable isotope ratio in the analysis due to the relatively high intensity of ^{34}S . Compared with fragment analysis (NSO^{2-}), parent compound analysis of FBSA required a much higher resolution (240 K) to fully resolve the isotopologues. We then focused on analyzing $\delta^{34}S$ using NSO^{2-} fragment and used topiramate ($C_{12}H_{21}NO_8S$) as a non-PFAS reference material. We optimized the fragmentation energies for source fragmentation and HCD fragmentation based on fragmentation patterns. We will compare $\delta^{34}S$ values obtained from Orbitrap MS with those from traditional isotope ratio mass spectrometry (e.g., IRMS) to assess the accuracy of our method. The analytical advancement of this project can expand the scope of isotope analysis using the orbitrap system and provide a solid base for further characterizing sources and transformation of various PFAS using their isotopic composition.