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Poster Session Day 2

Assessing stable isotope composition of per- and polyfluoroalkyl substances using electrospray ionization (ESI) Orbitrap mass spectrometry

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Per- and polyfluoroalkyl substances (PFAS) contamination has caused public health concerns due to their widespread occurrence and high persistence in environments. To fully understand the PFAS behavior in environments, identifying their sources, transformation pathways, and fate is essential. Here we introduce compound-specific isotopic analysis methods for various PFAS compounds with dual-inlet electrospray quadrupole-Orbitrap mass spectrometry (Orbitrap MS). Using perfluorobutane sulfonamide (FBSA, $C_4F_9NH_2SO_2$) as a model PFAS compound, we quantified its major isotopologues ($\delta^{13}C$, $\delta^{15}N$, $\delta^{18}O$, and $\delta^{34}S$) and found that $\delta^{34}S$ yielded the most reliable isotope ratio in the analysis due to the relatively high intensity and lack of isobaric interference. Compared with fragment analysis (NSO_2^-), parent compound analysis of FBSA required a much higher resolution (240K) to fully resolve the isotopologues. To ensure the high ion counts and precision, we decided to focus on analyzing $\delta^{34}S$ using NSO_2^- fragment and use topiramate ($C_{12}H_{21}NO_8S$) as a non-PFAS reference material with 60K resolution. We optimized the fragmentation energies for source fragmentation and higher-energy collision dissociation (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.