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Stable Isotopic Analysis of Per- and Polyfluoroalkyl Substances (PFAS) by Nanoflow-HPLC-Orbitrap-MS

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Per- and polyfluoroalkyl substances (PFAS) are industrially derived fluorinated organic compounds that persist in the environment and are detrimental to human and ecosystem health. Recent studies have demonstrated stable isotopic differences in individual PFAS molecules like perfluorooctanoic acid (PFOA) and perfluorooctane sulfonic acid (PFOS) that might be exploited for source apportionment of contaminated environmental samples. Orbitrap mass spectrometry (Orbitrap-MS) is gaining popularity for isotope analysis. It presents a unique opportunity for the isotopic characterization of PFAS: 1) electrospray ionization (ESI) is a soft ionization technique thus intact molecules are introduced into the mass spectrometer 2) combustion of the molecules to simple gases is not required, and 3) significantly less material is required to make an isotopic measurement. Derivatization of PFAS molecules for isotopic analysis can be difficult and most PFAS do not combust using traditional isotope ratio mass spectrometry reactors. Additionally, Orbitrap mass spectrometry allows for the possibility of performing multi-element compound-specific isotope analysis, where the isotopic composition for a single molecule in multiple isotope systems is determined all at once. By combining multiple isotopic tools, we can separate different sources and processes in multi-dimensional space using a “fingerprinting” approach. We present results of a method developed for determining the isotopic compositions of PFOA, PFOS, PFBS, and HFPO-DA using HPLC-Orbitrap-MS and compare our results to traditional isotopic characterization of PFOA and PFOS using elemental analyzer-isotope ratio mass spectrometry (EA-IRMS) and thermal conversion elemental analyzer-isotope ratio mass spectrometry (TCEA-IRMS).