Goldschmidt 2025 Abstract
https://doi.org/10.7185/gold2025.31960

A new method for Compound Specific Isotope Analysis (CSIA) of Perfluoroalkyl substances (PFAs)

EDUARDO DI MARCANTONIO[1], ORFAN SHOUAKAR-STASH[2], MASSIMO MARCHESI[1] AND LUIGI DALLAI[1]

[1]Sapienza University of Rome
[2]Isotope Tracer Technologies Inc. - IAGC

Per- and polyfluoroalkyl substances (PFAs) are a group of emerging contaminants that have come to public attention due to their harmful health effects and environmental persistence. Their non-volatile and polar nature prevent direct Gas Chromatography (GC), limiting the application of a useful tool like Compound-Specific Isotope Analysis (CSIA) by GC-Isotope Ration Mass Spectrometry (IRMS) for tracking their origin and behavior.

To overcome this limitation, a derivatization method was applied to Perfluorocarboxylic acids (PFCAs), a particularly concerning subclass of PFAs and among the most frequently detected in environmental samples, then analyzed with GC-Combustion-IRMS (GC-C-IRMS) for CSIA. Perfluoroheptanoic acid (PFHpA), Perfluorooctanoic acid (PFOA), and Perfluorodecanoic acid (PFDA) were successfully analyzed, achieving measurement errors below 0.5 ‰, which aligns with the generally accepted error for CSIA of other commonly studied organic pollutants like hydrocarbons and chlorinated solvents. Instead, for the Perfluorooctane sulfonate (PFOS) this method is not suitable, suggesting the need of a different preparation or analysis procedure.

In order to assess the suitability of the method for real samples, different real matrices for the solution, such as rain water and tap water, have been successfully tested. While the detection remains relatively high (from 50 μg/L) compared to the concentrations usually found in most of the environmental matrices (in the range of ng/L), preconcentration treatments can successfully be used in real field samples to reach the minimum concentrations needed for CSIA.

Additionally, analysis of various PFCAs from different manufacturers using Elemental Analysis-IRMS (EA-IRMS) revealed carbon isotopic differences up to 10 ‰, significantly exceeding the analytical error and confirming the potential of the method for source differentiation.

This approach offers a promising pathway to develop a solid analytical tool for tracing and monitoring PFCA contamination, improving efforts to manage and remediate pollution in complex environmental matrices.