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Direct and simultaneous species-specific isotope ratio determination of inorganic and methyl mercury

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The isotopic composition of Hg is increasingly used to trace its sources and environmental pathways, with species-specific isotopic ratios providing essential insights into transformation processes such as methylation and demethylation. Distinguishing between the isotopic signatures of inorganic mercury (iHg) and the most abundant organic species, namely methylmercury (MeHg), is crucial for understanding their fate in the environment [1].

Current analytical methods for species-specific Hg isotope analysis rely primarily on chromatographic separations coupled to on- or off-line detection by multi-collector inductively coupled plasma mass spectrometry. While effective, these techniques involve time-consuming sample preparation, like derivatization and solvent extraction, as well as complex instrumental setups requiring the coupling of GC [2] or HPLC [3] to MC-ICPMS for on-line procedures. Additionally, the latter methods provide transient signals that may reduce the precision of the data.

We propose a novel procedure using soft ionization that preserves molecular integrity, enabling direct, species-specific Hg isotope ratio determination. The procedure features the complexation of inorganic Hg and methylmercury, its introduction into an ESI source, subsequent collisional dissociation of the complexes, followed by the direct simultaneous detection of inorganic mercury and MeHg isotopic patterns by an Orbitrap™ mass spectrometer. This approach circumvents derivatization and chromatographic steps, as it preserves molecular information, leading to simplified sample preparation and reduced processing time.

We will present the status of optimization and validation of the procedure and assess its accuracy, reproducibility, and applicability across different environmental matrices. We will also discuss the advantages and limitations compared to existing methods. It is also expected that this approach may be extended to the species specific detection of several elements and their isotopic ratios, offering a more efficient means of investigating metal species fractionation and cycling in natural and contaminated systems.

References

[1] Tsui, Blum & Kwon (2020), *Science of the Total Environment* 716, 135386.

[2] Suárez-Criado, Queipo-Abad, Rodríguez-González & García Alonso (2024), *Journal of Analytical Atomic Spectrometry* 39, 508-517.

[3] Entwisle, Malinovsky, Dunn & Goenaga-Infante (2018), *Journal of Analytical Atomic Spectrometry* 33, 1645–1654.