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Simple Metal Ion Isotope Ratio Measurement with ESI-Orbitrap HRMS: Concept Validation and Preliminary Performance Evaluation

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Conventional methods for isotope ratio (IR) determination such as TIMS and MC-ICP-MS require extensive sample preparation [1] and struggle with isobaric interferences [2]. This study introduces a novel approach to convert a conventional Orbitrap™ MS into a platform for metal IR measurement, without any hardware modifications, allowing for a rapid and interference-free metal IR analysis.

The method exploits metal-ligand complexation to enhance ionization efficiency, followed by quadrupole filtering to isolate precursor ions. Subsequent collision-induced dissociation releases free metal ions for direct isotopic analysis with ultra-high resolution.

The isotopic patterns of several metal ions, namely Cr, Fe, Ni, Cu, Ga, In, Tl and Pb, were measured using EDTA as a complexant. The Orbitrap™ mass spectrometer effectively resolved isobaric interferences such as ^{54}Cr-^{54}Fe, ^{58}Fe-^{58}Ni, and ^{64}Ni-^{64}Zn. Simultaneous multi-isotope and multi-element detection was achieved in a single scan, significantly improving throughput.

A proof-of-concept study on Pb isotopes was conducted, carefully evaluating the impact of chemical and instrumental parameters, to maximize precision and accuracy: under tuned conditions, the method demonstrated optimal accuracy within 2–14 ppm of reference values after mass bias correction. Precision was conversely in the range 0.11% - 0.023% as RSD% when measured over a long-term, 12 hours run. While precision is currently 10 to 50 times lower than TIMS and MC-ICP-MS, and comparable to single-collector ICP-MS, further optimization is undergoing to reduce inaccuracies in the measurements.

This method, though at an early stage, is a promising alternative for IR measurements that leverages the unique capabilities of Orbitrap™, offering a streamlined, interference-free approach to IR determination. Future work will focus on expanding the range of analyzable elements and suitable ligands, improving precision, with the potential to complement conventional techniques.

[1] Penanes, Galán, Huelga-Suarez, Rodríguez-Castrillón, Moldovan & Garcia Alonso (2022), *J. Anal. At. Spectrom. 37*, 701–726.

[2] Van Acker, Theiner, Bolea-Fernandez, Vanhaecke & Koellensperger (2023), *Nat. Rev. Methods Prim. 3*, 1–18.