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Unravelling new isotopic dimensions of oxyanions by ESI-Orbitrap

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Oxyanions represent water-compatible forms of key elements required for life. The abundance of oxyanions has been extensively used to study biogeochemical cycles of the major elements that make up all organic matter (carbon, oxygen, nitrogen, phosphorus, sulphur), together with the abundance of their singly isotopically substituted variants. The nitrate and phosphate oxyanions belong to the two most anthropogenically disrupted nutrient cycles with the global impact on ecosystem stability and resilience. Higher nitrate and phosphate concentrations result in eutrophication and anoxic water conditions. Because the nitrogen and phosphorus cycles are interlinked and heavily disrupted by human activity with global consequences for the ecosystems, it is crucial to have a thorough understanding of the environmental dynamics of these elements of life.

We will present a newly established method [1,2] for isotopic analysis of the oxyanions that can overcome issues of currently used methods. We extend the recently developed method using electrospray ionization (ESI)-Orbitrap mass spectrometry from its initial application to biomolecules towards singly substituted oxyanions. Unlike the current methods, ESI-Orbitrap offers fast and simultaneous measurement of the analytes as a whole, with low detection limit and high mass resolution. Therefore, the technique provides access also to doubly substituted isotopic species (“clumped isotopes”) that have not yet been explored thoroughly and are hypothesized to overcome shortcomings of the singly substituted species. The technique will be applied to study isotopic signatures of the oxyanions in environmental samples. These studies will bring so far analytically inaccessible information about the clumped isotopes and triple oxygen isotopes (^{16}O, ^{17}O, ^{18}O) that have the potential to enable significant insights into the biogeochemical cycling of the elements of life in nature. A key piece for expanding this powerful methodology is developing easy-to-use sample purification protocols. Thus, the ESI-Orbitrap method can extend routine measurements in research laboratories with isotope analysis.

[1] Neubauer, Crémière, Wang, Thiagarajan, Sessions, Adkins, Dalleska, Turchyn, Clegg, Moradian, Sweredoski, Garbis & Eiler (2020), Anal. Chem. 92, 3077-3085.

[2] Hilkert, Böhlke, Mroczkowski, Fort, Aizikov, Wang, Kopf & Neubauer (2021), Anal. Chem. 93, 9139-9148.