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Thermo Scientific™ Orbitrap Exploris™ Isotope Solutions: tools for comprehensive characterization of polyisotopocules

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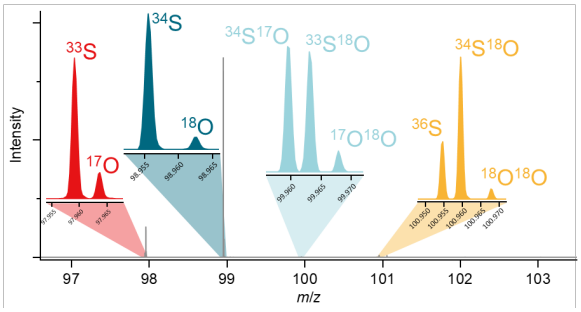

Orbitrap™ Isotope Ratio MS, both electrospray and gas source, is becoming increasingly accepted in the community as a unique and complimentary approach to classical IRMS techniques for measuring relative abundances of isotopically substituted species. Electrospray ionization offers the specific advantage of performing “soft” ionization, which produces intact molecular ions and provides unique insight into the molecular anatomy of polar compounds in aqueous solutions. In contrast to classical approaches, no chemical manipulation or gas conversion reactions are required and as a result, no intramolecular information is lost from sample to analysis. Similar to classical approaches, the principles of identical treatment and rigorous sample standard bracketing have been retained and are the key to achieving precise and accurate relative abundance measurements.

Currently, this approach is being applied to oxyanions and small organic molecules. Utilizing the HRAM capabilities of the Thermo Scientific™ Orbitrap Exploris™ MS platform, resolving singly and doubly substituted polyisotopocule molecular ions is achieved in routine measurements. Methods have been developed for nitrate ($\delta^{15}N$, $\delta^{18}O$, $\delta^{17}O$, $\Delta^{17}O$, $\Delta^{15}N^{18}O$, $\Delta^{15}N^{17}O$, $\Delta^{18}O^{18}O$), sulfate ($\delta^{33}S$, $\delta^{34}S$, $\delta^{36}S$, $\delta^{17}O$, $\delta^{18}O$, $\Delta^{17}O$, $\Delta^{33}S$, $\Delta^{36}S$, $\Delta^{34}S^{17}O$, $\Delta^{33}S^{18}O$, $\Delta^{34}S^{18}O$, $\Delta^{17}O^{18}O$, $\Delta^{18}O^{18}O$)(Figure), phosphate ($\delta^{18}O$, $\delta^{17}O$, $\Delta^{17}O$, $\Delta^{17}O^{18}O$, $\Delta^{18}O^{18}O$), which achieve sub-‰ precision for isotope ratios of singly substituted isotopologues. We are actively developing methods for small organic molecules such as MSA, caffeine, vanillin and amino acids.

Here we will present progress in method development including sample introduction, methods and measurement approaches. We will also touch on future directions and development opportunities in a wide range of topics in biochemical cycles, ecology and paleoclimate reconstructions.