

# Comprehensive Isotope Ratio MS with Electropray-Orbitrap

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A new, comprehensive approach to Isotope Ratio MS using an electrospray ionization (ESI) Orbitrap has been developed. It gives access to a wide range of isotopic information from intact polar compounds in liquid samples. It delivers isotope ratios of singly substituted isotopologs, mass independent fractionation, clumped isotopes and, for organic molecules, position specific isotope analysis.

We have developed two sample introduction methods and automation, applying IRMS specific rules by using nitrate as a model compound. In total, 7 isotopologs of nitrate can be quantified simultaneously opening multiple pathways for calculating  $\delta^{15}\text{N}$ ,  $\delta^{18}\text{O}$ ,  $\delta^{17}\text{O}$  and  $\delta^{17}\text{O}$  values with sub-‰ precision and accuracy (2021, Hilkert et.al). It also opens a unique way to measure non-random isotopic distributions (“clumping”) in oxyanions.

High precision and accuracy were achieved by combining IRMS strategies like sample/standard comparison and referencing schemes with Orbitrap technology. In addition, a simple and more direct application of real-life samples has been discovered.

The general validity of this new development was proven by a full characterization of S-MIF1 and 2, two recently published sulfate reference materials for sulfur isotope ratio MS, with in total 13 isotope ratios and triple isotope results.

Recently published data on methionine using the ESI-Orbitrap (2018, Neubauer et.al) complement the methodology and show the extension of comprehensive IRMS into position specific and clumped isotope analysis in organic molecules.

Comprehensive Isotope Ratio MS with Orbitrap technology measures the isotopic anatomy of intact organic and inorganic molecules reading nature's fine print in a single compound. Features by which a molecule now can be described can cover but are not limited to sources, metabolism, formation, transformation and diagenetic effects.

We will present latest results and discoveries in combination with the essential milestones of this new development.

