INV-05

Session 5b) Novel Methodology 2: Technical Development

High accuracy isotope analysis with the Orbitrap Exploris MS

Nils Kuhlbusch[1,3], Andreas Hilkert[1], Issaku E. Kohl[2], Brett Davidheiser[1], Dieter Juchelka[1], & Heiko Hayen[3]*

[1] Thermo Fisher Scientific

[2] University of Utah, Department of Geology and Geophysics

[3] University of Muenster

*Presenting Author Email: andreas.hilkert@thermofisher.com

Orbitrap-based Isotope Ratio MS is becoming increasingly visible. It provides a unique and complimentary tool to classical Isotope Ratio MS techniques to measure the relative abundance of isotopologues. The soft Electrospray Ionization of the Orbitrap produces intact molecular ions that can optionally be fragmented by higher energy collisional dissociation. Combining these features with the high-resolution accurate mass of Orbitrap analyzers can give insights into compound specific as well as position specific isotope ratios.

Precision and accuracy of Orbitrap-based isotope ratio analysis can be significantly improved by utilizing sample-standard bracketing to correct for instrument drift and inaccuracies via isotope ratio calibration. Two approaches are currently state of the art. The dual syringe inlet approach, which uses a diverter valve switching between two syringes filled with a sample and a standard or using an HPLC autosampler for alternating injections of sample and standard solutions.

In this talk we will show a combined workflow for an improved isotope ratio standardization. This new workflow utilizes two flows of liquid controlled by a switching valve, one flow from the HPLC autosampler for sample introduction, and a second flow for standard introduction. This fully automated setup allows the injection of a standard during the washout period of the HPLC autosampler loop. This reduces wasted time while simultaneously improving the quality of the measurements. Precision and accuracy can now be verified by drift correction and one- or two-point calibration.

Isotope ratio calibration using the novel strategy for sample and standard introduction will be demonstrated on latest applications for inorganic (e.g. sulfate) and organic (e.g. vanillin) samples showcasing unique insights into the isotopic anatomy of molecules.