INV-01 Opening talk

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The radical advance of the isotomics of natural materials

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The study of the properties and natural distributions of molecule isotopologues has entered a new era in which nearly any ppm or greater abundance isotopic form of nearly any recognized molecule can be studied with meaningful precision, even for the trace components of complex mixtures that typify environmental, geological and extraterrestrial samples. This capability has roots in diverse technologies and methods reaching back many decades, but practical capabilities have expanded with dizzying speed and scope due to the development and rapid spread of Orbitrap-based isotope ratio analysis. These devices are challenging to master and possess fundamental limitations; nevertheless, their intrinsic power for isotopologue research, the sophistication of the platforms in which they are integrated, and the relative accessibility and uniformity of such instruments mean our community has finally reached 'open water', where our measurements and applications are more limited by our imaginations and ambitions than by the capabilities of our machines.

The state of the art in Orbitrap-based isotope ratio measurements, and their relationships to other technologies that are preferable for specific targets, will be well illustrated by other presentations at this symposium. I will explore four questions that will shape the way in which our field takes advantage of our new capabilities to advance longstanding scientific questions: How can we most effectively develop and disseminate technical mastery of the complex, unfamiliar instruments now used for compound-specific, site-specific and clumped isotope analyses of molecules? How can first-principles theory and experiments most usefully enable rigorous interpretation of the vast number of new measurements we can now make? How will the rapidly expanding use of machine-learning and other advanced data science tools aid us in the design, execution and interpretation of complex, many-dimensional mass spectrometric measurements of isotopologues? And, what technologies will enable our field to reach deeply into its next vast analytical frontier: the isotopologues of condensed materials, particularly macromolecular organics?