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Orbitrap Isora Opens New Frontiers for Molecular-Level Isotope Analysis

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Thermo Fisher Scientificâ??s Mario Tuthorn and University of Glasgowâ??s Prof. Douglas Morrison discuss how high-resolution isotope analysis can accelerate research across environmental forensics, human health, food authenticity and astrobiology.

Isotope analysis is moving beyond specialised laboratories towards broader, molecular-level applications. **In this BioSpectrum Asia interaction, Mario Tuthorn and Prof. Douglas Morrison explore how the Orbitrap Isora workflow enables isotope and isotopologue measurements directly from intact molecules,** helping researchers gain deeper insights into their origin, transformation and pathways. From tracing PFAS contamination to uncovering extraterrestrial molecules in meteorites, the technology could open new possibilities across environmental science, metabolism, food research and human health.

What has been the biggest technical barrier preventing isotope ratio analysis from becoming more widely adopted, and how does the Orbitrap Isora workflow address this?

MT: Classical isotope ratio mass spectrometry (IRMS) is a highly established and powerful approach that continues to play an essential role in isotope research. At the same time, isotope ratio analysis can require specialized instrumentation, sample-conversion workflows and significant method-specific experience, which can present barriers for laboratories looking to expand into different types of isotope measurements.

The Orbitrap Isora workflow is designed to lower some of these barriers by bringing isotope analysis onto a dedicated Orbitrap mass spectrometry platform. With Orbitrap technology, isotope and isotopologue ratios can be measured directly from intact molecular ions using high-resolution accurate-mass detection, rather than having to convert samples to a simple gas and lose important molecular information. Studying isotopies from intact molecules provides deeper analytical insights to understanding where a compound came from and what molecular processes shaped it.

The Orbitrap Isora workflow also offers high sensitivity, enabling researchers to detect low-abundance isotopologues that can reveal additional information about individual molecules. It can measure multiple isotopes in a single run, building a richer picture of a compound’s origin and transformation. For suitable analytes, electrospray ionization can also reduce the need for chemical conversion or derivatization, simplifying sample preparation.

Together, these capabilities help streamline the path from sample to isotopic insight, while opening broader application spaces for researchers to connect isotope information with molecular structure and gain deeper insight into the origin, transformation and pathways of compounds.

Moving isotope ratio analysis from specialised laboratories to a broader research community could significantly expand its applications. Which research areas could see the most immediate impact from this increased accessibility?

MT: We see particularly strong opportunities in environmental science, geochemistry and biogeochemistry, where stable isotopes are already important tools for understanding natural and anthropogenic processes.

Beyond environmental research, there are also important opportunities in metabolism research, where isotopic information may add insight into how molecules are formed and routed through biochemical pathways, and in food research, where molecular isotope signatures may provide additional evidence related to origin and authenticity.

Across these areas, isotope information adds a complementary analytical dimension alongside concentration measurements and molecular identification, helping researchers build a richer picture of the processes and histories associated with individual compounds.

The workflow reduces analysis from days to hours. Beyond speed, how could this change how laboratories design experiments, handle larger sample volumes and undertake isotope-based research?

MT: The impact goes beyond receiving a result more quickly. A more streamlined workflow may support broader experimental designs, including larger sample sets, additional replicates, more time points or more systematic comparisons between conditions.

The Orbitrap Isora workflow connects rapid sample/reference injections using the Thermo Scientific™ Vanquish™ Duo UHPLC System with Thermo Scientific™ Isotope Discoverer™ Software, which takes data from raw spectra through calibration, visualization and reporting. This helps reduce manual data handling while delivering the accurate measurements and calibration that are fundamental to isotope ratio analysis.

For researchers, this may make it more practical to incorporate isotope measurements across a study—for example, in time-course experiments, source-tracing studies or investigations of environmental and biological pathways.

The scientific value is therefore not simply speed. A more connected workflow may support more extensive and systematic use of isotope information while allowing researchers to focus more attention on interpreting the resulting isotopic patterns.

For environmental applications such as PFAS contamination, how can molecular-level isotope information help researchers move beyond simply detecting a contaminant towards identifying its source and understanding how it moves through the environment?

MT: PFAS is a good example of why source information matters. Measuring concentration tells us which PFAS compounds are present and at what level, but the same compound may originate from different manufacturing sources or enter the environment through different release pathways. That makes attribution particularly challenging.

Stable isotope signatures provide an additional, intrinsic characteristic that may contribute to environmental forensic investigations. Recent research (Rapid Communications in Mass Spectrometry; Analytical Chemistry (July 9, 2026); Analytical Chemistry (July 16, 2026)) has demonstrated differences in stable isotope composition among PFAS materials from different suppliers and production lots, indicating that isotope signatures may provide useful information for distinguishing potential sources. Compound-specific Orbitrap-based methods have also demonstrated the measurement of PFAS isotope signatures, including work extending this approach to multiple elements and adding further dimensions for source differentiation.

The value lies in combining isotopic fingerprints with other evidence, such as PFAS composition, isomer patterns, co-contaminants and environmental context. Together, these complementary data may provide stronger evidence for distinguishing potential sources and investigating the origin of PFAS contamination.

This remains an emerging area of environmental forensics and the research is building an important foundation for adding source-related information to established PFAS detection and characterization approaches.

Professor Morrison, your research spans areas ranging from meteorite samples to malnutrition, gut inflammation and malaria. Could you share one example where Orbitrap-based isotope analysis revealed an insight that would have been difficult to obtain using conventional analytical approaches?

DM: How did life begin on Earth is still one of the most intriguing questions in science. We think meteorites may have been a source of early “prebiotic” chemicals necessary for life — but we have a problem — contamination!

In our meteorite work with Orbitrap-based isotope analysis, we examined the Winchcombe meteorite which landed in the UK in 2021. Winchcombe is important because it had limited exposure to Earth’s organic “contaminants” and limited exposure to water which can alter the isotopic fingerprint of molecules. The isotopic composition of molecules imprints evidence of their past history: of chemical reactions, of physical processes and even how they were formed through a process called isotopic fractionation.

For Winchcombe, we took a standard life sciences approach to look for unknown molecules by Orbitrap (called untargeted identification) to characterise the molecular inventory. We identified a group of organic sulfur molecules which were potentially of extraterrestrial origin. To nail this down, we looked at their carbon (13C) and hydrogen (2H or deuterium) isotopes (deuterium is especially interesting as it varies more wildly in extraterrestrial systems compared with Earth). We found compelling evidence of extraterrestrial origin because their deuterium composition is so wildly different to anything we find on Earth. Intriguingly, we see anomalies in the sulfur and oxygen isotope signatures that may tell us about their unique formation history and perhaps about the early solar system. All this information was gathered on a tiny fragment of meteorite (~50 mg) and molecules only present in the femtogram to picogram range. This would not have been possible with conventional molecular isotope measurement capability. Undoubtedly, Orbitrap-based isotope analysis will help unlock the isotopic secrets of extraterrestrial organics and may one-day provide more certainty in answering the long-standing question — how did life begin on Earth?

Looking ahead over the next three to five years, where do you see molecular-level isotope analysis creating the greatest scientific or societal impact, particularly across human health, sustainability, food security and environmental research?

MT: One of the most exciting opportunities is in metabolomics and human health research, where molecular isotope information may add a complementary layer of insight alongside established metabolite profiling.

By combining information on metabolite abundance with natural isotope patterns, researchers may gain a richer view of metabolic pathways, nutrient utilization, microbiome-host interactions and disease-related metabolic changes. Emerging work is also exploring whether subtle isotope fingerprints can provide additional information about metabolic processes in complex biological samples.

There are also important opportunities in food research, where molecular isotope information can complement existing analytical approaches for questions around origin, authenticity and nutrition. More broadly, adding isotopic information to the analytical toolbox may support a more complete understanding of biological and food systems.