High-precision and accuracy measurements of the isotopic contents and structures of extra-terrestrial organic molecules

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The OSIRIS-REx mission will return organic-bearing samples from Bennu, providing an opportunity to explore extra-terrestrial organic chemistry from an known environment. Stable isotope compositions (D, ^{13}C, ^{15}N, $^{17,18}O$, $^{33,34,36}S$) of returned organics will provide constraints on their precursors and formation mechanisms and conditions.

We are developing technology and methods for the analysis of stable isotope distributions in organic compounds returned from Bennu, including bulk molecular isotope composition, intramolecular position-specific isotopic differences, and proportions of multiply-substituted isotopologues. We are using the Thermo Fisher Q Exactive GC and LC instruments — Orbitrap-based mass spectrometers — coupled with novel methods for sample introduction and mass analysis. The high mass resolution ($M/\Delta M$ ~10^5-10^6), mass range (functionally ~50-500 amu), and capacity to simultaneously study multiple peaks permit the analysis of many molecular and fragment species and their isotopologues. We demonstrate precision in the range 0.1-1 ‰ for H, C, N, O and S isotope analyses of amino acids, fatty acids, and various aromatic hydrocarbons, including position-specific and multiply substituted species, on ~nmol sample sizes. Where known, measured properties are shown to be accurate within analytical precision. However, several instrumental fractionations must be controlled to achieve these levels of performance. Measurements can be integrated with on-line GC or LC separation. We will present illustrative applications to abiotic alanine and meteoritic PAHs.