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Position-specific carbon isotope measurements in alanine by high-resolution gas-source IRMS

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Measurements of site-specific and multiply-substituted isotope distributions can provide constraints on molecular origins and histories that are complementary to traditional methods of stable isotope measurement, which average the isotopic compositions across all isotopologues within a given molecule.

We are developing technology and methods for per-mil-level-precision analysis of the stable carbon isotope distributions in alanine perturbed through biological and enzymatic processes, measured with the Thermo Fisher Q Exactive GC and LC instruments – Orbitrap-based mass spectrometers – coupled with novel methods for sample introduction.

Alanine, the smallest chiral amino acid, plays an important indirect role in the tricarboxylic acid cycle, as it is formed directly from pyruvate via the alanine aminotransferase (ALT) enzyme, and can be converted back to pyruvate as needed. Because the conversion of alanine to pyruvate involves breaking alanine's C-N bond (the central carbon site) to make a C=O bond in pyruvate without changing the carbon structure, it is a useful reaction for studying site-specific isotopic fractionations within this molecule.

We are examining this chemistry through two experiments: in the first, alanine is consumed by *E. coli* and the residual, unconsumed alanine is examined for its whole-molecule, site-specific and multiply-substituted isotopic composition, relative to the starting composition; in the second, alanine is placed in solution with the ALT enzyme to be converted to and from pyruvate, and then analyzed similarly to study expected equilibrium isotope effects. Initial results show ¹³C enrichment in the residual whole molecule collected from the first of these two experiments; these findings soon will be complemented by site-specific and multiply-substituted analysis of these experimental residues.