



Highest-Magnetic-Field Ion Cyclotron Resonance Reveals Hidden Complexity of Natural Organic Matter

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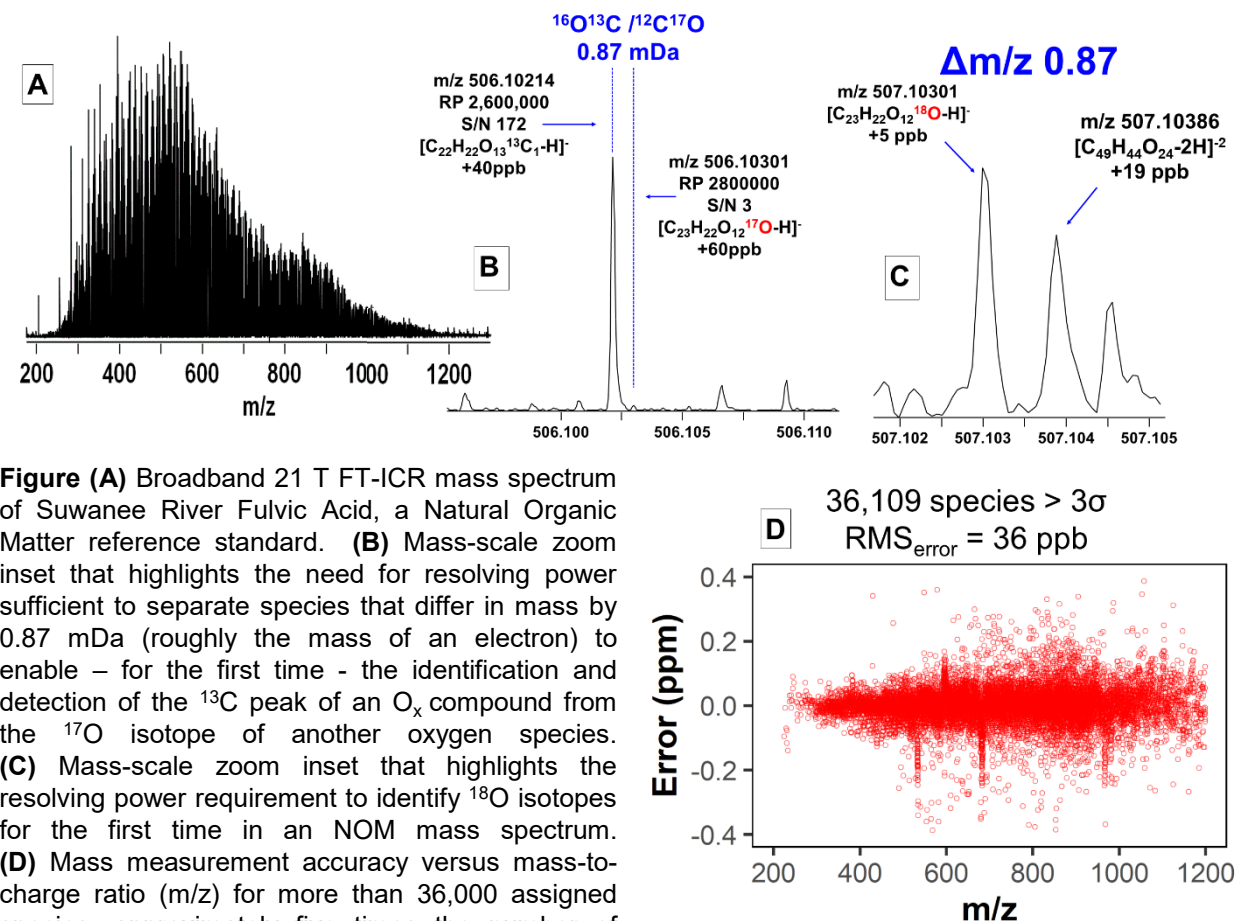
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Fourier transform ion-cyclotron resonance mass spectrometry (FT-ICR MS) is the only technique that can resolve the molecular complexity of natural organic matter and confidently assign thousands of detected elemental compositions. Active research on natural organic matter presently includes complex analyses of glacial thaw and permafrost, as well as the detection of emerging contaminants in food, water, and soil.

FT-ICR MS instruments that use lower magnetic fields (7-15 tesla) typically enable researchers to identify from a single complex mixture roughly 10,000 different molecules by their elemental formulas. In this work, MagLab users leverage the improved performance (higher dynamic range, resolving power, and mass measurement accuracy) of a custom built, 21 tesla hybrid linear ion trap/FT-ICR mass spectrometer to resolve and identify more than 36,000 species in one of the most commonly used reference standards for NOM, Suwanee River Fulvic Acid. The mass resolving power of five-million-to-one for molecules with $m/z \sim 200$ enables resolution of isobaric overlaps across the sample molecular weight range, a capability only achievable by 21T FT-ICR MS. For the first time, researchers resolve and identify ^{18}O and ^{17}O isotopologues that differ in mass from other species by as little as 0.87 mDa (roughly the mass of an electron).

The root-mean-square (rms) mass error for the 36,000 assigned species is 36 parts-per-billion, which is the most accurate measurement to date on a mixture this complex. The unique capabilities of the MagLab's 21T FT-ICR mass analyzer provide unparalleled insight into the molecular complexity of natural organic matter. These users are providing the molecular catalogue of this highly utilized reference standard to scientists worldwide via the Open Science Framework.



Facilities and instrumentation used: ICR Facility: MagLab's 21 T hybrid linear ion trap FT-ICR MS.

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