Annotation of Compound-Specific Molecular Structures in Aquatic Natural Organic Matter Using Liquid Chromatography Coupled witth Mass Spectrometry

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Natural organic matter (NOM), a complex assembly of biomolecules, is intimately involved in global carbon fluxes, in sustaining soil health for agriculture, and in the fate of contaminants. Limitations in methodologies for NOM characterization prevent a fundamental understanding of NOM dynamics. Unique molecular masses in NOM can be generated via Fourier transform ion cyclotron mass spectrometry (MS). However, elucidation of specific molecular structures in NOM is largely evasive. To overcome this challenge, we applied ultra high-performance liquid chromatography (LC) coupled with high-accurate orbitrap MS technology. Using a metabolomics approach, we have achieved annotation of compound-specific structures in the labile low molecular-weight (i.e., low mass-over-charge, *m/z)* portion in aquatic NOM samples, Suwannee River NOM and its alkaline (i.e., humic substance) extracts. Importantly, our method does not require a derivatization procedure. Thus far, we obtained simultaneous LC-MS detection of nearly 60 compounds, which are directly linked to metabolic pathways in microbial and plant biotia. This new methodological approach offers a molecular paradigm to track NOM genesis, transformation, and transport in the ecosystem.

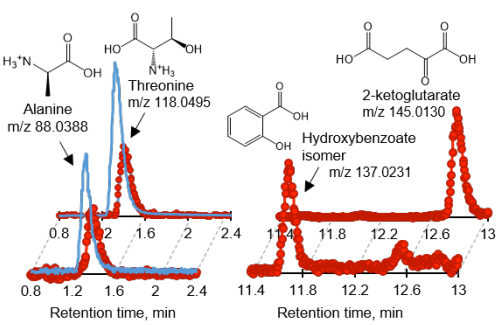

Figure 1. LC-MS spectra of NOM (red) with multiple detection of amino acids (left) and other organic acids (right) exhibiting different retention time and *m/z* values. Spectra from amino acid standard solutions are shown in blue.