

## Exploring the Soil Microbiome and Elemental Cycling via Advanced Mass Spectrometry at EMSL

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Given that over 90% of microbial community members cannot be cultivated (and thus have unknown functions and identities), together with exceptional diversity and lack of representative assembled genomic databases, microbiome omics data is extremely challenging to acquire, analyze and interpret, particularly with temporal and spatial resolution needed to decipher functional roles within the microbiome. Additionally, a limited understanding of the molecular composition and dynamics of natural organic matter (e.g. soil or dissolved organic matter) within microbial habitats limits our ability to interpret (bio)(geo)chemical processes within complex matrixes (e.g. soil). Therefore, successful development of molecular profiles that link soil microbiology with soil carbon (C) to ascertain soil vulnerability and resilience to climate change would have great impact on assessments of the soil ecosystems and their response to climate change. Fourier transform ion cyclotron resonance (FTICR) offers the highest mass resolving power and accuracy of any mass analyzer; nevertheless, even higher resolution and accuracy is required to capture the full range of information for increasingly complex natural mixtures (e.g., soil organic matter) and biological complexity (e.g., proteomics, metabolomics, metallomics). Herein, we will describe advanced mass spectrometry (MS) capabilities available at EMSL, a DOE national scientific user facility located at PNNL, to address the key knowledge gaps in functional understanding of how complex microbiomes influence and are influenced by their environment and present selected applications to oceanic, freshwater and soil microbiome field studies. Special emphasis will be on the novel high magnetic field (i.e. 21T) Fourier transform ion cyclotron resonance (FTICR) mass spectrometer recently brought online at EMSL. This capability will arguably provide that next level of performance needed to understand e.g. chemistry and dynamics of the belowground carbon cycle. Identification and quantitation of intact molecular structures derived from higher plants and soil microbiome within their native 3D inorganic soil matrix are essential for advancing molecular-scale mechanistic understanding of the role of physical, geochemical, and biological processes belowground. 21T FTICR platform will dramatically increase spectral acquisition rate and attainable sensitivity, and thus enable characterization of intact molecular structures in soil (and other complex matrixes) while addressing spatial relationships and heterogeneity, particularly in combination with other imaging modalities, e.g. FISH and/or nanoSIMS.