Novel analysis approach and new insights from FTICR-MS of soil organic matter

NANCY J. HESS[1], MALAK M. TFAILY[1], NIKOLA TOLIC[1], ALEJANDRO HEREDIA-LANGNER[1] AND E. ROBBY ROBISON[1]

[1]Pacific Northwest National Laboratory, Richland WA 99352 USA

The focus on ecosystem stress and climate change is currently relevant as researchers and policymakers strive to understand the feedbacks between soil C dynamics and climate change. The rhizosphere, where plant roots and their exudates meet microbial and fungal communities their metabolites, is a critical zone of dynamic C exchange and transformation in the belowground ecosystem. Successful development of molecular profiles that can link plant and microbial metabolic processes with soil C chemistry would greatly facilitate assessments of soil C dynamics and sustainability in response to changes in land use and climate.

Fourier transform ion cyclotron resonance mass spectrometry (FTICR-MS) has enabled the examination of organic molecules, directly from soil matrices, with ultrahigh mass resolution and sub-ppm mass accuracy. In this study, EMSL's extensive expertise and capabilities in FTICR-MS proteomics were leveraged to develop extraction protocols for the characterization of carbon compounds in SOM, thereby providing the chemical and structural detail needed to develop mechanistic descriptions of soil carbon flow processes. Using statistical approaches to analyze the mass spectrum we have been able to differentiate closely related soils prior to assigning chemical formula. Using molecular assignments we identify thousands of individual compounds in complex soils from diverse ecosystems within the USA. We found that **t**he yield of the chemical extraction was largely dependent on the type of solvent used and its polarity. Using this approach and metabolic network analysis we have identified possible chemical reactions relating classes of organic molecules that reflect abiotic and biotic processes which impact soil carbon composition. Examples of this approach will be presented from field studies of simulated climate change, vegetation restoration of long-term agricultural fields, and natural fire events. These novel approaches better enable soil scientists to address the challenging socioeconomic demands on the soil ecosystem.