# Novel analysis approach and new insights from UHR MS of soil organic matter

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**Abstract:**

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. 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 soil ecosystems in response to climate change. Additionally, a limited understanding of the molecular composition of SOM prohibits the ability to routinely decipher chemical processes within soil and predict how terrestrial C fluxes will response to changing climatic conditions. The use of ultra-high resolution Fourier transform ion cyclotron resonance mass spectrometry (UHR 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 UHR 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. In particular, we present a new extraction approach for more representative characterization of SOM thereby providing the necessary details needed to develop mechanistic descriptions of soil C 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 soil mixtures with a wide range of C content representing diverse ecosystems within the USA. We found that the yield of the chemical extraction was dependent on (1) the type of solvent used and its polarity, (2) sample-to-solvent ratios and (3) the chemical and physical nature of the samples including their origins. We have developed a sequential extraction protocol that permits sampling diverse classes of organic compounds while minimizing ionization competition in ICR cell. Using this approach 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.