Metabolomics, Lipidomics, and Metagenomics: Multiple Lines of Evidence for Monitored Natural Attenuation

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Background/Objectives. When monitored natural attention (MNA) is the desired strategy for a site, understanding the health of the microbial community is critical. Current molecular biological tools provide a wealth of information about the microbial community but none have the ability to inexpensively assess the health of the microbial populations present along with the potential for degradation. Recent advances in liquid chromatography–mass spectrometry (LC–MS)-based metabolomics and lipidomics have furthered understanding of metabolism in a variety of systems. Not only can such techniques be used to discover biomarkers for the physiological state of the system, they can also be used to probe the global metabolism of a sample by providing information on the concentration of thousands of molecules (i.e., the metabolome and lipidome) from a single analysis. These small molecules are the products of microbial metabolism and can provide key insights into the microbial community's health and function. Metabolomics can be used as an inexpensive screening tool to better understand the microbial community dynamics and function across an entire site. This information has the potential to greatly reduce overall analytical costs and provide a direct line of evidence for MNA.

Approach/Activities. Several analytical methods using ultra performance LC–high resolution MS (UPLC–HRMS) and UPLC–tandem mass spectrometry (UPLC-MS/HRMS) have been employed to ensure a broad coverage for the detection of metabolites from a variety of biological samples derived from many environments and all kingdoms of life. Using the metabolomics techniques, 90-180 known metabolites and 1500-5000 spectral features arising from water-soluble molecules with unknown structures can be detected. The lipidomics platform detects 400-600 known lipids with 5000-8000 spectral features from unknowns. The combination of high resolution MS data to determine molecular formulae and fragmentation data to help elucidate structure is a powerful tool to characterize water- and lipid-soluble intercellular metabolites as well as extracellular carbon-containing compounds.

Results/Lessons Learned. Data from multiple sites will be presented to compare metabolomic profiles from wells with and without active degradation of chlorinated hydrocarbons and petroleum hydrocarbons, and the presentation will describe how metabolomics can be a low-cost screening tool in site assessment. The information gained from these metabolomic samples will be shown coupled with other traditional molecular biological tools, such as metagenomics, to demonstrate their value and show how an approach using multiple lines of evidence will aid in determining which wells and sites are most appropriate for MNA.