# Using Environmental Metabolomics to Improve Decision Making at Chlorinated Solvent Sites

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**Background/Objectives.** Through bioremediation of chlorinated solvents, microorganisms break down harmful groundwater contaminants. Under the right conditions the microbes are able to destroy the toxins completely, transforming the original chemicals into harmless compounds. If the conditions are not right, the process can stall, resulting in a buildup of carcinogenic intermediates in our groundwater. Current tools and methods are limited in their abilities to determine if the microbial communities can efficiently detoxify a contaminated site or if stalls are likely to occur. Recent advances in liquid chromatography–mass spectrometry (LC–MS)-based metabolomics 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 the organisms within a sample by providing information on the relative abundance of thousands of molecules (i.e., the metabolome) 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. Patterns in metabolomics data can be used to differentiate between healthy and efficient communities of chlorinated solvent degraders or slowing and inefficient communities as well as to predict bioremediation stalls.

**Approach/Activities.** An ultra-high performance liquid chromatography–orbitrap high-resolution mass spectrometer (UHPLC–Orbitrap HRMS) is 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, 1500 to 5000 spectral features arising from water-soluble molecules with unknown structures can be detected. Patterns within these thousands of metabolites are analyzed via statistical tools and correlated with bioremediation efficacy.

**Results/Lessons Learned.** Data from multiple field sites will be presented to compare metabolomic profiles from background locations and wells with and without active degradation of chlorinated hydrocarbons. 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 or biostimulation.