Evaluation of Metabolomics as a Monitoring Tool at Chlorinated Solvent Sites

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Background/Objectives. Metabolomics is an emerging molecular biological tool (MBT), which involves using highly sensitive instrumentation to probe environmental samples (e.g., groundwater or soil extracts) to obtain a measure of all the small organic compounds present. These compounds can be collectively referred to as the metabolome (e.g., corrinoids, electron shuttling compounds, signaling compounds for organismal communication) and can provide key insights into microbial community health and function. Nucleic acid-targeted quantitative tools (i.e., qPCR) to enumerate biomarker genes and transcripts inform site assessment and remedial decision making (i.e., technology selection) at chlorinated solvent-contaminated sites. A shortcoming of this DNA-based monitoring approach is that the quantitative assessment of biomarker genes informs merely about the genetic potential, but not actual activity of the bacteria present. Efforts to integrate quantitative measurements of biomarker transcripts and/or proteins are ongoing and will enrich the MBT "toolbox"; however, the potential value of metabolomics to generate information about the biodegrading community has not been explored. Metabolomics has the potential to identify manipulations (e.g., more/less electron donor, trace nutrients) required to enhance activity of microbial groups relevant for process(es) of interest, and thereby serve as a powerful diagnostic tool in environmental monitoring regimes. We have begun to probe the utility of metabolomics as a direct measure of reductive dechlorination activity both on its own and in combination with other MBTs through the use of both axenic cultures, dechlorinating consortia, and in environmental samples.

Approach/Activities. Technological advances over the past decade have enabled researchers to obtain an unprecedented view of cellular metabolism, and we employ techniques that rely on liquid chromatography (LC) separation coupled with mass spectrometry (MS) detection as they are well suited to measure compounds whose structures are very diverse. The Orbitrap-based methods measure a panel of ~300 highly conserved intracellular metabolites and ~500 lipids, as well as tens of thousands of spectral features of compounds currently not represent in our standard library. These "new" compounds will add valuable information concerning the role that novel metabolites play in these systems. The endo- and exometabolomes of several representative axenic organohalide-respiring Chloroflexi grown with chlorinated solvents were measured and compared to the profiles obtained with the commercial bioaugmentation consortium SDC-9TM. The data gleaned from these experiments are being assessed for the ability to determine metabolite biomarkers for productive bioremediation in at sites impacted with chlorinated solvents.

Results/Lessons Learned. New MBTs that provide a direct measure of microbial activity and can be deployed easily in the field offer promise in aiding the monitoring of bioremediation activities. The metabolomics data collected from these experiments will provide a starting point to find metabolite biomarkers that could be used to monitor the activity of organohalide-respiring Chloroflexi.