The Use of NMR Based Metabolomics to Determine Biomarkers for Environmental Stressors

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Metabolomics is the study of small molecule metabolite profiles produced by specific cellular processes in an organism in response to normal physiological events or to an external stressful event. It is considered a complimentary 'omics' approach with genomics and proteomics. Nuclear Magnetic Resonance (NMR) based metabolomics can be used to rapidly assess the metabolic status of an organism and provide insight into the effects of environmental stressors. Through the use of NMR, metabolites in a biological sample may be measured in an unbiased manner with a targeted or non-targeted approach. Recent results of an international intercomparison exercise for NMR-based environmental metabolomics show that NMR metabolome analysis yields robust results with consistent trends in metabolite-based biomarker identification among laboratories (Viant et al. 2009). This type of demonstrated comparability is necessary as the technique is considered for regulatory environmental studies.

We propose to measure the metabolomic response of marine organisms to relevant stressors in lab experiments as well as field experiments. We hypothesize that particular metabolites in the organism of interest will provide information about the pathophysiological response of the organism. In turn, these measurements will be related to the overall health of the environment. To begin this study, the metabolic profile (in the form of a 1D NMR spectrum) of laboratory-grown *Spartina*, a sea grass native to the Atlantic coasts and prevalent in the Charleston area, has been analyzed. Exploratory polar and non-polar metabolite extractions were performed, and 1D and 2D NMR data collected using 700 MHz and 800 MHz instruments. Spectral annotations indicate the presence of sulphur cycle compounds as well as a host of others including amino acids, sugars, and others typical of the plant metabolome. These types of studies are key to understanding the effects of anthropogenic and natural stressors in coastal regions.

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