A Workflow for Archiving and Integrating Diverse Data for Structural Characterization of Biomass

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Project Goals: The BioEnergy Science Center (BESC) is focused on the fundamental understanding and elimination of biomass recalcitrance. BESC's approach to improve accessibility to the sugars within biomass involves 1) designing plant cell walls for rapid deconstruction and 2) developing multitalented microbes for converting plant biomass into biofuels in a single step (consolidated bioprocessing). BESC biomass formation and modification research involves working directly with two potential bioenergy crops (switchgrass and *Populus*) to develop varieties that are easier to break down into fermentable sugars. We are using both testing and generation of large number of natural and modified plant samples as well as developing genomics tools for detailed studies into poorly understood cell wall biosynthesis pathways. BESC researchers in characterization, modeling, and data management areas are engaged in 1) applying advanced technologies to analyze chemical and structural changes within biomass and 2) storing, tracking, analyzing and integrating data and understanding across the Center.

Terrestrial biomass is a highly complex material comprised primarily of secondary plant cell walls. The molecular structures of the biopolymers that constitute these cell walls vary depending on a large number of factors, including the plant species and the genetic makeup of the plant as well as growth, harvest, drying and storage conditions. The observable differences include variation in cell wall composition (i.e., relative proportions of various biopolymers), the molecular structures of these biopolymers and the overall infrastructure of resulting composite. These differences, in turn, lead to differential susceptibilities of the individual cell wall components to chemical and/or enzyme-catalyzed solubilization and saccharification. Although complete structural and ultrastructural characterization of the cell walls contained in different biomass samples is beyond our current technological capabilities, considerable structural information can be obtained using a wide range of spectroscopic, chemical and immunochemical methods. Each of these methods provides unique information, and interpretation of the data generated by one method almost always requires information provided by another method. Therefore, we have designed a workflow to collect diverse types of complementary analytical data from each biomass sample under study and archive this data in a dedicated database that facilitates integration and analysis of the global data set. This will provide an experimental basis for interpretation of each data set and the identification of correlations (e.g. covariance) among the different data sets. For example, changes in the molecular structure or amount of a specific polysaccharide might be correlated to changes in the capacity of a specific antibody to bind to the biomass, suggesting that antibody binding depends on the specific structure that changed. Correlation of such data to measured variations in biomass recalcitrance should lead to testable hypotheses regarding the molecular basis for recalcitrance and the development of genetic or agronomic approaches to modulate recalcitrance.

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