SAND2007-1828C

Enhanced Biomass-Bioenergy Conversion through Enzyme Engineering

"Energy crops" and agriculture waste are preferred long-term solutions for renewable, cheap and globally available feedstocks for biofuels. Biomass is converted to fermentable sugars for biofuels production using pretreatments, disrupting cellulose cross-links (e.g., lignocellulose) and allowing for "deconstruction" of cellulose into starch. A key area of this biomass conversion is the use of enzymes to covert biomass into the desired end-products to replace the current cost- and energy-intensive practices. The enzymes used in nature to accomplish this conversion are a part of a complex consortium of metabolic pathways that have been produced by evolutionary forces to be optimal for their specific operating environment. In order to be utilized effectively in artificial industrial settings which are significantly different than those normal operating conditions, changes must be made to both the structural and active components of these natural catalysts.

We are utilizing molecular modeling based approach to engineering proteins and metabolic pathways to adapt these for the increased conversion efficiency of biomass to bioenergy. The primary proteins targets that are being investigated for enhanced catalytic activity are cellulases derived from extremophiles. The target enzymes function to convert cellulose to intermediate hydrolytic products like cellobiose and have catalytic activity at high temperatures and extremes of pH, conditions that are compatible with the pretreatment processes in cellulosic deconstruction in a consolidated biorefinery. We are using our expertise in sequence-based structural and functional modeling to generate targets for enzyme engineering to produce a catalytically more efficient and active enzyme for the conversion of biomass. Initial efforts have focused on making a site directed mutations of enzyme targets, primarily cellulase (EC 3.2.1.4; GH families 9 and 12) based on a list of target sites and preferred mutant gene sequences generated by numerical modeling. This is coupled to a high-throughput strategy of enzyme screening for the rapid and reliable identification of desired enzymatic characteristics.