POPULAR SCIENTIFIC ABSTRACT

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Microscopic Characterization of Lignocellulosic Systems Mediated by Spectral Entropy and Simplex Optimization

The recalcitrance of lignocellulosic biomass is widely regarded as one of the major impediments of producing cellulosic biofuels, alongside the cost of cellulolytic enzymes for hydrolysis. Indeed, the economic challenges of utilizing enzymes for hydrolysis were described more than 25 years ago, triggering decades of intense research in the mechanisms of enzymatic hydrolysis by individual enzymes, as well as the origins of synergistic effects between multiple cellulolytic enzymes.

Current insights in the mechanisms of enzymatic hydrolysis have predominantly been established from studies on model cellulose systems. While these insights provide a fundamental, mechanistic understanding of cellulose hydrolysis, the extent by which these observations are transferable to lignocellulosic systems is largely unknown. This project posits that a major determinant precluding interrogation of mechanisms of enzymatic hydrolysis in lignocellulosic biomasses, is that tools for characterization of biomass microstructure are currently not compatible with the requirements for studying enzymatic hydrolysis.

The current project develops, benchmarks and demonstrates a combined multivariate framework and imaging methodology for detection, discrimination and mapping of chemical constituents using label-free hyperspectral data, with a view to moving toward label-free, in-liquid characterization of the lignocellulosic matrix and its concerted recalcitrance toward enzymatic depolymerization. It is shown that concurrent microscopic characterization of biomass microstructure and chemical composition can be achieved by considering the chemically-specific but mixed ‘fingerprints’ measured using microspectroscopic methods, as a ‘Cocktail Party Problem’. Based on blind signal separation, chemically-specific source signals in hyperspectral data are located, and used for reconstructing images with chemical specificity. It is demonstrated that the technique can be extended from 2D imaging to 3D imaging of plant microstructure, in in-liquid environments at atmospheric pressure, and without the use of fluorescent dyes.