Molecular Mechanisms Driving Biomass Deconstruction

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Lignocellulosic biomass, a potentially important renewable organic source of energy and chemical feedstock, resists enzymatic degradation to glucose in industrial hydrolysis processes and thus requires expensive thermochemical pretreatments. Understanding the mechanism of biomass breakdown during these pretreatments will lead to more efficient use of biomass. By combining neutron scattering experiments with molecular dynamics (MD) simulations, we reveal two fundamental processes responsible for the morphological changes in biomass during steam explosion pretreatment: cellulose dehydration and lignin- hemicellulose phase separation [1]. We further determine the mechanism of the tetrahydrofuran (THF)-water interactions with cellulose and lignin that render the co-solvent system highly effective for the fractionation and pretreatment of biomass [2]. Finally, we elucidate a detailed mechanism of how lignin reduces cellulase efficiency: lignin binds preferentially both to the elements of cellulose to which the cellulases also preferentially bind (the hydrophobic faces) and also to the specific residues on the cellulose-binding module of the cellulase that are critical for cellulose binding of *Tr*Cel7A (Y466, Y492, and Y493). Lignin thus binds exactly where for industrial purposes it is least desired, providing a simple explana- tion of why hydrolysis yields increase with lignin removal [3].

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