

### **139h Molecular Modeling of Cellulose Hydrolysis: the Hydrated Cel7a Linker Peptide**

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Plant biomass is the most abundant source of fermentable carbohydrates in the world, which when converted to fuels such as ethanol, holds the potential for significant environmental, economic, and strategic gains. Currently, chemical or biological conversion of biomass is too costly to permit ethanol to compete as a viable alternative fuel. For this reason, understanding the mechanisms of biological degradation of biomass, with special emphasis on the depolymerization of cellulose, is an active area of research.

In particular, cellobiohydrolase I (Cel7A), from *Trichoderma reesei*, is one of the most active cellulases known. Cel7A is a multi-domain exoglucanase enzyme, consisting of a large catalytic domain containing an active site tunnel and a small cellulose binding module joined to one another by a 27 residue linker peptide. Although the spatial conformation adopted by the linker domain is yet to be determined, it is thought to play an important role in the enzymatic hydrolysis of cellulose. This enzyme, which is found in fungal cellulase systems, is believed to hydrolyze cellulose in a “processive” manner, beginning from a reduced end of a cellodextrine chain, liberating cellobiose residues. Unfortunately, the exact mechanism is not known.

Since the linker peptide is relatively small, it is possible to study the energetic conformations adopted by the linker through molecular mechanics and molecular dynamics techniques. In this work, we will present results of computer simulations of the *O*-linked glycosylated linker peptide in an aqueous environment in order to gain insight into the role the linker may play in cellulose hydrolysis. Preliminary results will also be presented for the interaction of the peptide with a cellulose surface in order to study possible interactions of the linker with the surface.