INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
SHORT ABSTRACT OF THESIS

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Programme of Study	:	Ph.D.

Thesis Title: Production, characterization, *in silico* and crystal structure analyses of recombinant endo-**β**-1,3-glucanase of family 81 glycoside hydrolase (GH81) from *Clostridium thermocellum* ATCC 27405 and synthesis of laminarioligosaccharides for prebiotic applications.

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SHORT ABSTRACT

The thermophilic bacterium *Clostridium thermocellum* contains multienzyme complex called cellulosome which is known to degrade recalcitrant substrates. In this study one of the cellulosomal enzymes, β-1,3-glucanase (*Ct*Lam81A) of family 81 GH from *Clostridium thermocellum* was explored. *Ct*Lam81A was highly thermostable and displayed endo β-1,3-glucanase activity. The *in silico* and X-ray crystal structure of *Ct*Lam81A showed N-terminal β-sandwich domain, a $(\alpha/\alpha)_6$ domain and a short β-sandwich domain at C-terminal. Structural analysis of *Ct*Lam81A displayed the inverting hydrolytic mechanism. The docking of laminari-oligosaccharides to *Ct*Lam81A revealed that the active site can occupy maximum 5 glucose residues of β-1,3-glucan. The aromatic amino acid residues create the binding pocket at active site of *Ct*Lam81A to hold the ligand. The laminari-oligosaccharides generated by hydrolysis of curdlan by *Ct*Lam81A displayed prebiotic properties. They showed resistance or low digestibility against artificial gastric juice, intestinal fluid and α-amylase than inulin indicating their bioavailability to the probiotic bacteria present in the gastrointestinal tract of human. Therefore, laminari-oligosaccharides can be used for functional food additives.