Exploring Polysaccharide lyases of PL-5 family through the lens of structure, function, and dynamics

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Polysaccharide lyases are the biologically and industrially important enzymes, which catalyze non-hydrolytic degradation of polysaccharides via a beta-elimination reaction mechanism. There are 40 families of PLs in the CAZY database; classified based on their secondary structure elements and the folds. The PL-5 family enzyme adopts (alpha/alpha)\textsubscript{3,5} fold with an N-terminal lid-loop interaction giving rise to a pseudo-toroid architecture. Our research group work is focused on delineating the structure-function-dynamics for PL-5 family enzymes. To this end, the biochemical characterization has been carried on the selected among PL-5 enzymes to identify substrate specificity and enzyme efficiency. We have determined the X-ray crystal structures of the enzymes in apo and substrate-bound forms to understand structural aspects of substrate acquisition and specificity as a function of pH and the enzyme-substrate interactions. Further, the molecular dynamic simulation performed on the X-ray structures suggest the potential dynamics in loop configuration of the molecule to a closed and open state; providing mechanistic insights into functioning, and the mechanism of substrate acquisition and product expulsion in the PL-5 family enzymes.

Keywords: beta-elimination, pseudo-toroid, Molecular dynamic simulation, substrate acquisition