

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

Prerana Dash<sup>1,2</sup>, Rudresh Acharya<sup>1,2</sup>

<sup>1</sup>*National Institution of science education and research, Bhubaneswar, India;*

<sup>2</sup>*Homi Bhabha National Institute, Training School Complex, Anushakti Nagar, Mumbai 400094, Maharashtra, India*

*prerana.dash@niser.ac.in*

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)<sub>5,5</sub> 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