

Engineered enzymes to enhance selective degradation of PET to original monomers

Polyethylene Terephthalate (PET) is a widely used synthetic polymer due to its versatile material properties. The annual production of PET exceeds 73.39 million metric tons, out of which only 30% is recycled, leading to terrestrial and aquatic ecosystems pollution. Indeed, current mechanical or chemical recycling techniques are not techno-economically feasible to recycle PET. Recently, commercially applicable promising biocatalytic (enzyme or whole-cell) technologies have been developed to enable PET recycling and upcycling (make high-value products). However, the enzyme's kinetic parameters and thermal stability need to be improved to increase the PET degradation efficiency. Hence, our goal is to develop an efficient enzyme system that selectively degrades PET into monomers ethylene glycol (EG) and terephthalic acid (TPA). We will leverage the Molecular Dynamics (MD)-simulation to understand the molecular mechanism and mutants to enhance the PET degradation enzymes (**Fig. 1**). The Identified mutants via MD simulation will be introduced to the enzyme, and we will perform the *in vitro* and *in vivo* investigation to demonstrate the efficiency of PET degradation by engineered enzymes.

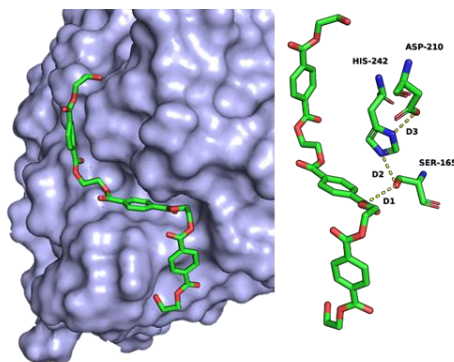


Fig.1 Optimized atomic configuration of MHET/Leaf Branch Compose Cutinase enzyme obtained from MD simulations (results from a simulation performed by a Physics Major undergraduate Kurtis Sanders)