

Fragment Based Active Site Exploration of Polyurethane Degrading Enzymes for Structure-guided Protein Engineering

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Polyurethane (PU) plastics are extremely durable and hard to recycle by conventional methods due to crosslinked and branched molecular structure. Recent discoveries of enzyme that target carbamate (urethane) bond in the PU provide alternative way of PU recycling by means of biocatalytic degradation. EnZync center has been established to discover, characterize and engineer novel enzymes for PU degradation. So far we have discovered several enzymes by computational searches and experimental ways. The critical steps to establish rational basis of protein engineering campaign is the understanding of Plastic-enzyme interactions at molecular level. To pursue structural characterization of "PURases" we have two different but complementary methods to characterize active site of PURases: i) Fragment Based Active site Exploration (FASE) of PURases by using small molecule fragment libraries and soluble PU analogs and ii) time-resolved serial crystallography by cryocapturing catalytic intermediate (for slow-millisecond kinetics) and ambient temperature (fast-microsecond) crystallography. We have completed FASE approaches for one of our patented enzymes and now we are starting to perform serial crystallography approach with promising preliminary data.

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