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STRUCTURAL INSIGHTS INTO THE CATALYTIC MECHANISMS OF PLASTIC-DEGRADING ENZYMES

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The accumulation of plastic waste in terrestrial and marine ecosystems poses a severe environmental threat nowadays. With an estimated 450 million metric tons of plastic waste produced annually, developing effective recycling methods is critical to achieve sustainability (Ritchie et al., 2023). While current solutions for end-of-life plastics include mechanical recycling, incineration, and landfill disposal, biochemical recycling -particularly via enzymatic depolymerization- is gaining attention as a greener method that operates under milder conditions (Shalem et al., 2024; Qiu et al., 2024). The incorporation of enzymes that tackle different plastic polymers (e.g poly(ethylene terephthalate)-PET or poly(lactic acid)-PLA) in cocktails could enable selective depolymerization of plastic mixed waste, addressing an additional key challenge behind the low rates of plastic recycling.

In this study, we focus on two enzymes, an engineered leaf-branch compost cutinase (LCC_ICCG) (Tournier et al., 2020) and a glucuronoyl esterase from Sporotrichum thermophile (StGE) (Taxeidis et al., 2024). LCC_ICCG displays enhanced thermostability and has been used as a template for engineering efforts aimed at developing variants with enhanced catalytic properties. LCC_ICCG displays activity strictly on PET, while StGE is able to tackle PET as well as amorphous PLA polymers. The goal of the present study is to define the structural determinants that define hydrolytic activity towards the aforementioned substrates and propose modifications that could increase catalytic efficiency. The crystal structure of apo LCC_ICCG was determined to 1.64 Å resolution. Docking simulations with PET oligomers reveal subsites that mediate terephthalate binding as well as hydrophobic residues that form critical interactions with the substrate. Moreover, docking simulations of PET and PLA oligomers using the crystal structure of StGE (PDB ID 4G4G) highlight interactions that determine the promiscuous nature of this enzyme.

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