Decoding Plastic Waste: Novel AI-Guided Engineering of PETase Mutants for Enhanced PET Plastic Bioremediation

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Polyethylene terephthalate (PET) represents one of the most prominent forms of synthetic plastic pollution, accounting for over 50 million tons of annual waste worldwide. Although the discovery of natural PET-degrading enzymes like PETase has provided a foundational base for biological recycling through bioremediation, the native enzyme exhibits limitations including low thermal tolerance, poor activity against high-crystallinity PET, and narrow pH ranges. To overcome these challenges, I developed PETase-M14, a computationally engineered PET hydrolase derived from Ideonella sakaiensis PETase, enhanced via an AI-guided design framework. My engineering strategy utilized a transformer-based neural network (StructuRiNet) to predict mutation fitness, integrated with a probabilistic regression model (BayesRegression) that estimates PET hydrolytic efficiency using structural, thermodynamic, and biochemical descriptors. Through iterative silico selection, I introduced 14 synergistic mutations designed to enhance thermal stability, folding energetics, and PET substrate binding. Experimental characterization of PETase-M14 revealed a substantial increase in degradation activity over wild-type PETase on untreated amorphous PET films, alongside a significant improvement in thermal stability (+19–22°C Tm). The enzyme retained >90% of peak activity across a broad pH range (6.0–8.5) and temperature window (30–55°C). PETase-M14 also efficiently degrades postconsumer plastics, achieving up to 92.8% mass reduction within 120 hours. This work demonstrates the power of AI-assisted enzyme engineering to accelerate bioremediation optimization and provides a practical route toward enzymatic PET recycling under environmentally realistic conditions.

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