Title:	Synergistic action of different thermostable esterases in pet degradation: improvement of activity against intermediate degradation products by protein engineering
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Abstract:	Polyethylene terephthalate (PET) is high molecular weight polymer of terephthalate (TPA) and ethylene glycol (EG) which constitutes a rapidly increasing environmental threat. It is broken down to bis- (BHET) and mono -(MHET) hydroxyethyl-terephthalate and ultimately to TPA. The bacterium, Ideonella sakaiensis 201-F6, uses PET as a primary carbon source, and contains a two-component PET-degrading system consisting of a PET/BHET-degrading esterase, which aggregate at temperatures above 30 °C, and a MHET-degrading esterase/lipase with optimal function at 30 °C. The glass transition temperature (Tg) of PET, anticipated to enhance rates of hydrolysis by increasing access of enzymes to PET chains is ~70 °C, creating scope for development of thermostable PETases. Promising thermophilic enzymes such as Thermobifida fusca cutinase (TfCut2), metagenomic leaf/branch compost cutinase (LCC), and certain carboxylesterases (CEs) show PET-degrading ability. LCC outperforms I. sakaiensis PETase, and is the most efficient PET-degrading enzyme known; however, it has too high a binding affinity for PET to display disseminated degradation of crystalline PET, and also aggregates at high temperatures, and is inhibited by MHET. We determined amino acid residues crucial to PET binding and hydrolysis in LCC, TfCut2 and an uncharacterized CE from Thermus thermophilus (TTCE), using molecular docking, MD simulations with 2-HE(MHET)4 and structural-biochemical considerations. Attempts were then made (using rational mutagenesis based on residue changes inspired by I. sakaiensis PETase) to enhance catalytic efficiency in TTCE and TfCut2, reduce aggregation of LCC, reduce binding of PET by LCC, reduce MHET-based inhibition, and cause synergistic degradation of PET and BHET by different pairs of enzyme. Amongst other results, we report a pair of variants that are more effective than LCC in PET degradation, and have additional benefits.
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