Sustaining Tomorrow: AI Solutions Toward Biological Recycling of Polyurethane Plastic Waste

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Escalating plastic waste demands breakthroughs. Promising biological plastic recycling (BPR)—using microbial-origin enzymes, is little explored for poorly recycled polymers like polyurethanes (PU). Highly researched PET-BPR uses time-consuming, resource-intensive, IsPETase laboratory evolution for critically needed enzyme improvements. To address slow BPR progress, this science project, 1) created, 2) validated and 3) applied an original and efficient workflow, harnessing for the FIRST-time ProteinMPNN and AlphaFold2 for depolymerization-enzyme engineering. Both are cutting-edge deep-learning-based, open-source AI tools. The workflow with 3 simple, web-based, input-output steps, presents >50,000-fold acceleration over current experimental methods. In ~10 minutes, ProteinMPNN replicated 5 of 5 IsPETase amino acid replacements reported from years of research. Next, by redesigning a 2023-reported, PU-degrading, metagenomic (from plastic-waste-facility soil) wild-type urethanase (WTU), the study presents the applicability of the workflow beyond PET. WTU structure being unknown, structure prediction by AlphaFold2 enabled the ProteinMPNN step, generating a FIRST urethanase protein structure (PDB-search confirmed). In another FIRST, the resulting AI-evolved urethanase—AIU, had 22.6% ($p=0.002$) increased expression (an indicator of yield) in E. coli. This confirmed the workflow is compatible with an enzyme-production system so that AIU can be tested for industrial utility. In conclusion, this study is among the first to demonstrate urethanase engineering as a proof of concept for PU-BPR, a hard-to-recycle polymer. Novel AIU and the innovative, fast, reliable, low-cost, enzyme-design approach, lay the groundwork for expedited BPR to ultimately help curb plastic pollution.