# GAP: A Novel Genetic Algorithm Design of PETase Variants Optimized to Biodegrade Crystalline PET

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Polyethylene terephthalate (PET) is one of the most common plastics used worldwide, and is used to create products like water bottles, food packaging, and textiles. PET is difficult to break down in the environment. In particular, high-crystallinity PET, which makes up most bottle-grade plastic, has tightly packed polymer chains. While current PETase enzymes can degrade PET under laboratory conditions, their activity drops significantly when acting on crystalline PET, creating a major barrier to applying scientific solutions to the real world. My project uses a computational model to design PETase variants with a higher bonding efficiency with crystalline PET. ProteinMPNN-DDG, an AI model that can predict the impact of single mutations on stability, was used to optimize PETase to maximize stability. Each mutation was checked for its impact on the geometries, flexibility, dynamics, acidity, and electrostatics of the enzyme. Additionally, a fast docking software was used to improve the PET's docking. The results identified several PETase variants with improved predicted binding to the PET compared to the original enzyme. In the future, I hope to verify my work using wet lab methods and compare my modified PETase with WT PETase and FAST-Petase.

**Awards Won:**