Nouveau-AI-Plastic-Degen: A Novel Approach Using AI-Based Enzyme Engineering To Design New and Highly Efficient Marine Plastic Degrading Enzymes

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In this project through machine learning guided directed evolution, a novel Marine plastic degrading enzyme “Eco-Enzyme” was designed to reduce plastic pollution. It is estimated that there is at least 14 million tons of plastic in our oceans. In 2016, researchers discovered PETase, a naturally occurring enzyme that breaks down PET. However, PETase is not the best enzyme for degrading environmental marine plastics, as it functions optimally at a relatively high temperature (Topt) of 44.2 °C. In 2019, another enzyme Thermobifida-fusca-Cutinase(TfCut) that broke PET down at lower temperature (40.35 °C), was identified. In this project, Machine Learning guided directed evolution was used to design a novel mutant enzyme of TF-Cut with an optimal temperature within the average range of ocean surface temperatures(20-25°C), allowing the enzyme to degrade marine plastic with a high efficiency. Three machine learning models: Logistic and Linear Regression, and Random Forest; were trained to predict Topt with high performance, using a data set built of enzymes from the BRENDA database online. Following training, Random Forest, the best performing model, was used to implement ML-guided directed evolution. In this process, my algorithm generated hundreds of mutants of TF-Cut, selected the mutants with the lowest Topt, and used the lowest Topt mutant for future mutation. After 35 iterations, a novel mutant of TF-Cut(“Eco-Enzyme”) was generated with Topt of 24 degrees Celsius. This enzyme has the potential to be the first enzyme to break down marine plastic. The next steps are lab validation of “Eco-Enzyme” and introducing it into Cyanobacteria.

Awards Won:
Third Award of $1,000
Arizona State University: Arizona State University ISEF Scholarship (valued at up to $52,000 each)