# High School Workshop Plan: AI Empowering Biological Experiments

## 1. Workshop Basic Information

- Theme: AI Empowering Biological Experiments – From Plastic-Degrading Enzyme Design to Practical Exploration
- Time: August 20th, 2025 (14:00 - 17:00 p.m.)
- Participants: NEBS-VCA team members & KVIS high school students
- Core Objectives:
  - Help students understand AI's application principles in biological experiments (focus on plastic-degrading enzyme R&D) and the "AI-assisted enzyme design - experimental verification" process.
  - Guide students to use simplified software for AI-based target screening simulation and co-design small-scale verification experiment plans.

## 2. Workshop Agenda Design

### Background Introduction

- Each member gives a self-introduction, covering their iGEM project direction (integrating "plastic pollution" "biological enzymes") and interesting "AI + Biology" scenarios.
- Background Introduction: NEBS-VCA team uses data to explain traditional biological experiment shortcomings, highlighting the urgency of AI to speed up biological enzyme.

### Core Knowledge: AI in Biological Experiments

*3 Stages of AI-Assisted Biological Experiments*

1. AI "Clear Observation" via MD Simulation: Use GROMACS/AMBER to simulate PETase-PET interaction, observe enzyme active pocket's PET accommodation and identify essential amino acids, providing structural info for AI.
2. "Intelligent Screening": AI uses "sequence + structure + dynamics" data to select mutations that improve thermal stability/catalytic efficiency, avoiding blind experiments.
3. "Result Verification": Lab-test AI-predicted mutants (e.g., E. coli expression purification) to form "AI design - experimental verification" loop.

*Practical Tools*

- Pross Server: Online input of PETase sequence to predict thermally stable mutants.
- Simplified AlphaFold2: Rapidly generate mutant 3D structures, compare active pocket differences between wild-type and AI-designed PETase to explain mutation effectiveness.

### 3. Discussion

1. "Can AI completely replace biological experiments?" (AI is a tool, experiments are core – based on "AI predictions need experimental verification".)
2. "How to use AI to design specific enzymes for Thailand’s common plastic waste (e.g., fishing nets)?"