

SCIENTIFIC ENGLISH IMMERSION WITH HANDS-ON EXPERIMENTATION ON MICROBIAL PLASTIC DEGRADATION IN VIETNAM

Computer-Assisted Molecular Modeling of Plastic-Eating Enzymes

Prof. Meden F. Isaac-Lam

Project Leader 1

Fulbright Alumni Exchange Program
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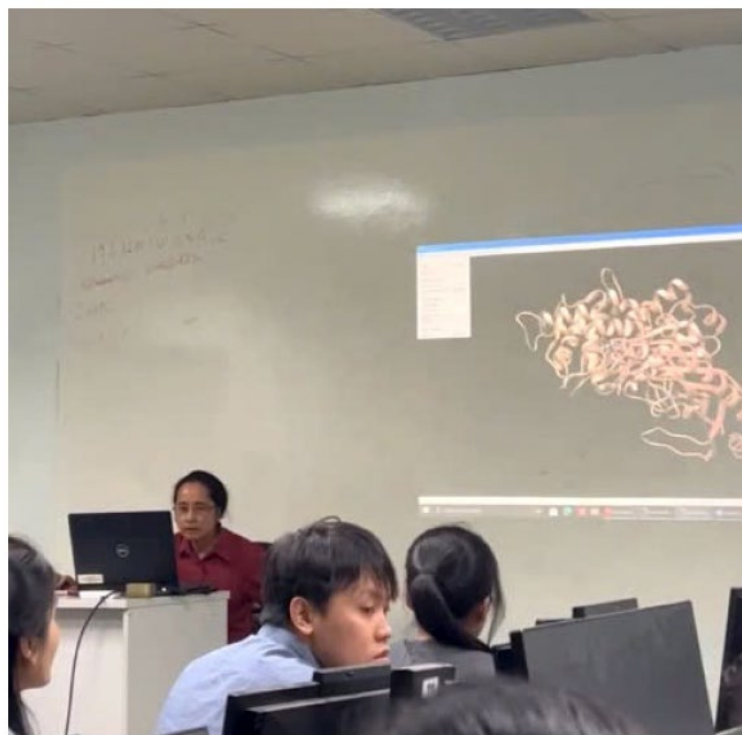
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AI-INSPIRED COMPUTER SIMULATION



CDAF Team Leader 1 Prof. Meden F. Isaac-Lam introduced three-dimensional protein structure as key concept in understanding the role of enzymes to biodegrade plastics. Participants attending the lecture on August 6, 2024 include Vi Nha Tran from Can Tho University (left), Nguyễn Thảo Trang from University of Social Sciences and Humanities Nguyễn Van Hai from Nong Lam University, Lương Thị Mỹ An from Golden Gate University, (middle photo: right to left), and others (right photo) in the computer lab at TTU. Team Lead 1 discussed the open-source molecular modeling software Chimera, an extensible program for visualization of molecular structures and related data developed by UCSF (University of California, San Francisco) Resource for Biocomputing, Visualization and Informatics (RBVI).

AI-INSPIRED COMPUTER SIMULATION

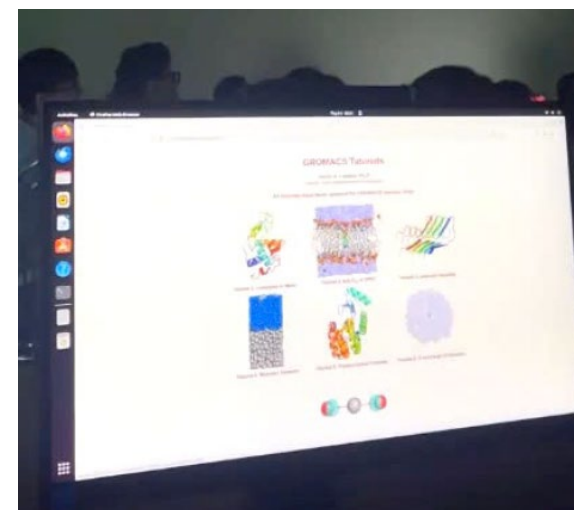
Team Lead 1 was assisted by Teaching Assistant Phạm Thị Ngọc Hân (Ton Duc Thang University, Institute of Chemical Technology) and staff Nguyễn Ngọc Mai Phuong to demonstrate the use of Gromacs (bottom right), a free and open-source suite for molecular dynamics and output analysis. The software provides high performance algorithmic optimizations in its codes primarily designed for biochemical molecules such as proteins, lipids and nucleic acids as well as non-biological systems including polymers, plastics and fluid dynamics to understand and calculate complicated bonded and non-bonded interactions. Protein-substrate, as exemplified by enzyme-ligand, specifically, PET (polyethylene terephthalate) hydrolase-PET degradation product, was shown as a docking experiment wherein a partially-degraded plastic product interacts with enzyme found to be isolated in bacterial gut. Both Chimera and Gromacs were presented as part of the in-person activities for the participants to recognize the application of AI (Artificial Intelligence) in probing the biochemical mechanism of enzymatic microbial degradation of plastic, which is one of the core objectives of our CDAF project in providing a possible solution to the plastic pollution in Vietnam. With this activity, participants gained knowledge regarding the best cutting-edge technology incorporating AI platforms into biological processes.



Prof. Meden F. Isaac-Lam with project assistants Phạm Thị Ngọc Hân and Nguyễn Ngọc Mai Phuong.



Phạm Thị Ngọc Hân
MS Chemistry student



Gromacs software

PLASTIC-EATING ENZYME WITH PLASTIC PRODUCT

Example of computer simulation experiment to visualize the interaction of plastic degradation product with a plastic-eating enzyme shown to the participants.

