Electronic and Atomic Protein Modeling (EAPM)

Our team focuses on the theoretical modelling of biochemical and biophysical processes at a molecular, atomic, and electronic level of detail. We place emphasis both on development of methods and on their

application to specific systems. Particular areas of interest include: protein engineering, drug design and software development.

Objectives

Main objectives include:

- Developing our in-house code Monte Carlo (PELE) for better sampling of protein/DNA-ligand interactions
- Improving the user experience in interactive molecular modelling by combining biophysics/biochemistry software with state-of-the-art graphics, High Performance Computing and Artificial Intelligence.
- Develop new approaches for mapping in silico protein engineering focusing on: protein mutation, substrate migration and chemical process.
- Application studies of our (and others') modelling techniques for addressing specific biomedicine and biotechnology problems. Here we aim to establish collaboration with top experimental labs and industries.

Current EU funded projects:

- FuturEnzymes
- OXIPRO

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