Electronic and Atomic Protein Modeling (EAPM)

Our team focuses on the theoretical modelling of biochemical and biophysical processes placing emphasis both on development of methods and on their application to specific systems. For this, we combine different modeling techniques including: quantum mechanics electronic structure, molecular modeling (Monte Carlo and molecular dynamics techniques), bioinformatic statistical analysis, machine learning, etc. Particular areas of interest involve two main topics: biomedical applications and industrial biotechnology

Objectives

Main objectives include:

- Developing our in-house code Monte Carlo (PELE) for better sampling of biomolecular interactions.
- Integrating machine learning techniques and molecular modeling methods for an optimal efficiency-speed ratio in (large) biomolecular sampling strategies: bioprospecting, engineering, screening, etc.
- 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
- ROBUSTO
- LWNVIVAT
- BIOMACHINE

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