MOL 910 BIOSTRUCT – Biomolecular Modeling

ECTS

10 ECTS

Teaching methods

Lectures: 37 h, Lab exercises: 37 h lab.

Course contents

The course provides an introduction to key techniques for modeling of biological molecules with a focus on molecular structure and function. Techniques to analyze and validate computations are also central in the course. The course focuses on three main areas: i) molecular mechanics: force field, composition and evaluation techniques, and simulation techniques; ii) conformational sampling by geometry optimization, molecular dynamics, and Monte Carlo simulations; iii) free energy calculations: determination of binding energies using free energy perturbation, linear interaction energy, and simplified scoring approaches.

Objective of the course

The candidate will acquire a theoretical knowledge and hands on experience to understand, plan and execute a simple molecular modeling project.

The successful student will:

Knowledge

- Molecular mechanics concepts and basics of statistical thermodynamics
- Main algorithms used for geometry optimization, molecular dynamics and Monte Carlo simulations
- Principles and approximation behind main free energy calculation methods
- Principles and techniques for molecular docking

Skills

- Perform geometry optimization on biomolecules
- Set up and conduct molecular dynamics simulations projects, including data analysis
- Calculate binding free energies with different methods, and pick the most appropriate approach
- Set up and conduct a docking project

General competence

- Independent planning and execution of a protein modeling project, be it to study structure-function relationship or ligand binding
- Ability to choose the modeling methods appropriate to a given project and a given question