Universidad Zaragoza

Academic Year/course: 2024/25

68454 - Simulations of Biomolecules

Syllabus Information

Academic year: 2024/25
Subject: 68454 - Simulations of Biomolecules
Faculty / School: 100 - Facultad de Ciencias
Degree: 626 - Máster Universitario en Biofísica y Biotecnología Cuantitativa / Master in Biophysics and Quantitative Biotechnology
ECTS: 6.0
Year: 01
Semester: First semester
Subject type: Compulsory
Module:

1. General information

This course covers the state of the art of molecular simulations applied to Biomolecules and it is design to provide the students an understanding on these techniques and also to be capable to perform calculations for their own projects using the available computer codes. The student will be able to:

1. understand tridimensional structures of biomolecules and the main forces acting on the atoms
2. know the main methodologies and approximations employed for (bio)molecular simulations
3. choose the most adequate computational technique for a given biomolecular problem
4. understand the main features of drug design in pharmaceutical companiesv) be proficient, at a user level, with specialized software to simulate and study protein flexibility or protein ligand interactions

These approaches and objectives agree with the following Sustainable Development Goals (SDGs) of the United Nations Agenda 2030 (https://www.un.org/sustainabledevelopment/es/), in such a way that the acquisition of the learning results of this subject provides training and competence to contribute to a certain extent to its achievement:

- Goal 3: Health and wellness
- Goal 4: Quality education

Students should have a basic chemical and/or physics background on molecular structure and properties and intermolecular interactions. Basic knowledge on UNIX environment is recommended.

2. Learning results

- The main goal of this subject is to know the main structural features of biological molecules and the interactions that are at their origin.
- To understand the theoretical basis of the most used techniques for the simulation of biomolecules.
- To be able to apply these techniques to simple problems using computer programs.
- To recognize the limitations of the studied techniques and to choose among them the most suitable for a given problem.

The understanding of the different simulation techniques and the ability of carry out calculations using computer programs is a basic skill which is essential for the design of new Biotechnological projects and for a future career as a researcher within this field.

3. Syllabus

1. Introduction to computational models in physics and chemistry.
2. Experimental determination of biomolecular structures: X-ray, NMR, electronic microscopy, protein data

bank.

3. Molecular Dynamic simulations I. Force fields for biomolecules.
4. Molecular Dynamic simulations II. Force fields, minimizations and algorithms.
5. Molecular Dynamic simulations III. Tools in statistical mechanics. Thermostats.
6. Molecular Dynamic simulations IV. Design and analysis of simulations.
7. Quantum Mechanics I: Molecular models and simulation methods.
8. Quantum Mechanics II: Hybrid QM/MM methods.
9. Docking techniques for Protein-ligand interaction.
10. Structure-activity relationships. Molecular descriptors. Quantitative structure-activity relationships (QSAR).

4. Academic activities

The course includes 6 ECTS organized according to:

1. Lectures (2 ECTS): 20 hours. In these classes students are presented with the basic theoretical knowledge of the course and the participants are continuously requested active participation
2. Laboratory sessions (3 ECTS): 30 hours. Workshops, practical work, and individual work in the computer classroom will take place in groups of up to 10 people. They will cover aspects presented in lectures and / or practice sessions in the computer classroom. Individual work with computer is also used
3. Assignments (1 ECTS): 10 hours. Presentation of an assignment or seminar: Students will collect individual or group information on a specific topic, led by the teacher. In general, the analysis of the information will lead to the elaboration of a report organized in Introduction, Methods, Results, Discussion, Conclusions, and Bibliography, as well as to its presentation and discussion in class.
4. Autonomous work: 90 hours

5. Assessment system

The course evaluation consists of two parts: theoretical contents and practical activities, which will be evaluated as follows:

Written exam on theoretical contents (**60%** of the overall grade). To be able to average with the practical activities, a minimum grade of 3.0/10 is required.

Evaluation of practical activities (**40%** of the overall grade). The evaluation of practical activities can be done in two ways:

- Completion of a given project. For that, **attendance to at least all but 2 of the practical activities is required**. In this case, the **grade for the practical activities will be the grade for the project minus 1 point for each practical activity missed without justification**.
- Practical exam. A theoretical-practical exam on the content of the practical lessons. Taking the exam will be mandatory if more than two practical activities are missed. Similarly, students may choose to take the practical exam instead of completing the project.