Universidad Zaragoza

Curso Académico: 2023/24

68454 - Simulación de Biomoléculas

Información del Plan Docente

Año académico: 2023/24
Asignatura: 68454 - Simulación de Biomoléculas
Centro académico: 100 - Facultad de Ciencias
Titulación: 626 - Máster Universitario en Biofísica y Biotecnología Cuantitativa / Master in Biophysics and Quantitative Biotechnology
Créditos: 6.0
Curso: 01
Periodo de impartición: Primer semestre
Clase de asignatura: Obligatoria
Materia:

1. Información básica de la asignatura

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. Resultados de aprendizaje

- 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. Programa de la asignatura

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. Actividades académicas

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. Sistema de evaluación

1. Written work (35% of the final grade). Elaboration of a report, on a topic related to the subject. The memory will be realized individually or in groups of 2 students. It will be assessed if the work follows a coherent structure in blocks (introduction, methods, results, discussion, conclusions and biography), clearly describes the problem's approach, describes the methods and results in a logical and sequential, provides original ideas in the description, provides justifiable conclusions of the work, and provides an appropriate bibliography
2. Written exam (50 % of the final grade). The written test will consist of questions that require short answers (limited response tests) or that require a broad development of the subject (free and open test or response tests). The former will allow a broad sampling of the student's knowledge on the subject, and the latter will allow to assess their capacity for expression, to present and sustain arguments, and to make critical judgments. The written test will be based on the programmed learning activities program
3. Seminar work (15% of the final grade). Elaboration of memory, exhibition and public defense of a work on a topic related to the subject. The memory will be realized individually or in groups of 2 students. The work will be exhibited and defended by each group of students in seminar-type sessions. The time available for the presentation and defense of the topic during the seminar sessions will be 10-15 minutes. It will be assessed if the work follows a coherent structure and provides an appropriate bibliography. During the presentation, the clarity and order of the exhibition will be evaluated, as well as the maturity of the debate.