Universidad Zaragoza

Academic Year/course: 2021/22

68454 - Simulations of Biomolecules

Syllabus Information

Academic Year: 2021/22
Subject: 68454 - Simulations of Biomolecules
Faculty / School: 100 - Facultad de Ciencias
Degree: 626 -
ECTS: 6.0
Year: 01
Semester: First semester
Subject Type: Compulsory
Module:

1. General information

1.1. Aims of the course

This course explains the fundamentals of molecular simulations and their applications to biomolecular systems. The student will be able to: i) understand tridimensional structures of biomolecules and the main forces acting on the atoms, ii) know the main methodologies and approximations employed for (bio)molecular simulations, iii) choose the most adequate computational technique for a given biomolecular problem, iv) understand the main features of drug design in pharmaceutical companies, v) be proficient, at a user level, with specialized software to simulate and study protein flexibility or protein ligand interactions

1.2. Context and importance of this course in the degree

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.

1.3. Recommendations to take this course

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 goals

2.1. Competences

Basic and general:

CG 01 ? To arrange, analyze critically, understand and synthesize information

CG 02 ? To obtain information from different types of sources and evaluate their reliability

CG 03 ? To learn efficiently through autonomous study and acquire a significant level of independence

CG 04 ? To implement the acquired knowledge and solve problems in new or unfamiliar environments within broader (or multidisciplinary) contexts related to the study area

CG 05 ? To formulate, analyze, evaluate and compare new or alternative solutions for different problems

CG 06 - Being able to work in multidisciplinary and international teams.

CG 07 ? To develop capacity for criticism and self-criticism.

CG 08 ? To make decisions taking into account social, ethical and legal responsibilities

CG 09 - Be able to develop a project, participating in the stages of bibliographic search, planning of experiments, obtaining results, interpretation, and dissemination of the same

CB 6 ? To have and understand knowledge that provides a basis or opportunity to be original in the development and / or implementation of ideas, often in a research context

CB 7 ? The students know how to implement the acquired knowledge and their ability to solve problems in new or little

known environments within broader (or multidisciplinary) contexts related to their area of ??study

CB 8 ? The students are able to integrate knowledge and face the complexity of provide opinions based on information that, being incomplete or limited, includes reflections on social and ethical responsibilities linked to the application of their knowledge and opinions.

CB 9 - The students know how to communicate their conclusions and the latest knowledge and reasons that support them to specialized and non-specialized audiences in a clear and unambiguous way

CB 10 - The students have the learning skills that allow them to continue studying, largely self-directed or autonomous.

Transversals

CT 01 - Properly management of the available resources and time for solving a problem or developing a project

CT 02 ? To communicate own conclusions and the last knowledge and reasons that support them - to specialized and non-specialized audiences in a clear and unambiguous way.

CT 03 - To Transmit oral, writing or graphically information using appropriate presentation tools and with the limitations imposed by time or space.

CT 04 - Fluently communication in English (understanding of scientific texts, writing reports, talks, colloquiums, exhibitions, etc.).

Specifics

CE01 ? Understand the relationship between the structure of a biomolecule (folding, stability, ?) and its function within (and without) the physiological context for research or biotechnological goals.

CE12 - To carry on simulations for the study of dynamical, structural and functional properties of theoretical models of biological interest (biomolecules, biological networks, ?) using the most suitable algorithms for simulation and analysis of results

CE14 ? Search, visualize and interpret information on the three dimensional structure of molecules of biological interest

CE15 ? To handle computer packages of molecular dynamic simulation, molecular coupling and molecular modelling, and simulation of hybrid classical/quantum systems as well.

2.2. Learning goals

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.

2.3. Importance of learning goals

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. Assessment (1st and 2nd call)

3.1. Assessment tasks (description of tasks, marking system and assessment criteria)

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

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

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.

4. Methodology, learning tasks, syllabus and resources

4.1. Methodological overview

The methodology followed in this course is oriented towards achievement of the learning objectives. Lectures will generally use computer screen projections (PowerPoint), including small animations, videos and offline browsing. Blended learning will be used to exchange information with the students and to guide them on the presentation of their individual assignment.

The preparation of seminars and individual assignments will train students in the search for relevant information on the Internet, the use of databases, scientific bibliography and network applications. Students will be encouraged to use original scientific material (scientific publications, patents) to interpret it, for the presentation of the information to both a specialized and a general public. This activity will teach students how to communicate conclusions ?the ultimate knowledge and reasons behind them? in a clear and unambiguous way.

Laboratory practice sessions or workshops in the computer room: the teacher will provide the scripts of the laboratory practices through the platforms of semi-classroom teaching, and after the theoretical presentation, they will be discussed in the laboratory or computer classroom. These activities will instruct the students on how to approach experimental techniques or computational methods, and present the data and results provided by their application. Finally, the results will be shared and discussed with peers. This part of the course requires both group and individual work by the student. These activities will allow the student to acquire the necessary skills and abilities to describe, quantify, analyze and critically evaluate the obtained results, as well as to independently use the experimental techniques and methods related to this Master's and to design technical and methodological alternatives.

Workshops and debates. The discussion of a research topic or relevant technological development that has shown significant progress in recent years will allow students to express their opinions on the subject in question, as well as to propose alternatives to the solutions presented for them.

4.2. Learning tasks

The course includes 6 ECTS organized according to:

- **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.

- **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

- **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.

- **Autonomous work**: 90 hours

4.3. Syllabus

The course will address the following topics:

Topic 1. Introduction to computational models in physics and chemistry.

Topic 2. Experimental determination of biomolecular structures: X-ray, NMR, electronic microscopy, protein data bank.

Topic 3. Molecular Dynamic simulations I. Force fields for biomolecules.

Topic 4.Molecular Dynamic simulations II. Force fields, minimizations and algorithms.

Topic 5. Molecular Dynamic simulations III. Tools in statistical mechanics. Thermostats.

Topic 6. Molecular Dynamic simulations IV. Design and analysis of simulations.

Topic 7. Quantum Mechanics I: Molecular models and simulation methods.

Topic 8. Quantum Mechanics II: Hybrid QM/MM methods.

Topic 9. Docking techniques for Protein-ligand interaction.

Topic 10. Structure-activity relationships. Molecular descriptors. Quantitative structure-activity relationships (QSAR).

4.4. Course planning and calendar

For further details concerning the timetable, classroom and further information regarding this course please refer to the "Facultad de Ciencias" website (https://ciencias.unizar.es).

The course is taught throughout the first semester (November-January).

Examinations: one exam at the end of the semester

4.5. Bibliography and recommended resources

http://psfunizar10.unizar.es/br13/egAsignaturas.php?codigo=68454