# 63101 - Biomolecular Simulation

**Información del Plan Docente**

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| **Academic Year** | 2018/19 |
| **Subject** | 63101 - Biomolecular Simulation |
| **Faculty / School** | 100 - Facultad de Ciencias |
| **Degree** | 572 - Master's in Quantitative Biotechnology |
| **ECTS** | 6.0 |
| **Year** | 1 |
| **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 understand tridimensional structures of biomolecules and the main forces acting on the atoms. The student will be able to choose the most adequate computational technique for a given biomolecular problem. To understand protein-ligand interactions at the molecular level. Also, to prepare input files, to carry on the simulation and to interpret the output files.

### 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 this 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.

## 2.Learning goals

### 2.1.Competences

Basic and general:

01 - Sort, analyze critically, interpret and synthesize information

02 - Obtain information from different types of sources and evaluate their reliability

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03 - Learning efficiently through autonomous study and acquiring a significant degree of independence

04 - Apply the acquired knowledge and solve problems in new or unfamiliar environments within broader (or multidisciplinary) contexts related to the area of study

05 - Formulate, analyze, evaluate and compare new or alternative solutions to different problem

06 - Be able to work in multidisciplinary and international teams

07 - Develop capacity for criticism and self-criticism

08 - Make decisions taking into account social, ethical and legal responsibilities

09 - Be able to develop a project, participating in the stages of bibliographic search, planning experiments, obtaining results, interpreting, and disseminating them

CB6 - Possess and understand knowledge that provides a basis or opportunity to be original in the development and / or application of ideas, often in a research context

CB7 - That the students know how to apply the acquired knowledge and their problem solving capacity in new or little known environments within broader (or multidisciplinary) contexts related to their area of study

CB8 - That students are able to integrate knowledge and face the complexity of making judgments from information that, incomplete or limited, includes reflections on social and ethical responsibilities linked to the application of their knowledge and judgments

CB9 - That 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

CB10 - That the students possess the learning abilities that allow them to continue studying in a way that will have to be to a great extent self-directed or autonomous

Specific:

06 - Find, visualize and interpret information about the tridimensional structure of biological macromolecules (proteins, nucleic acids, ...), organic molecules or organometallic complexes.

07 - Employ force field techniques to evaluate the energy and the forces of a system containing biological relevance molecules.

08- Choose the most suitable minimization and integration algorithms and to set up control variables to carry out a molecular simulation.

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09- Carry out molecular dynamics simulations to describe the temporal evolution of a system of biological molecules (description of the native set, folding/unfolding reactions, associative/dissociative protein ligand interactions).

10 - Design and perform Monte Carlo simulations for conformational sampling and calculation of averaged properties.

11 - Carry out analysis of simulations using principal component analysis (PCA), vibrational normal modes and free energy differences.

12 - Understand the principles of quantum mechanics simulations and their relationship to molecular dynamics simulations.

13 - Carry out hybrid simulations (QM/MM) for the study of enzymatic reactions.

14 - Carry out protein/protein and protein/ligand docking using different approaches for conformational flexibility.

15 - Link coupling tests between a target and a ligand library.

## 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 clearly 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:

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- **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:** 10 hours. 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. Experimental determination of biomolecular structures: X-ray, NMR, electronic microscopy, protein data bank.

Topic 2. Potential energy surfaces in biomolecules. Intermolecular forces. Molecular mechanics (MM): Force fields.

Topic 3. Molecular Dynamic simulations.

Topic 4. Algorithms and thermostats for molecular dynamic simulations.

Topic 5. Conformational sampling using Monte Carlo methods.

Topic 6. Analysis of the simulations. Principal Component Analysis, normal modes, free energies.

Topic 7. Quantum mechanics (QM) for enzymatic catalysis.

Topic 8. Mixed models for molecular simulations in enzymatic catalysis: QM/MM methodology.

Topic 9. Docking techniques for Protein-ligand interaction. 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

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"Facultad de Ciencias" website (https://ciencias.unizar.es).

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

Examinations: one exam at the end of the semester

## 4.5.Bibliography and recommended resources

Molecular Modeling and Simulation: An Interdisciplinary Guide. Tamar Schlick Springer

Understanding Molecular Simulation, Second Edition: From Algorithms to Applications Daan Frenkel Academic Press

Essentials of Computational Chemistry: Theories and Models Chris Cramer Wiley