COURSE DATA

Data Subject	
Code	44983
Name	Computational biochemistry
Cycle	Master's degree
ECTS Credits	5.0
Academic year	2022 - 2023

Study (s)

Degree	Center	Acad. year	Period
2245 - Master's Degree Erasmus Mundus in Theoretical Chemistry and Computational M	Faculty of Chemistry	1	Annual

Subject-matter

Degree	Subject-matter	Character
2245 - Master's Degree Erasmus Mundus in Theoretical Chemistry and Computational M	3 - Optativas de primero	Optional

Coordination

Name	Department
TUÑON GARCIA DE VICUÑA, IGNACIO NILO	315 - Physical Chemistry

SUMMARY

English version is not available

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

There are no specified enrollment restrictions with other subjects of the curriculum.

Other requirements

There are no previous prerequisites

COMPETENCES (RD 1393/2007) // LEARNING OUTCOMES (RD 822/2021)

2245 - Master's Degree Erasmus Mundus in Theoretical Chemistry and Computational M

- Students should apply acquired knowledge to solve problems in unfamiliar contexts within their field of study, including multidisciplinary scenarios.
- Students should be able to integrate knowledge and address the complexity of making informed judgments based on incomplete or limited information, including reflections on the social and ethical responsibilities associated with the application of their knowledge and judgments.
- Students should communicate conclusions and underlying knowledge clearly and unambiguously to both specialized and non-specialized audiences.
- Students should demonstrate self-directed learning skills for continued academic growth.
- Students should possess and understand foundational knowledge that enables original thinking and research in the field.
- Students are able to foster, in academic and professional contexts, technological and scientific progress within a society based on knowledge and respect for: a) fundamental rights and equal opportunities between men and women, b) The principles of equal opportunities and universal accessibility for persons with disabilities, and c) the values of a culture of peace and democratic values.
- Students demonstrate their knowledge and understanding of the facts applying concepts, principles and theories related to the Theoretical Chemistry and Computational Modeling.
- Students acquire an overview of the different applications of the Theoretical Chemistry and modeling in the fields of Chemistry, Biochemistry, Materials Sciences, Astrophysics and Catalysis.
- Students are able to solve problems and make decisions of any kind under the commitment to the defense and practice of equality policies.
- Students are able to adapt their selves to different cultural environments by demonstrating that they are able to respond to change with flexibility.
- Students are organized at work demonstrating that they know how to manage their time and resources.
- Students have the ability of analyze and synthesize in such a way that they can understand, interpret and evaluate the relevant information by assuming with responsibility their own learning or, in the future, the identification of professional exits and employment fields.
- Students have the ability to handle the main sources of scientific information related to Theoretical Chemistry and Computational Modeling. They are able to search for relevant information in web pages of structural data, physical chemical experimental data, databases of molecular calculations, databases of scientific bibliography and scientific works.

- Students understand the theoretical and practical bases of computational techniques with which they can analyze the electronic, morphological and structural structure of a compound and interpret the results adequately.

LEARNING OUTCOMES (RD 1393/2007) // NO CONTENT (RD 822/2021)

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. To recognize the limitations of the studied techniques and to choose among them the most suitable for a given problem.

DESCRIPTION OF CONTENTS

1. Topics and sub-topics

1. Introduction. Biomolecules and their properties. Structural databases of biomolecules. Structure-energy relationship: Biomolecules modeling.

2. Potential energy surfaces in biomolecules. Molecular mechanics force fields. Conformational exploration. Minimization: Reaction coordinate. Molecular Dynamics and Monte Carlo methods. Structure prediction methods. .

3. Advanced MD methods. Ab initio Born-Oppenheimer MD, hybrid QM/MM MD simulations. Enhanced sampling techniques, free energy simulations and Metadynamics .

4. Mixed QM/MM models. Electrostatic and polarizable embedding. Continuum solvation models. Extension to excited states .

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

6. Protein-ligand interaction. Docking techniques

WORKLOAD

ACTIVITY	Hours	% To be attended
Laboratory practices	20,00	100
Theory classes	20,00	100
Tutorials	10,00	100
Development of individual work	16,00	0
Study and independent work	59,00	0
TOTAL	**125,00**	

TEACHING METHODOLOGY

Lecture: The Professor will deliver lectures about the theoretical contents of the course during two-hour sessions. The presentations will be based on the different materials available at the Moodle platform.

Network teaching: All the tools available at the Moodle website (http://www.uam.es/moodle) will be used (uploading of teaching materials, utilization of work team strategies, wiki, blogs, e-mail, etc.).

Teaching in computer room. Teaching will be conducted in a computer room. The classes, in sessions from two to four hours, will include a brief theoretical introduction, in which the teacher will present the basic concepts, followed by practical applications, in which the student will learn through the resolution of practical examples.

Tutoring sessions: The professor can organize either individual or group tutoring sessions about particular topics and questions raised by students.

Written reports: Orientation and supervision in the preparation of written reports.

EVALUATION

Ordinary assessment

The knowledge acquired by the student will be evaluated along the course. The educational model to follow will emphasize a continuous effort and advance in training and learning.

The final student mark will be based on exercises that must be done during the course. The next criteria will be followed for assessment of student exercises:

- 10% attendance and participation in class,

- 90% practical case study. Part of this percentage may be applied to the performance of tests.

Extraordinary assessment

The student will have to face a final exam, including both theory and practical exercises. The student mark will be obtained from:

- 60% theoretical exam,

- 40% practical exam.

REFERENCES

Basic

- 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