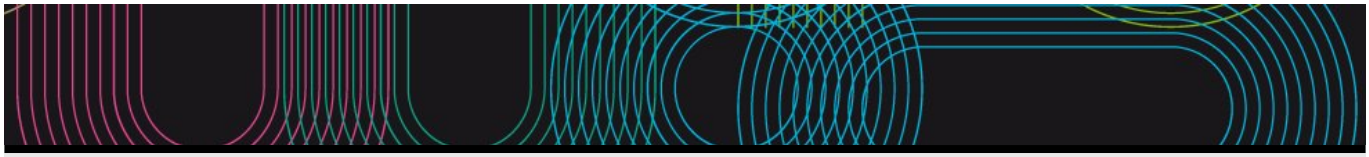

IDENTIFYING DATA				
Computational modeling of biomaterials				
Subject	Computational modeling of biomaterials			
Code	V11M188V01110			
Study programme	Máster Universitario en Nanociencia y Nanotecnología			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	3	Optional	1st	1st
Teaching language	Spanish Galician English			
Department				
Coordinator	Pérez Juste, Ignacio Mandado Alonso, Marcos			
Lecturers	Hervés Beloso, Juan Pablo Mandado Alonso, Marcos Pérez Juste, Ignacio Renero Lecuna, Carlos			
E-mail	mandado@uvigo.es uviqpipj@uvigo.es			
Web	http://www.usc.gal/gl/estudos/masteres/ciencias-saude/master-universitario-nanociencia-nanotecnoloxia/20212022/modelizacion-computacional-biomateriais-17798-17030-3-99009			
General description	This course seeks for the student to know the possibilities offered by the latest computational modeling methods, as fundamental complementary tools in the rational design of biomaterials of biological or biotechnological interest (peptides, proteins, membranes, surfactants, etc.), as well as in elucidation at the atomic level of its mechanism of action. To this end, the main methods of molecular modeling and dynamic simulation applied to biomaterials will be studied, along with the algorithms and approximations necessary to carry out these studies, as well as the most common calculation methods for estimating ligand-biomolecule affinity, active conformations, etc. The subject also seeks to provide basic notions on how to use a supercomputer to carry out computational simulations of biomolecules, as well as knowing how to use some of the main computational tools for simulating biomaterials: computer engines, analysis packages, molecular displays, force fields, public servers for specific calculations, file formats, etc.			

Training and Learning Results
Code

Expected results from this subject	
Expected results from this subject	Training and Learning Results

Contents
Topic

CHAPTER 1. Introduction to the computational simulations of biomaterials. Historical evolution and projection.

CHAPTER 2. Main methods of modeling and simulation. Docking, Montecarlo and Molecular Dynamics.

CHAPTER 3. Force fields and resolution levels. Advantages and limitations. Multi-scale mappings.

CHAPTER 4. Algorithms and approximations. Consideration of short and long range forces, barostats, thermostats, periodic conditions.

CHAPTER 5. Analysis: deviations and fluctuations, density profiles, diffusion coefficients in 2 and 3 dimensions, autocorrelation functions, radial distribution functions, etc.

CHAPTER 6. Methods of calculation of Gibbs energies for different processes.

CHAPTER 7. Software and hardware: main computer tools and how to manage hardware resources. Computing engines, analysis packages and visualizers.

CHAPTER 8. Practical cases: self-association of small molecules, study of supramolecular aggregates, folding-deployment of macromolecules, micelles and membranes.

Planning

	Class hours	Hours outside the classroom	Total hours
Lecturing	6	12	18
Seminars	4	12	16
Laboratory practical	12	29	41
Objective questions exam	0	0	0
Presentation	0	0	0

*The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.

Methodologies

	Description
Lecturing	Presentation by the teacher of the contents on the subject under study, theoretical and / or guidelines for a job, exercise or project to be developed by the student.
Seminars	Activity focused on the work on a specific topic, which allows to deepen or complement the contents of the subject. They can be used as a complement to the theoretical classes.
Laboratory practical	Activities application of knowledge to specific situations and basic skills acquisition and related procedural matter under study. They are developed in specific spaces with specialized equipment (Laboratories, computer rooms, etc ...)

Personalized assistance

Assessment

Description	Qualification	Training and Learning Results

Seminars	The continuous assessment will have a weight of 50% in the mark of the subject and will consist of two components: Active participation in seminars and practical classes (30% of the mark). This evaluation will be carried out through the resolution of questions and problems raised in class, the presentation of tasks and the participation in the discussion that may arise. The maximum score will be 3 points.	30
Objective questions exam	The assessment of this subject will be done through continuous evaluation and the completion of a final exam. The final exam will be about basic content of the subject (50% of the mark). The examination of the subject, which will be held on the date indicated in the corresponding course guide, will consist of short questions and problem solving. The maximum score will be 5 points. A minimum mark of 2 points on the exam is required, in order to account the other two items that are considered in the assessment.	50
Presentation	(ii) Oral presentations (20% of the mark). Expository clarity and the ability to answer the proposed questions will be assessed. The maximum score will be 2 points.	20

Other comments on the Evaluation

For the evaluation, the Moodle (virtual campus) and MS Teams platforms can be used.

Sources of information

Basic Bibliography

H.-D. Holje & G. Folkers, **Molecular Modeling: Basic Principles and Applications**, VCH, Weinheim, 2008

Herman J. C. Berendsen, **Simulating the Physical World: Hierarchical Modeling from Quantum Mechanics to Fluid Dynamics**, Cambridge University Press, 2007

GROMACS 5.0.7 User manual: ftp://ftp.gromacs.org/pub/manual/manual-5.0.7.pdf,

Amber 2020 Reference User manual. https://ambermd.org/Manuals.php,

Daan Frenkel, **Understanding Molecular Simulation: From Algorithms to Applications, Computational Science Series, Vol 1**, Academic Press, 2001

Michael P. Allen, Dominic J. Til, **Computer Simulation of Liquids**, 2ª, OUP Oxford, 2017

Complementary Bibliography

Recommendations