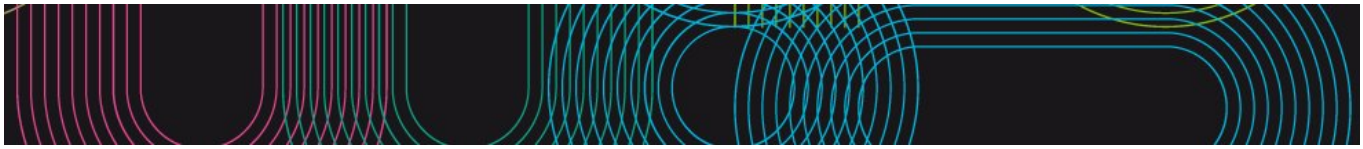

IDENTIFYING DATA				
Structural Biology				
Subject	Structural Biology			
Code	V02M123V01211			
Study programme	(*)Máster Universitario en Ciencias Biolóxicas: Bioloxía Molecular, Computacional e Ambiental e Bio-Industrias			
Descriptors	ECTS Credits	Type	Year	Quadmester
	6	Optional	1st	2nd
Language	English			
Department				
Coordinator	Nieto Faza, Olalla			
Lecturers	Nieto Faza, Olalla Pérez Rodríguez, Martín Silva López, Carlos			
E-mail	faza@uvigo.es			
Web	http://faitic.uvigo.es			
General description	In this course, computational models and simulation techniques, together with visualization tools are going to be used to describe and investigate the structure and dynamics of biomolecular systems.			

Competencies		
Type A	Code	Competences Specific
	A1	(*)To know the scientific method and the correct use of the scientific terminology as well as to acknowledge the contribution that scientific research provides to the overall knowledge and professional practice.
	A2	(*)Ability to describe and to analyse biological diversity, the mechanisms determining the interactions with the biotic and abiotic environment and being able to select those which might have technical applications.
	A3	(*)Ability to manage and/or to develop basic tools for validating and analysing data by means of statistics and bioinformatics.
	A4	(*)To know the ethical and legal aspects governing the collection and the handling of biological samples, organisms and habitats.
	A5	(*)Ability to design, evaluate and implement models of biological structures, systems and processes.
	A6	(*)To learn the sampling techniques and the instrumental methodologies, in the field and laboratory, for their application in the Biological Sciences
	A7	(*)To have an integrated view of the R&D processes and their possible transfer to the industrial sector. Planning and supervising facilities together with managing their human and economic resources.
	A8	(*)Ability to classify, evaluate, conserve, restore and manage natural and productive systems. Developing and implementing land management and sustainability plans.
	A9	(*)To understand and know how to apply quality control systems and safety protocols in any biological laboratory of the public or private sector.
	A10	(*)To acquire the professional ability to teach and spread Biology and to offer expertise advice for elaborating scientific, technical and socioeconomic biology reports. Address environmental consulting.
	A11	(*)To perform an individual Master Project (critical and in-depth study) under the supervision of a tutor in a research or working environment demonstrating that skills have been acquired.

Type B	Code	Competences Transversal
	B1	(*)Dissemination of results and conclusions of the biological studies, in oral and written English, through complex presentations that address ideas related with R&D in Biology.
	B2	(*)Managing computational, laboratory, field and industrial techniques in order to obtain, process and apply the acquired information.
	B3	(*)Disseminating and broadcasting ideas in contexts both academic and non-specialised.
	B4	(*)Reflecting on social and ethical responsabilities.

Learning aims

Subject competences	Typology	Competences
Being able to predict the structure of biomolecules at different levels	Know How	A1 A3 A5 B2
To evaluate DNA/RNA/protein/ligand/solvent interactions	know Know How	A1 A3 A5 B2
Being able to understand different static and dynamic simulation methods, to select those appropriate for a given problem and to apply them to provide significative answers.	know Know How	A1 A3 A5 B1 B2
To visualize, analize and interpret simulations of biomolecular systems.	know Know How	A1 A3 A5 A10 B1 B2 B3

Contents

Topic	
A. Structure and representation of biomolecules	1. Chemical bonding in biomolecules. Non-covalent interactions. Solvation. 2. Structure of biomolecules: proteins, nucleic acids, carbohydrates. 3. Representation of biomolecules: formats and software. Repositories. Protein Data Bank.
B. Molecular modeling	4. Fundamentals of molecular modeling. Potential energy surfaces. Time and size scales. Multiscale methods. 5. Quantum models: ab-initio, semiempirical methods, DFT. 6. Molecular Mechanics. Force fields. 7. Coarse-grain models.
C. Simulation techniques	8. Homology Modeling and Docking in drug discovery. 9. Introduction to Molecular Dynamics and MD advanced techniques. 10. Applications (structural problems, drug-receptor interactions, catalysis, etc.)

Planning

	Personalized attention	Assessment	Ordinary class hours A	Face-to-face hours outside the classroom Guided academic environment B	Student's work factor C	Outside the classroom hours D	Total hours (A+B+D) E
Master Session	☐	☒	20	0	0.5	10	30
Classroom work	☒	☒	10	0	0	0	10
Autonomous troubleshooting and / or exercises	☒	☒	0	0	0	108	108

Multiple choice tests	☒	☒	2	0	0	0	2
Total hours E:							150
Work load in UVIGO ECTS credits:							6
*The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.							

Methodologies

	Description
Master Session	The instructor explains concepts and introduces tools.
Classroom work	The students do computational work with the instructor.
Autonomous troubleshooting and / or exercises	The students do computational work on their own.

Personalized attention

	Description
Classroom work	The instructors are available online (through forums, discussion lists or chats) to answer the students' questions. When needed, help will be also provided in person through e-mail or regular office hours.
Autonomous troubleshooting and / or exercises	The instructors are available online (through forums, discussion lists or chats) to answer the students' questions. When needed, help will be also provided in person through e-mail or regular office hours.
Multiple choice tests	The instructors are available online (through forums, discussion lists or chats) to answer the students' questions. When needed, help will be also provided in person through e-mail or regular office hours.

Assessment

	Description	Qualification
Master Session	Students are expected to have read the assigned material and to actively participate in the classroom discussions. Evaluation can be done either through class observation or short quizzes.	5
Classroom work	Students are expected to have read the assigned material, worked through the proposed activities and to actively participate in the classroom discussions. Evaluation can be done either through class observation or short quizzes.	5
Autonomous troubleshooting and / or exercises	Students have to deliver a report on their computational assignments.	60
Multiple choice tests	A multiple choice test will evaluate the mastery of the course contents.	30

Other comments and second call

Sources of information

Tamar Schlick , Molecular Modeling and Simulation: An Interdisciplinary Guide, , 2010 Springer

Christopher Cramer, Essentials of Computational Chemistry: Theories and Models., , 2008 Wiley

Daan Frenkel, Understanding Molecular Simulation: From Algorithms to Applications, , 2002 Academic Press

Recommendations

Subjects that continue the syllabus

Systems Biology/V02M123V01212

Subjects that it is recommended to have taken before

Molecular Evolution/V02M123V01210
Knwledge Discovery/V02M123V01113
Computational Genomics/V02M123V01209
Statistical and Mathematical Methods in Bioinformatics/V02M123V01112
Progrmming for Bioinformatics/V02M123V01111