UAB
Universitat Autònoma de Barcelona

Structure and Function of Proteins and Drug Design

Code: 42398
ECTS Credits: 12

2025/2026

Degree	Type	Year
Bioinformatics	OT	0

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Teachers

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Teaching groups languages

You can view this information at the end of this document.

Prerequisites

To take this module it is necessary to have previously passed both compulsory modules I and II (Programming in Bioinformatics and Core Bioinformatics). Basic notions of Chemistry and/or Biochemistry are also needed.

The student must have the B2 Level in English or equivalent.

Objectives and Contextualisation

Proteins are the subject of intensive research in many different areas, from being the target of drug design projects to the design of new enzymes to be used as biocatalysts in new industrial processes of interest and/or in a more environmentally friendly way.

Molecular modelling is a very powerful tool in all these areas, in which it has become an essential part of the conducted research, both in academia and in companies.

In this module, students will be provided with the fundamental and practical knowledge to become skilled scientists in the field.

Thus, the objective of this module is to provide students with theoretical and practical knowledge on:

- the physical grounds that sustain the different molecular modelling techniques

- the basic and state-of-the-art methods applied in the field

- an overview of main areas of application, with special emphasis in drug design

Competences

- Analyse and interpret data deriving from omic technology using biocomputing methods .
- Communicate research results clearly and effectively in English.
- Design and apply scientific methodology in resolving problems.
- Identify the biocomputing needs of research centres and companies in the biotechnology and biomedicine sectors.
- Possess and understand knowledge that provides a basis or opportunity for originality in the development and/or application of ideas, often in a research context.
- Propose biocomputing solutions for problems deriving from omic research.
- Propose innovative and creative solutions in the field of study
- Understand the molecular bases and most common standard experimental techniques in omic research (genomics, transcriptomics, proteomics, metabolomics, interactomics, etc.)
- Use and manage bibliographical information and computer resources in the area of study
- Use operating systems, programs and tools in common use in biocomputing and be able to manage high performance computing platforms, programming languages and biocomputing analysis.

Learning Outcomes

1. Carry out searches (virtual screening) in chemical structures bookshops.
2. Communicate research results clearly and effectively in English.
3. Create models of pharmacophores using the structures of ligand sets.
4. Describe and apply modelling techniques for homology in the three-dimensional protein structure.
5. Describe and characterise computing techniques for molecular dynamics in studying the structure and function of proteins.
6. Describe and classify techniques for predicting the secondary structure using amino acid sequence.
7. Describe the operation, characteristics and limitations of techniques for analysing and visualising protein structures.
8. Design and apply scientific methodology in resolving problems.
9. Establish the corresponding relationships between aminoacidic sequence, three-dimensional structure and proteic function using sources of biological data and the foundations of biocomputing analysis.
10. Identify and apply techniques for CAD, computer assisted drug design
11. Possess and understand knowledge that provides a basis or opportunity for originality in the development and/or application of ideas, often in a research context.
12. Propose innovative and creative solutions in the field of study
13. Recognise and apply different prediction methods of the functions and three-dimensional structure of proteins.

14. Recognise the strategic importance of the protein model in the area of human health, especially in personalised medicine applications and pharmacogenomics.
15. Simulate the union of the ligand and the receptor using ?docking? techniques and molecular dynamics
16. Understand the biomolecular and pharmacological techniques used in functional protein assays.
17. Understand X-ray crystallography and NMR techniques to obtain protein structures
18. Use and manage bibliographical information and computer resources in the area of study
19. Use programs for calculating structure.
20. Use programs for calculating structure-activity relationships.
21. Use programs for visualising structure.

Content

MODULE 4: Structure and Function of Proteins and Drug Design

Part I MOLECULAR MODELING. Basic concepts.

Basic concepts

Introduction

Energy calculation (PES, QM, Force fields, Hybrid QM/MM)

Conformational Exploration (other than MD: MC, GA, NMA)

Part II STRUCTURE CHARACTERIZATION AND MODELLING

Methods for Determining Protein Structure

X-ray crystallography

NMR

Cryo-electron microscopy

Structural modeling

Homology modeling

AlphaFold

Part III MOLECULAR DYNAMICS (MD)

Molecular dynamics, an essential technique

Basics

MD in water

MD in the membrane environment

Coarse graining

Scripting & Analysis

Enhanced sampling methods (metadynamics, GaMD, …)

Free energy: TI, FEP, MM/PBSA

Part IV DRUG DESIGN

Basics in pharmacology

Hot targets and currently marketed drugs: Kinases, Nuclear receptors, G protein-coupled receptors, Membrane transport proteins

Molecular descriptors

ADME-Tox

Ligand-based and structure-based pharmacophore modelling

Docking

Ligand-protein docking

Protein-protein docking

Virtual screening

MD applications in drug design.

Activities and Methodology

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Seminars	2	0.08	2
Solving problems in class and work in the computing lab	40	1.6	2, 3, 7, 4, 5, 6, 1, 8, 9, 10, 12, 13, 15, 11, 20, 19, 21, 18
Theoretical classes	32	1.28	16, 17, 2, 7, 4, 5, 6, 8, 9, 10, 12, 13, 14, 11, 18
Type: Autonomous			
Regular study	224	8.96	16, 17, 3, 7, 4, 5, 6, 1, 8, 9, 10, 12, 13, 14, 15, 11, 20, 19, 21, 18

The methodology will combine theoretical classes, solving problems in class, practices in the computers lab, seminars and independent study and delivarable tasks. The virtual platform of the UAB will be used.

Annotation: Within the schedule set by the centre or degree programme, 15 minutes of one class will be reserved for students to evaluate their lecturers and their courses or modules through questionnaires.

Assessment

Continous Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Individual theoretical and practical tests	40%	2	0.08	16, 17, 3, 7, 4, 5, 6, 1, 9, 10, 13, 14, 15, 20, 19, 21
Soft skills	10%	0	0	2, 8, 12, 11, 18
Works done and presented by the student (student's portfolio)	50%	0	0	16, 17, 2, 3, 7, 4, 5, 6, 1, 8, 9, 10, 12, 13, 14, 15, 11, 20, 19, 21, 18

The evaluation system is organized in three main activities. There will be, in addition, a retake exam. The details of the activities are:

Main evaluation activities

- Soft skills (10%): attendance and participation in class, transversal competences.
- Student's portfolio (50%): works done and presented by the student all along the course. None of the individual assessment activities will account for more than 50% of the final mark.
- Individual theoretical and practical test (40%): a final exam will take place at the end of this module.

Retake exam

To be eligible for the retake process, the student should have been previously evaluated in a set of activities equaling at least two thirds of the final score of the module. The teacher will inform the procedure and deadlines for the retake process.

Not valuable

The student will be graded as "Not Valuable" if the weight of the evaluation is less than 67% of the final score.

This subject/module does not implement the single-evaluation system.

Use of AI (restricted use model): For this course, the use of Artificial Intelligence (AI) technologies is permitted exclusively for bioinformatics tasks that require it and for support tasks, such as bibliographic or information searches, text correction, or translations. Regarding its use in support tasks, the student must clearly identify which parts were generated using this technology, specify the tools used, and include a critical reflection on how these tools have influenced the process and the final outcome of the activity. Failure to transparently disclose the use of AI in this graded activity will be considered a breach of academic integrity and may result in a partial or total penalty on the activity's grade, or more severe sanctions in serious cases.

Bibliography

Molecular Modeling principles and applications, A. Leach, Ed. Pearson (i.e. second edition ISBN-13: 978-0582382107) (physical document available at the UAB library services)

Essential of Computational Chemistry, C. J. Cramer, (i.e. second Edition, ISBN-13: 978-0470091821) (physical and electronic documents available at the UAB library services)

Introduction to Computational Chemistry. Frank Jensen. JohnWiley § Sons Ltd. (ISBN: 0470011874, 2007) (electronic document available at the UAB library services)

Python, how to think like a computer scientist [http://www.greenteapress.com/thinkpython/] (electronic document available at the UAB library services)

Computational and Visualization techniques for structural bioinformatics using chimera, Forbes J. Burkowski, CRC press (electronic document available at the UAB library services)

Software

On Linux:

UCSF Chimera
UCSF ChimeraX
PyMol
Gaussian
Gaussview
VMD
AMBER
Ambertools
Modeller
AlphaFold
Gromacs
LigandScout
Datawarrior
Conda
grace
Jupyter Notebook
Matplotlib
Python

Rasmol
ssh
xxdiff

Groups and Languages

Please note that this information is provisional until 30 November 2025. You can check it through this link. To consult the language you will need to enter the CODE of the subject.

Name	Group	Language	Semester	Turn
(PLABm) Practical laboratories (master)	1	English	first semester	morning-mixed
(SEMm) Seminars (master)	1	English	first semester	morning-mixed
(TEm) Theory (master)	1	English	first semester	morning-mixed