UAB
Universitat Autònoma de Barcelona

Structural Biology

2026/2027

Code: 107534
Credits: 6

Degree programme	Type	Course
Biotechnology	OP	4

Contact lecturer

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Teaching staff

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Teaching staff (external to UAB)

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Group languages

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

Prerequisites

Students must have passed the courses: Basic instrumental techniques, Advanced instrumental techniques and Chemistry and protein engineering.

Objectives

The general objective of the subject is the structural and functional study of biological macromolecules.

The subject includes a description of the current techniques of resolution and prediction of the three-dimensional structure of biological macromolecules, as well as experimental and computational methodologies for the study of their dynamic behavior and functions.

Top priority will be given to the practical application of the subject, so that students can experience the techniques described by themselves and simulate the behavior of macromolecules and their complexes in a biological context.

Finally, the structural-functional analysis of macromolecules and the prediction of supramolecular complexes will be applied to practical examples of identification of the molecular basis of diseases and drug design.

Learning outcomes

- CM25 (Work collaboratively in teams to solve problems in the field of systems biology.) Work collaboratively in teams to solve problems in the field of systems biology.
- KM25 (Describe the physical and chemical bases of the methodology and instrumentation used in genomic, transcriptomic, proteomic, interactomic and metabolomic analysis.) Describe the physical and chemical bases of the methodology and instrumentation used in genomic, transcriptomic, proteomic, interactomic and metabolomic analysis.
- SM24 (Quantitatively model a biological process or system.) Quantitatively model a biological process or system.
- SM25 (Analyse information from databases and software necessary for the study of correlations between structure, function and evolution of macromolecules.) Analyse information from databases and software necessary for the study of correlations between structure, function and evolution of macromolecules.

Contents

THEORY

Lesson 1. Biological applications of synchrotron radiation

Introduction to the production and characteristics of synchrotron light. X-ray and infrared microscopies: introduction to techniques and applications in biomedicine.

Lesson 2. Advanced Microscopy techniques

Electron cryomicroscopy, cryotomography; determination of the structure of single particles; transmission electron microscopy, scanning electron microscopy. Atomic force and tunneling microscopies; force spectroscopy; nanotribology. Applications in Biotechnology and Biomedicine.

Lesson 3. X-ray crystallography and applications

Basic theoretical foundations of determining the three-dimensional structure of macromolecules by crystallography and X-ray diffraction; properties of crystals; diffraction data processing and 3D model reconstruction. New methodologies with 4th generation synchrotron light sources (free electron lasers, serial crystallography, time resolution experiments and molecular films). Tools for the analysis of functional regions in macromolecules.

Lesson 4. Bioinformatics tools for the study of proteins

Introduction to structural bioinformatics. Sequence and structure comparison. Protein structure prediction: secondary structure, transmembrane regions, and artificial intelligence-based methods (AlphaFold). Homology modelling. Introduction to force fields and molecular dynamics of biomolecules. Molecular docking and virtual screening strategies to study macromolecule-ligand interactions.

PROBLEMS

The resolution of practical problems will be proposed to facilitate the consolidation of the theoretical concepts taught. Most of the problem sessions will be taken in the computer room, where structural prediction software will be applied.

PRACTICUM

Three Practical blocks will be carried out according to the course syllabus.

1st block (Topics 1 and 2) Practicals at the Electron Microscopy Service: Analysis of biological samples using high-resolution optical microscopy and transmission electron microscopy (negative staining and CryoTEM). Practicals in the SID computer classroom: Structure determination by Electron Microscopy.

2nd block (Topic 3) Practicals on three-dimensional structure determination by X-ray Crystallography in the SID computer classroom. Analysis of functional regions in macromolecules in the SID computer classroom.

3rd block (Topic 4)

Visualization and structural analysis: use of PyMOL to explore, represent, and analyze protein structures and macromolecular complexes.

Modeling and molecular interactions: construction of three-dimensional models and study of macromolecule-ligand interactions through molecular docking.

Molecular dynamics: introduction to molecular dynamics simulation to analyze the flexibility, stability, and dynamic behavior of biomolecules.

SEMINAR:

It is planned to include a specialized seminar

Field trip:

Guided tour of the ALBA synchrotron light laboratory. Seminar by Dr. Fernando Gil and explanation of the operation of the stations: BL-09, X-ray microscopy; BL-11, Non-crystalline diffraction and BL-13, Crystallography of macromolecules.

Tutorials

Tutorial sessions may be held during the semester. The objective of these sessions is to resolve doubts and review concepts.

Learning activities and methodology

Title	Hours	ECTS	Learning outcomes
Problems	10	0.4	
Practicum	9	0.36	
Autonomous work	52.5	2.1	
solving of practical cases	41	1.64	
Theoretical lectures	30	1.2	

Theoretical master classes

The teacher will explain the contents of the program with the support of audiovisual material that will be available for students at the Moodle/Virtual Campus section. This support material will be written in English, Catalan or Spanish.

Optionally, seminars by specialists in the field will be held.

Problem cases

Throughout the course you will attend 8 hours of problems' teaching. Classes will include sessions at the computer room.

Practices

There will be guided tours to large installations with specialized equipment. The Protocol of practices will be available at the Virtual Campus before the practice session. Practices will also include sessions at the computer room.

Students must attend the practice session with the Protocol (available at the Virtual Campus) printed and read beforehand and bring a notebook to write down observations and data.

Practices, as well as its evaluation, will be carried out individually or in groups of two people. Attendance at practical sessions is mandatory, except in cases where there is a justified reason to prove the student absence.

Tutorials

Several tutorial sessions can be held during the semester. The aim of these sessions is to answer questions and review concepts with a high level of difficulty.

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

Continuous assessment activities

Title	Weight	Hours	ECTS	Learning outcomes
Problems Evaluation	15%	1.25	0.05	CM25, SM24, SM25
Evaluation 1st+ 2nd part Theory Exam	70%	5.25	0.21	KM25, SM24, SM25

Practicum evaluation	15%	1	0.04	CM25, SM25

Description

The qualification will be based on the following elements:

1 - Final test of theoretical content: a maximum of 7 points

2 - Problems' reports: maximum 1.5 points

3 - Participation in practices: maximum 1.5 points

The content of the course will be evaluated in two partial exams.

The proportional weight in the final mark for each of the issues will be proportional to the number of hours taught by each teacher.

The course will be overcome when the final mark is equal to or greater than 50 for a maximum of 100.

Other considerations

Students who cannot attend an individual evaluation test due to a justified cause must provide an official documentation to the Coordinator of the course and shall be entitled to perform the corresponding test in a different date.

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 course or module. Thus, the student will be graded as \"No Avaluable\" if the weighth in of all conducted evaluation activities is less than 67% of the final score

Rules for improving your mark:

It is possible to improve the note of the midterms exam on the occasion of the Recovery Examination. The second note obtained will be considered as final if this one is higher than the one obtained in the first test.

When the obtained note at the second chance is less than 1 point or more than the first note obtained, the final note considered will be the average of the two notes.

The student will have 10 minutes at the start of the test to decide whether or not to perform the test.

For the maximum award of honours qualification priority will be given to qualifications obtained in midterms' exam.

Calculation of the final mark:

Final mark = 0.70 * Theory + 0.15 * Problems + 0.15 * Practices

To pass the course the final mark must be$\geq$ 5

Single evaluation:

Students who take advantage of the single evaluation must carry out all the sessions of laboratory practices, practices in the computer room and field trip (visit to the synchrotron).

The single assessment consists of a single synthesis test (with questions of variable format on the contents of the sessions of all types). All assignments commissioned during the course must be delivered either during the corresponding session or on the day of the final exam.

The single assessment test shall be carried out coinciding with the date fixed in the calendar of the final examination for the continuous assessment and the same recovery system shall be applied as for the continuous assessment.

The calculation of the final grade for students who request the single evaluation will be as follows:

Final grade = 0.80 *Theory + 0.10 *Problems + 0.10 *Practices

Fraud and improper use of AI.

The commission of any irregularity in an assessment activity (academic fraud, plagiarism, or improper use of AI, unless such use is expressly authorized in the course guide), which may lead to a significant variation in the grade, means that this activity will be graded with a 0. If the course guide establishes that obtaining a minimum grade in this assessment activity is an essential requirement to pass the subject, or if several irregularities occur in the assessment activities of the same subject, the final grade for that subject is 0. In addition to this, a disciplinary process may be initiated against the student who commits any of these irregularities.

Bibliography

Web links

- Training Protein Data Bank Portal

https://pdb101.rcsb.org

- Protein Crystallography course. Structural Medicine. MRC-LMB Cambridge University:

http://www-structmed.cimr.cam.ac.uk/course.html

- University of Cambridge. Crystallography. Teaching and Learning packages.

http://www.doitpoms.ac.uk/tlplib/crystallography3/index.php

- Department of structural biology. CSIC, Madrid

http://www.xtal.iqfr.csic.es/Cristalografia/index-en.html

Llibres electrònics de lliure accés a la biblioteca de la UAB:

Integrative Structural Biology with Hybrid Methods Advances in Experimental Medicine and Biology. Vol. 1105. Haruki Nakamura; Gerard Kleywegt; Stephen K. Burley and John L. Markley. Springer. Cohen et al. editors. 2018

BOOKS

Molecular Biology of Assemblies and Machines.A. C. Steven et al. (2016) Garland Science.

Proteins. Structures and Molecular Properties. T.E. Creighton, (1993) 2ed Freeman W.H.and co

Introduction to Biophysical Methods for Protein and Nucleic Acid ResearchGläsel and Deutscher (1995) Academic Press

Crystal Structure Analysis for Chemists and Biologists.J.P. Glusker, M. Lewis and M. Rossi (1994) VCH Publishers, Inc.

Computational tools for Chemical Biology. [2018]. Editor: S. Martín-Santamaría. London. Chemical Biology series. Royal Society of Chemistry. ISBN: 978-1-78262-700-5. DOI: 10.1039/9781788010139.

Software

UCSF Chimera; CCP4i2; Coot, Phenix; Modeller, AutoDock, AlphaFold, Pymol, RosettaFold

Course groups and languages

The information provided is provisional until November 30. After this date, you will be able to consult the language of each group through this link. To access the information, you will need to enter the course CODE