UAB
Universitat Autònoma de Barcelona

Advanced Structural Analysis

Code: 100907
ECTS Credits: 6

2024/2025

Degree	Type	Year
2500252 Biochemistry	OT	4

Contact

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Teachers

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Teaching groups languages

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

Prerequisites

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

Objectives and Contextualisation

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.

Competences

- Act with ethical responsibility and respect for fundamental rights and duties, diversity and democratic values.
- Apply the principal techniques used in biological systems: methods of separation and characterisation of biomolecules, cell cultures, DNA and recombinant protein techniques, immunological techniques, microscopy techniques, etc.
- Clearly perceive current advances and possible future developments by reviewing scientific and technical literature in the area of biochemistry and molecular biology.
- Collaborate with other work colleagues.
- Define the structure and function of proteins and describe the biochemical and molecular bases of their folding, intracellular traffic, post-translational modification and replacement.
- Design experiments and understand the limitations of experimental approaches.
- Identify molecular structure and explain the reactivity of the different biomolecules: carbohydrates, lipids, proteins and nucleic acids.
- Integrate scientific and technological knowledge.
- Interpret experimental results and identify consistent and inconsistent elements.
- Introduce changes in the methods and processes of the field of knowledge to provide innovative responses to the needs and demands of society.
- Read specialised texts both in English and one's own language.
- Stay abreast of new knowledge of the structure, organisation, expression, regulation and evolution of genes in living beings.
- Think in an integrated manner and approach problems from different perspectives.
- Understand the language and proposals of other specialists.
- Use the basics of mathematics, physics and chemistry that are required to understand, develop and evaluate the chemical procedures of living matter.

Learning Outcomes

1. Act with ethical responsibility and respect for fundamental rights and duties, diversity and democratic values.
2. Collaborate with other work colleagues.
3. Describe in detail the biophysical methods used to reveal the dynamic structure and properties of DNA and chromatin.
4. Describe the scientific and technical principles underpinning knowledge of the structure and chemical properties of biomolecules.
5. Design experiments and understand the limitations of experimental approaches.
6. Explain in detail the biophysical methods used to reveal the dynamic structure and properties of proteins.
7. Explain the basic physical principles, and applications to biochemistry and molecular biology, of advanced techniques in electron and atomic force microscopy and in the study of individual biomolecules.
8. Identify fundamental issues in present-day biophysics.
9. Identify scientific and technical advances in biophysics.
10. Identify the applications of emerging technologies (especially those linked to Synchrotron radiation and nanotechnology) to biochemistry and molecular biology.
11. Interpret experimental results and identify consistent and inconsistent elements.
12. Introduce changes in the methods and processes of the field of knowledge to provide innovative responses to the needs and demands of society.
13. Read specialised texts both in English and one's own language.
14. Think in an integrated manner and approach problems from different perspectives.
15. Understand the language and proposals of other specialists.

Content

THEORY

Lesson 1. 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; nanotribiology. Applications in Biotechnology and Biomedicine.

Lesson 2. Biological applications of synchrotron radiation.

Introduction to the production and characteristics of synchrotron light. X-ray and infrared microscopy: introduction to the technique and applications in 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 applied to the structural analysis of macromolecules.

Introduction to structural bioinformatics. Methods of prediction and comparison of structures. Identification of functional domains. Applications of artificial intelligence in the prediction of the structure of biomolecules. Docking strategies and applications in drug design. Molecular dynamics and prediction of structural conformations. Study of interaction networks in molecular complexes.

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.

PRACTICUM

There will be 3 sessions of Practices

1stsession: Practices of computer applications to the resolution of structures by Electron Microscopy in the laboratory of the Biophysics Unit.

2nd session: Practices of resolution of three-dimensional structures by X-ray crystallography in the computer room SID.

3rd session: Practices of analysis of functional regions in macromolecules in the SID computer room.

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.

Activities and Methodology

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Theoretical lectures	30	1.2	3, 4, 6, 7, 9, 8
Type: Supervised			
Practicum	9	0.36	2, 4, 5, 6, 11, 14
Problems	10	0.4	2, 3, 4, 5, 6, 7, 8, 11, 14
Type: Autonomous			
Autonomous work	52.5	2.1	2, 5, 15, 6, 7, 9, 8, 11, 13, 14
solving of practical cases	41	1.64	2, 5, 15, 6, 7, 9, 10, 11, 13, 14

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

Continous Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Evaluation 1st+ 2nd part Theory Exam	70%	5.25	0.21	2, 3, 4, 5, 15, 6, 7, 9, 10, 8, 11, 13, 14
Practicum evaluation	15%	1	0.04	2, 5, 9, 10, 11, 14
Problems Evaluation	15%	1.25	0.05	1, 2, 5, 7, 10, 11, 12, 14

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 weighthin 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 asfinal ifthis 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 awardof 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

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.

Software

UCSF Chimera; CCP4i2; Coot, Phenix; Modeller, Autodockv4, AlphaFold.

Language list

Name	Group	Language	Semester	Turn
(PAUL) Classroom practices	341	Catalan/Spanish	second semester	morning-mixed
(PLAB) Practical laboratories	341	Catalan/Spanish	second semester	morning-mixed
(SEM) Seminars	341	Catalan	second semester	morning-mixed
(TE) Theory	34	Catalan/Spanish	second semester	morning-mixed