Course guide
2703126 - SB - Structural Bioinformatics

Last modified: 30/01/2026

Unit in charge: Barcelona School of Informatics
Teaching unit: 1004 - UB - (ENG)Universitat de Barcelona.

Degree: BACHELOR'S DEGREE IN BIOINFORMATICS (Syllabus 2024). (Compulsory subject).

Academic year: 2025 **ECTS Credits:** 6.0 **Languages:** English

LECTURER

Coordinating lecturer: JOSEP LLUIS GELPI BUCHACA

Others: Segon quadrimestre:
JOSEP LLUIS GELPI BUCHACA - 11, 12

PRIOR SKILLS

Basic knowledge of macromolecule structure (Physical and organic chemistry, Biochemistry, Molecular Biology)
Knowledge of Thermodynamics and kinetics and evaluation of energies in macromolecules (Physical and organic chemistry, Biophysics)
Knowledge of molecular visualization tools
Knowledge of programming (python)

LEARNING RESULTS

Knowledges:
K1. Recognise the fundamental principles of biology, from the cellular to the organismic scale, and how they relate to current knowledge in bioinformatics, data analysis and machine learning, achieving an interdisciplinary vision with an emphasis on biomedical applications.
K2. Identify statistical and computational methods and mathematical models that can be used to solve problems in molecular biology, genomics, medical research and population genetics.
K5. Identify the nature of the biological variables that need to be analysed, as well as appropriate mathematical models, algorithms and statistical tests to develop and evaluate statistical analyses and computational tools.
K7. Analyse sources of valid and reliable scientific information to determine the state of the art of a bioinformatics problem and how to tackle it.

Skills:
S10. Apply acquired knowledge and bioinformatics problem-solving skills in new or unfamiliar environments in broader (or multidisciplinary) contexts related to bioinformatics and computational biology.
S7. Implement programming methods and data analysis based on the development of working hypotheses within the area of study.

TEACHING METHODOLOGY

- The theoretical classes will be expository with the help of graphic materials (slides, videos, computer demonstrations).

- The problem-solving session will detail the methodology for solving the selected problems. It will include expository and practical sessions.

- The guided structural analysis sessions will be held in "Hackathon" style working groups to solve the use of structural bioinformatics tools for the resolution of practical cases.

LEARNING OBJECTIVES OF THE SUBJECT

1.1. Recognition of the structural patterns of biomolecules and relationship with their biological function. The student must demonstrate understanding of the physicochemical descriptors of structure: terms of potential energy, solubility, acidity, hydrophobicity
2.2. Correlate three-dimensional structure of biomolecules with their biological function
Demonstrate understanding of:
- Relationship between sequence, structure, and function: global and local flexibility and similarity of the sequence, three-dimensional preservation of active centres, conservation of interactions with ligands and other proteins.
- Bases and applications of the homology concept. Identify the conserved residues in structure and describe its possible structural function.

3.3. Manage the software that allows processing data representing structures and sequences of biomolecules.

STUDY LOAD

Type	Hours	Percentage
Self study	90,0	60.00
Hours small group	30,0	20.00
Hours large group	30,0	20.00

Total learning time: 150 h

CONTENTS

Part 0. INTRODUCTION

Description:
Introduction to the course.Aims, position of structural bioinformatics within bioinformatics, main objectives. Application examples

Part 1. STRUCTURE AND MODELLING

Description:
Fundamentals of macromolecular structures. Conformational space. Experimental structure determination. Data sources and formats. Databases and Molecular visualization.
Structural data quality, common issues and fixes.Structure comparison, Sequence/structural alignment, structural families, the concept of homology. Structure prediction (1D, Threading, Comparative, Ab initio, Alphafold). Complex prediction (Docking)

Part 2. CONFORMATIONAL SPACE AND SIMULATION

Description:
Energy evaluation. Molecular force fields. System setup for simulation. Optimization of the simulation process and HPC. Strategies for improved comformation sampling. Simulation analysis. Quality control. Flexibility analysis. Strategies for entropy and free enegy evaluation. Advanced analysis. nmetwork analysis and AI-based methods

Part 3. STRUCTURES IN SYSTEM BIOLOGY

Description:
Protein domains. Interactions between chains and between domains. Predicting physical interactions based on domains. Transitive and permanent complexes. Other predictions of relationships between genes and proteins. Communication systems and signalling networks (phosphorylation). Study of interaction networks: Interactome. Large macromolecular complexes.

ACTIVITIES

Partial Exam

Description:
Mid-term exam (Problem solving)

Specific objectives:
1, 2, 3

Full-or-part-time: 2h
Guided activities: 2h

Final Exam

Description:
Final Exam.

Specific objectives:
1, 2, 3

Full-or-part-time: 3h
Guided activities: 3h

Theoretical sessions

Description:
Content presentation sessions. Slide presentations and guided demonstrations.

Specific objectives:
1, 2

Full-or-part-time: 47h
Theory classes: 27h
Self study: 20h

Guided problem solving

Specific objectives:
1, 2, 3

Full-or-part-time: 30h
Laboratory classes: 10h
Self study: 20h

Guided structural analysis

Description:
Resolution of practical cases on bioinformatics analysis tools, usually available via the web, or easily installableResolution of practical cases on bioinformatics analysis tools, usually available via the web, or easily installable

Specific objectives:
1, 2, 3

Full-or-part-time: 44h
Laboratory classes: 14h
Self study: 30h

Session on Project presentations

Description:
Short group presentations of the results of the analysis project

Specific objectives:
1, 2, 3

Full-or-part-time: 2h
Guided activities: 2h

Intregrated Analysis project

Description:
Free-subject project that involves the use of structural analysis or prediction tools developed during the course, applied to the understanding of the structure-function relationship of a protein system.

Full-or-part-time: 22h
Laboratory classes: 2h
Self study: 20h

GRADING SYSTEM

For the evaluation of the subject, the grade of the partial exam (MTE) and final exam (FE) and the grade of the practical sessions and the analysis project (Proj) will be taken into account according to the following formula:

Grade = MTE * 0.2 + FE * 0.6 + Proj * 0.2

A grade equal to or greater than 5 is required to pass.
The Practical Sessions and Project (Proj) qualification is conditional on a minimum in-person attendance of 60% in the practical/problem sessions.
Students who have failed with a grade equal to or greater than 3 may take the re-evaluation exam (RT). In this case, the grade of the subject will be 0.2 * Proj + RT * 0.8.

BIBLIOGRAPHY

Basic:

- Gu, Jenny; Bourne, Philip E.. Structural Bioinformatics. 2. Wiley Blackwell, 2009. ISBN 978-0-470-18105-8.
- Branden, Carl; Tooze, John. Introduction to protein structure. 2a ed. Garland, cop. 1999. ISBN 978-0-8153-2305-1.
- Leach, Andrew R. Molecular modelling : principles and applications. 2nd ed. Prentice Hall, 2001. ISBN 9780582382107.
- Creighton, Thomas E. The Biophysical chemistry of nucleic acids & proteins. Helvetian Press, 2010. ISBN 9780956478115.