COURSE DATA

DATA SUBJECT

Code: 42588
Name: Structural bioinformatics
Cycle: Master's Degree
ECTS Credits: 3
Academic year: 2025-26

STUDY (S)

Degree	Center	Acad. year	Period
2116 - Master's Degree in Bioinformatics	Escola Tècnica Superior d'Enginyeria	1	Second quarter

SUBJECT-MATTER

Degree	Subject-matter	Character
2116 - Master's Degree in Bioinformatics	Structural bioinformatics	COMPULSORY

COORDINATION

ARNAU LLOMBART VICENTE

SUMMARY

We will study the basic techniques of analysis and structure prediction of nucleic acids and proteins. Within the course will give an overview of the tools and data bases used in structural bioinformatics.

PREVIOUS KNOWLEDGE

RELATIONSHIP TO OTHER SUBJECTS OF THE SAME DEGREE

There are no specified enrollment restrictions with other subjects of the curriculum.

OTHER REQUIREMENTS

None

COMPETENCES / LEARNING OUTCOMES

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Be able to access the information required (databases, scientific articles, etc.) and to interpret and use it sensibly.

Be able to access to information tools in other areas of knowledge and use them properly.

Desarrollar la iniciativa personal y ser capaces de realizar una toma rápida y eficaz de decisiones en su labor profesional y/o investigadora.

Students should apply acquired knowledge to solve problems in unfamiliar contexts within their field of study, including multidisciplinary scenarios.

Students should be able to integrate knowledge and address the complexity of making informed judgments based on incomplete or limited information, including reflections on the social and ethical responsibilities associated with the application of their knowledge and judgments.

Students should communicate conclusions and underlying knowledge clearly and unambiguously to both specialized and non-specialized audiences.

Students should demonstrate self-directed learning skills for continued academic growth.

Students should possess and understand foundational knowledge that enables original thinking and research in the field.

To be able to assess the need to complete the scientific, historical, language, informatics, literature, ethics, social and human background in general, attending conferences, courses or doing complementary activities, self-assessing the contribution of these activities towards a comprehensive development.

Trabajar en equipo con eficiencia en su labor profesional y/o investigadora y con personas de diferente procedencia.

DESCRIPTION OF CONTENTS

1. Structure and biophysics of nucleic acids and proteins.

Structure and biophysics of nucleic acids and proteins. Basic concepts and obtain crystallographic protein structure by X-ray diffraction or NMR.

2. Database of protein structure, nucleic acids and small molecules

Accessing databases of protein structure, nucleic acids and small molecules.

3. Alignment and classification structure

A structural alignment is a type of alignment of sequences based on the comparison of the shape. We will study these concepts.

4. Structural genomics

We need to know not experimentally determined structures of known sequences of genes and proteins. Structural genomics is concerned with generating and analyzing these three-dimensional shapes.

5. Three-dimensional structure prediction of nucleic acids and proteins.

We will focus on three-dimensional structure prediction of nucleic acids and proteins.

6. Docking of small molecular structures on the surface of proteins.

Study the molecular coupling or docking of small molecular structures on the surface of proteins.

7. Applications for the development of new drugs

One of the main objectives of structural bioinformatics is its application to drug development. We will discuss this possibility with the techniques seen in this area.

WORKLOAD

PRESENCIAL ACTIVITIES

Activity	Hours
Theory	10,50
Laboratory	4,50
Total hours	**15,00**

NON PRESENCIAL ACTIVITIES

Activity	Hours
Attendance at other activities	2,00
Individual or group project	2,00
Independent study and work	22,00
Preparation of lessons	13,50
Preparation for assessment activities	6,00
Resolution of case studies	9,00
Total hours	**54,50**

TEACHING METHODOLOGY

MD1 - Task training of the teaching-learning environment interaction in the classroom through expository sessions. Previous assignments include preparation (information search, reading texts supplied by teachers), teaching sessions themselves and the later work of deepening.

MD2 - Learning through problem solving and case studies, through which it is acquiring skills on different aspects of materials and subjects.

MD3 - Hands-on lab. Include preparation, implementation of practices to monitor and teacher support, independent work online and reporting practices.

MD4 - Cross-disciplinary skills. Include attendance at courses, conferences or round tables organized by the CEC of the Master and / or conduct of a bibliographic work on issues that contribute to the integral. It produces a report of activities.

EVALUATION

In both sessions:

SE1 Continuous Assessment: 5%.
SE3 Laboratory: 55%.
SE4 Exams: 40%.

REFERENCES

Thomas E. Creighton. Proteins: Structures and Molecular Properties. W. H. Freeman (ed); 2 Sub edition (August 15, 1992). ISBN-10: 071677030X

Gregory A. Petsko & Dagmar Ringe. Protein Structure and Function. Sinauer Associates (eds) (January 2004). ISBN-10: 0878936637

Structural Bioinformatics, 2nd ed. (2009). Eds. Gu, J. & Bourne, P.E. John Wiley & Sons, New Jersey.

Introduction to Protein Structural Bioinformatics (2018). K. Anton Feenstra, Sanne Abeln. bioRxiv: 1801.09442https://doi.org/10.48550/arXiv.1801.09442

Kessel, A., & Ben-Tal, N. (2018). Introduction to Proteins: Structure, Function, and Motion, Second Edition (2nd ed.). Chapman and Hall/CRC.

Florencio Pazos & Mónica Chagoyen. Practical Protein Bioinformatics. Springer. (January 2015). ISBN 978-3-319-12727-9

Michael Eisenstein (2021). Artificial intelligence powers protein-folding predictions. Nature. 7886(599):706-708.