

**COURSE DATA****Data Subject**

<b>Code</b>	42588
<b>Name</b>	Structural bioinformatics
<b>Cycle</b>	Master's degree
<b>ECTS Credits</b>	3.0
<b>Academic year</b>	2023 - 2024

**Study (s)**

<b>Degree</b>	<b>Center</b>	<b>Acad. year</b>	<b>Period</b>
2116 - M.U. en Bioinformàtica 12-V.1	School of Engineering	1	Second term

**Subject-matter**

<b>Degree</b>	<b>Subject-matter</b>	<b>Character</b>
2116 - M.U. en Bioinformàtica 12-V.1	6 - Structural bioinformatics	Obligatory

**Coordination**

<b>Name</b>	<b>Department</b>
ARNAU LLOMBART, VICENTE	240 - Computer Science

**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



## OUTCOMES

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- 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.
- Be able to access the information required (databases, scientific articles, etc.) and to interpret and use it sensibly.
- Students should possess and understand foundational knowledge that enables original thinking and research in the field.
- Be able to access to information tools in other areas of knowledge and use them properly.
- 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.
- Desarrollar la iniciativa personal y ser capaces de realizar una toma rápida y eficaz de decisiones en su labor profesional y/o investigadora.
- Trabajar en equipo con eficiencia en su labor profesional y/o investigadora y con personas de diferente procedencia.

## LEARNING OUTCOMES

Mastering the basics of structural biology and biophysics and bioinformatics tools essential management structures of nucleic acids and proteins.

Understand the use and development of primary methods of predicting three-dimensional structure of nucleic acids and proteins.

## 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**

ACTIVITY	Hours	% To be attended
Theory classes	10,50	100
Laboratory practices	4,50	100
Development of group work	5,00	0
Development of individual work	10,00	0
Study and independent work	15,00	0
Readings supplementary material	10,00	0
Preparation of evaluation activities	10,00	0
Preparing lectures	5,00	0
Preparation of practical classes and problem	5,00	0
<b>TOTAL</b>	<b>75,00</b>	

**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 the two calls:

SE2 Activities: minimum 10 and maximum 50.

SE3 Laboratory: minimum 25 and maximum 75.

SE4 Exams: minimum 0 and maximum 40.



## REFERENCES

### Basic

- Referencia b1: Structural Bioinformatics. Jenny Gu, Philip E. Bourne. Ed. John Wiley & Sons, 2009.
- Belton JM, McCord RP, Gibcus JH, Naumova N, Zhan Y, Dekker J. 2012. Hi-C: a comprehensive technique to capture the conformation of genomes. *Methods* 58: 268-276.
- Cavalli G, Misteli T. 2013. Functional implications of genome topology. *Nature structural & molecular biology* 20: 290-299.
- Dekker J, Marti-Renom MA, Mirny LA. 2013. Exploring the three-dimensional organization of genomes: interpreting chromatin interaction data. *Nature reviews Genetics* 14: 390-403.

### Additional

- Referencia c1: Structural Bioinformatics: An Algorithmic Approach (Chapman & Hall/CRC Mathematical & Computational Biology). Forbes J. Burkowski. 2008 | ISBN-10: 1584886838.
- Referencia c2: Structural Bioinformatics. Ed. Aaron Philippe Toll. 2012. ISBN-10: 6200704244 | ISBN-13: 978-6200704245