

BASIC DETAILS:

Subject:	BIOINFORMÁTICA ESTRUCTURAL		
Id.:	33710		
Programme:	DOBLE GRADO EN FARMACIA Y BIOINFORMÁTICA. PLAN 2019		
Module:	BIOINFORMÁTICA		
Subject type:	OBLIGATORIA		
Year:	3	Teaching period:	Primer Cuatrimestre
Credits:	3	Total hours:	75
Classroom activities:	35	Individual study:	40
Main teaching language:	Inglés	Secondary teaching language:	Castellano
Lecturer:	R O I G M O L I N A , FRANCISCO JOSE (T)	Email:	fjroig@usj.es

PRESENTATION:

This course covers the algorithmic approaches used to predict the primary, secondary and tertiary structure of proteins. In addition to understanding the theoretical bases, we will study how to apply these methods in practice for structure prediction and expression analysis. Within the course, a general overview of the tools and databases most used in structural Bioinformatics will be given, emphasizing the input formats, parameters and interpretation of results common to many of them.

Upon completing the subject, the student will be able to:

- Interpret the information contained in public databases of proteins and chemical substances
- Use tools for the visualization, modification and analysis of proteins
- Model the secondary structure of proteins using the sequence of homologous amino acids of known structure
- Identify homologous proteins of known 3D structure and subsequent comparative 3D modeling
- Predict potential protein domains and their function
- Determine potential relationships between chemical structure and bioactivity

PROFESSIONAL COMPETENCES ACQUIRED IN THE SUBJECT:

General programme competences	G01	Use learning strategies autonomously for their application in the continuous improvement of professional practice.
	G02	Perform the analysis and synthesis of problems of their professional activity and apply them in similar environments.
	G03	Cooperate to achieve common results through teamwork in a context of integration, collaboration and empowerment of critical discussion.
	G04	Reason critically based on information, data and lines of action and their application on relevant issues of a social, scientific or ethical nature.
	G05	Communicate professional topics in Spanish and / or English both orally and in writing.
	G06	Solve complex or unforeseen problems that arise during the professional activity within any type of organisation and adapt to the needs and demands of their professional environment.
	G07	Choose between different complex models of knowledge to solve problems.
	G09	Apply information and communication technologies in the professional field.
	G10	Apply creativity, independence of thought, self-criticism and autonomy in the professional practice.
	Specific programme competences	E02
E03		Apply the fundamental concepts of mathematics, logic, algorithmics and computational complexity to solve problems specific to bioinformatics.
E04		Program applications in a robust, correct, and efficient way, choosing the paradigm and the most appropriate programming languages, applying knowledge about basic algorithmic procedures and using the most appropriate types and data structures.
E05		Implement well-founded applications, previously designed and analysed, in the characteristics of the databases.
E06		Apply the fundamental principles and basic techniques of intelligent systems and their practical application in the field of bioinformatics.
E07		Apply the principles, methodologies and life cycles of software engineering to the development of a project in the field of bioinformatics.

E12	Apply the principles and techniques of protein computational modelling to predict their biological function, their activity or new therapeutic targets (Structural Bioinformatics, Computational Toxicology).
E13	Apply omics technologies for the extraction of statistically significant information and for the creation of relational databases of biodata that can be updated and publicly accessible to the scientific community.
E14	Use programming languages, most commonly used in the field of Life Sciences, to develop and evaluate techniques and/ or computational tools.
E15	Infer the evolutionary history of genes and proteins through the creation and interpretation of phylogenetic trees.
E16	Plan linkage and association studies for medical and environmental purposes.
E17	Induce complex relationships between samples by applying statistical and classification techniques.
E18	Apply statistical and computational methods to solve problems in the fields of molecular biology, genomics, medical research and population genetics.
E21	Apply computational and data processing techniques for the integration of physical, chemical and biological concepts and data for the description and/ or prediction of the activity of a substance in a given context.

PRE-REQUISITES:

Not prerequisites needed.

SUBJECT PROGRAMME:

Subject contents:

1 - Proteins: Structure and function.
1.1 - What is a protein?
1.2 - Protein structure: Structuring levels
1.3 - Structure-function relationship
2 - Bioinformatics and proteins
2.1 - From sequence to function
3 - Databases and structural data formats
3.1 - Protein Data Bank
3.2 - SCOP and CATH
4 - Prediction of structures
4.1 - Secondary structure prediction
4.2 - 3D structure prediction using comparative modeling
4.3 - Model evaluation
4.4 - Software for structural analysis
4.4.1 - Visualization: Pymol and Rasmol
4.4.2 - Modeling: I-Tasser and Modeller
5 - Molecular coupling
5.1 - What is molecular coupling?
5.2 - Software
5.2.1 - AutoDock Vina and SwissDock
6 - Applications of structural bioinformatics.
6.1 - Functional identification
6.2 - Development of new drugs

Subject planning could be modified due unforeseen circumstances (group performance, availability of resources, changes to academic calendar etc.) and should not, therefore, be considered to be definitive.

TEACHING AND LEARNING METHODOLOGIES AND ACTIVITIES:

Teaching and learning methodologies and activities applied:

Master classes:

Teacher will explain the theory using TIC and physical resources on presential classes. Material will be available on the PDU in advance for previous reading. Students are highly recommended to perform the reading task.

Theoretical-practical classes:

Omics needed from practise. In this type of sessions the students will perform a reproduction of command execution done in theory and the completion of proposed exercises, in order to assure correct comprehension.

Self-learning based on critical-thinking:

Students will explore scientific publication and discuss between each other about oral presentation of the rest of students. This way, basic knowledge of the field will be reinforced for scientific process.

Learning based on projects:

Two projects will be performed time course of the subject in order to apply the acquired knowledge in the experimental design area:

a) The students will carry out the critical analysis of a publication in which a structural reconstruction performed using bioinformatics, analyzing the methodology, the type of results. Students are expected to be able not only to carry out a bibliographic analysis, but also to be able to understand the objectives, the methodology and the conclusions at a structural and biological level. This work will be 10% of the final grade. The work will be delivered in electronic format.

b) The students will carry out the reconstruction of the 3D structure of a protein sequence, looking for possible ligands. The work will be presented in the form of a scientific article and the execution of the analyzes will be presented in markdown format, preferably written in English. The starting data for the work may be provided by the teacher or selected by the students with the help of the teacher. This work will represent 35% of the final grade. The work will be in electronic format and presented in class virtually.

Both works will be presented in class on the date shown in the planning.

Tutoring sessions

The students will be able to ask the teacher any doubts that arise both from the face-to-face classes and from the autonomous or group work. The tutorials can be both face-to-face and using available technological means.

Student work load:

Teaching mode	Teaching methods	Estimated hours
Classroom activities	Master classes	16
	Tutorials	4
	Individual activities (essays, presentations, oral presentations, concept maps, problems ...)	10
	Evaluation tests (questionnaires and other instruments)	5
Individual study	Individual study	7
	Individual coursework preparation	10
	Project work	14
	Recommended reading	4
	Video class/Webinars/vidoelessons/ podcast	5
Total hours:		75

ASSESSMENT SCHEME:

Calculation of final mark:

Individual coursework:	45 %
Final exam:	55 %
TOTAL	100 %

*Las observaciones específicas sobre el sistema de evaluación serán comunicadas por escrito a los alumnos al inicio de la materia.

BIBLIOGRAPHY AND DOCUMENTATION:

Basic bibliography:

Fiser A. From Protein Structure to Function with Bioinformatics. Ridgen DJ, editor. Springer 2008.

Recommended bibliography:

Alberts, B., Johnson, A., Lewis, J., Raff, M., Roberts, K., & Walter, P. Molecular biology of the cell. New York: Garland Science.2002.

Bateman A. Protein families: relating protein sequence, structure, and function. New Jersey: John Wiley and Sons.2014

Berg JM, Tymoczko JL, Stryer L. Biochemistry. 5th edition. New York: W H Freeman. 2002.

Fiser A. Template-based protein structure modeling. Methods Mol Biol. 2010;673:73-94.

Persson B. Bioinformatics in protein analysis. EXS. 2000;88:215-231.

Roger Sayle and E. James Milner-White. RasMol: Biomolecular graphics for all. Trends in Biochemical Sciences (TIBS), September 1995, Vol. 20, No. 9, p. 374.

Webb B., Sali A. Comparative Protein Structure Modeling Using Modeller. Current Protocols in Bioinformatics 54, John Wiley and Sons, Inc., 5.6.1-5.6.37, 2016.

Xu Y, Xu D, Liang J. Computational methods for protein structure prediction and modeling volume 1: basic characterization. Berlin: Springer. 2007.

Xu Y, Xu D, Liang J. Computational methods for protein structure prediction and modeling volume 2: Structure Prediction. Berlin: Springer. 2007.

Yang, J. and Zhang, Y. Protein Structure and Function Prediction Using I-TASSER. Current protocols in bioinformatics, 2015;52, 5.8.1–5.8.15.

Recommended websites:

Protein Data Bank <https://www.rcsb.org/>