



Teaching Guide				
Identifying Data				2022/23
Subject (*)	Protein Structure and Dynamics	Code	610441012s	
Study programme	Máster Universitario en Bioloxía Molecular, Celular e Xenética (semipresencial)			
Descriptors				
Cycle	Period	Year	Type	Credits
Official Master's Degree	2nd four-month period	First	Optional	3
Language	SpanishEnglish			
Teaching method	Hybrid			
Prerequisites				
Department	BioloxíaDepartamento profesorado máster			
Coordinador	Cerdan Villanueva, María Esperanza	E-mail	esper.cerdan@udc.es	
Lecturers	Becerra Fernandez, Manuel Cerdan Villanueva, María Esperanza De Castro De Antonio, María Eugenia	E-mail	manuel.becerra@udc.es esper.cerdan@udc.es m.decastro@udc.es	
Web				
General description	This subject pretends to meet and manage the theoretical foundations and the experimental approaches to the analysis of the physical and chemical of biological macromolecules, especially proteins, properties in order to relate their structures with its function and biological activity. We will study the concepts needed for the description of the structures, computational and experimental methods for their study and the theoretical foundations that justify them.			

Study programme competences / results	
Code	Study programme competences / results
A3	Skills of understanding the functioning of cells through the structural organization, biochemistry, gene expression and genetic variability.
A9	Skills of understanding the structure and dynamics of proteins to individual and proteomic level, as well as the techniques that are necessary to analyze them and to study their interactions with other biomolecules.
B2	Skills of decision making for the problem solving: that are able to apply theoretical knowledges and practical acquired in the formulation of biological problems and the looking for solutions.
B3	Skills of management of the information: that are able to gather and to understand relevant information and results, obtaining conclusions and to prepare reasoned reports on scientific and biotechnological questions
B4	Organization and work planning skills: that are able to manage the use of the time as well as available resources and to organize the work in the laboratory.
C2	Ability to know and use appropriately the technical terminology of the field of knowledge of the master, in the native language and in English, as a language of international diffusion in this field
C3	Using ICT in working contexts and lifelong learning.
C8	Valuing the importance of research, innovation and technological development for the socioeconomic and cultural progress of society.

Learning outcomes			
Learning outcomes	Study programme competences / results		
Ability to understand concepts and theories related to the dynamics of proteins in cells	AR3 AR9	BR2	CC3 CC8
Familiarization with the bibliographic and information sources where you can get updated information	AR3 AR9	BR2	CC2 CC3 CC8
Know the systems for the determination of structures by x-ray diffraction	AR9	BR2	CC3 CC8



Learn different computer programs for the representation of proteins and their use	AR3 AR9	BR2	CC3 CC8
Learn the techniques to determine interactions between proteins and proteins with other biomolecules and ligands	AR3 AR9	BR4	CC8
Ability to interpret critically the data of a structure of a protein in a publication	AR3 AR9	BR3	CC2 CC3

Contents	
Topic	Sub-topic
Structural classification of proteins.	Structural domains of proteins. Classification of proteins according to its three-dimensional structure. Alpha proteins. Alpha/beta protein. Protein beta. Structural classes of proteins. CATH classification. SCOP classification. DALI classification. SMART classification.
Criteria for the choice of a method of purification and preliminary characterization.	Chromatographic techniques: gel filtration, ion exchange, affinity and hydrophobic interaction. Purification strategies. Preliminary characterization of the protein conformation: State of aggregation, compactness. Secondary structure and tertiary structure indicators. Quantification of proteins.
Experimental determination of the structure of proteins using diffraction X.	Crystallization techniques. Tools and strategies for diffraction data. Interpretation of the XRD. Obtaining and refinement of the molecular model. Parameters for calculating the convergence of the model. Modelling.
Interactions between biomolecules.	Interactions of proteins for the formation of complexes with proteins and other ligands. Experimental methods used to determine these interactions and their structure. The double hybrid method. The split-ubiquitin method. Pull-down. GST-Pull-down. FRET. EMSA trials. CHIP test. Other methodologies.

Planning				
Methodologies / tests	Competencies / Results	Teaching hours (in-person & virtual)	Student?s personal work hours	Total hours
Guest lecture / keynote speech	A9 C2	1	41	42
Case study	A9 B2 B3 B4 C8	1	9	10
ICT practicals	A3 C3	1	3	4
Mixed objective/subjective test	A9	2	12	14
Personalized attention		5	0	5

(\*)The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.

Methodologies	
Methodologies	Description
Guest lecture / keynote speech	The student will be able to attend the face-to-face sessions synchronously through TEAMS. Sessions will be recorded for viewing asynchronously.
Case study	Case study consists of simulations and works using the problem-based learning methodology.
ICT practicals	ICT allow display of protein structure models and design interaction experiments.
Mixed objective/subjective test	Combination of multiple choice questions and short of relationship questions

Personalized attention	
Methodologies	Description



Case study ICT practicals	The personalized attention that is described in relation to these methodologies are conceived as moments of face-to-face student work with the teacher through TEAMS by involving a compulsory student participation.
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Assessment			
Methodologies	Competencies / Results	Description	Qualification
Case study	A9 B2 B3 B4 C8	Students will have to answer questionnaires based on the case study.	15
Mixed objective/subjective test	A9	Test related to theoretical and practical knowledge. Students in blended mode, in addition to passing the test, must submit a series of tasks that will be requested throughout the course.	75
ICT practicals	A3 C3	Students in blended mode will carry out the practices through ICT on their own and will submit a report of the work carried out.	10

Assessment comments
<p>To get honours preference will be given to the students evaluated at the first opportunity in June.</p> <p>For the students who request the DECEMBER ADVANCE CALL, the current regulations will be applied, according to which the teaching guide of the current course governs.</p> <p>Implications of PLAGIARISM in the qualification: The current regulations will be applied, according to which the fraudulent performance of the tests or evaluation activities will directly imply the qualification of failure.</p>

Sources of information	
<b>Basic</b>	<p>Banaszak, L. J. (2000). Foundations of structural biology. Academic Press. Berg, J. M., Tymoczko, J. L., Stryer. L. (2003). BIOQUÍMICA. 5ª Edición. Reverté. Branden, C. &amp; Tooze, J. (1998). INTRODUCTION TO PROTEIN STRUCTURE. 2nd edition Garland Publishing, Inc, New York. Cerdán Villanueva, M. E. (2005). Curso avanzado de proteínas y ácidos nucleicos. Universidade da Coruña. Creighton, T. E. (1993). PROTEINS: STRUCTURES AND MOLECULAR PROPERTIES, 2nd edition. W.H. Freeman &amp; Company, New York. Gómez-Moreno, C. &amp; Sancho, J. (Coords). (2003). ESTRUCTURA DE PROTEÍNAS. Ariel Ciencia, Barcelona. Lesk, A. M. (2000). INTRODUCTION TO PROTEIN ARCHITECTURE. THE STRUCTURAL BIOLOGY OF PROTEINS. Oxford University Press, Oxford. Nelson, D. L., Cox, M. M. (2000). LEHNINGER PRINCIPLES OF BIOCHEMISTRY. Worth Publishers. Rodes, G. (2000). Crystallography. Made Crystal Clear. Academic Press.</p>



## Complementary

§ Carter, Jr., C.V. y Sweet, R. M. (1997). *Macromolecular Crystallography*, parts A and B. *Methods in Enzymology*, vols. 276 y 277. Academic Press. NY. § Casari, G., Sander, C., Valencia, A. (1995). A method to predict functional residues in proteins. *Nature Struct. Biol.*, 2: 171178. § Clore, G. M. y Gonenborg, A. M. (1998). New methods of structure refinement for macromolecular structure determination by NMR. *Proc. Natl. Acad. Sci.*, 95, 58915898. § Del Sol Mesa, A., Pazos, F., Valencia, A. (2003). Automatic methods for predicting functionally important residues. *J. Mol. Biol.*, 326: 12891302. § Ducruix, A., Giegé, R. (1999). *Crystallisation of Nucleic Acids and Proteins. A Practical Approach*, edn 2. Oxford University Press. Oxford. § Eyrich, V. A., MartiRenom, M. A., Przybylski, D., Madhusudhan, M.S., Fiser, A., Pazos, F., Valencia, A., Sali, A. y Rost, B. (2001). EVA: continuous automatic evaluation of protein structure prediction servers. *Bioinformatics*, 17: 12421243. § Ferentz, A.E. y Wagner, G. (2000). *NMR spectroscopy: a multifaceted approach to macromolecular structure*. *Quarter Rev. Biophys.* 33, 2965. § Fersht, A. R. (1999). *Structure and Mechanism in Protein Science*, Freeman and Co., NY. § Frank, J. (1996). *Three dimensional electron microscopy of macromolecular assemblies*. Academic Press, San Diego. § Harris, E. L. V. y Angel, S. (eds.) (1999): *Protein purification methods. A practical approach*. IRL Press. Oxford. § James, T. L., Dötsch, V. y Smith, U. (2001). *Nuclear Magnetic Resonance of Biological Macromolecules. Part A and B. Methods Enzymol.*, 338, Academic Press, San Diego. § Juan, D., Graña, O., Pazos, F., Fariselli, P., Casadio, R., Valencia, A. (2003). A neural network approach to evaluate Fold recognition results. *Proteins Mar 1,(4): 50, 600608.* § Kleanthous, C. (ed.) (2000). *Protein-Protein Recognition*. Oxford University Press, Oxford. § Mayo, K. H. y Daragan, U. A. (2003). *Protein dynamics using NMR relaxation*. World Scientific, Nueva Jersey. § McEwen, B. F. y Marcko, M. (2001). The emergence of electron tomography as an important tool for investigating cellular ultrastructure. *J. Histochem. Cytochem. Vol 49, 553563.* § McPherson, A. (2002). *Introduction to Macromolecular Crystallography*. John Wiley and Sons. Inc., NY. § Naomi, E. C. (2004). Turning Protein crystallisation from an art into a science. *Current Opinion in Structural Biology*, 14: 577583. § Sinha, N. y SmithGill, S. J. (2002). Protein structure to function via dynamics. *Protein Peptid Letters*, 9: 367377. § Van Heel, M. (2000). Single particle electron cryomicroscopy: towards atomic resolution. *Q. Rev. Biophys.* Vol. 33, 307369. § Igor Stagljar and Stanley Fields (2002). Analysis of membrane protein interactions using yeast-based technologies ? REVIEW . *Trends in Biochemical Sciences*, 27: 559-563. § Sandor Vajda and Carlos J. Camacho (2004). Protein-protein docking: is the glass half-full or half-empty? *Trends in Biotechnology*, 22: 110-116. § Dobrin Nedelkov and Randall W. Nelson (2003). Surface plasmon resonance mass spectrometry: recent progress and outlooks ? REVIEW *Trends in Biotechnology*, 21: 301-305. § Takashi Ito, Tomoko Chiba and Mikio Yoshida (2001). Exploring the protein interactome using comprehensive two-hybrid projects ? REVIEW . *Trends in Biotechnology*, 19 (Supplement 1): 23-27. § Valerio Orlando (2000). Mapping chromosomal proteins in vivo by formaldehyde-crosslinked-chromatin immunoprecipitation ? REVIEW . *Trends in Biochemical Sciences*, 25: 99-104. § Dobrin Nedelkov and Randall W. Nelson (2003) Surface plasmon resonance mass spectrometry: recent progress and outlooks ? REVIEW . *Trends in Biotechnology*, 21: 301-305. § Philippe I. H. Bastiaens and Rainer Pepperkok (2000). Observing proteins in their natural habitat: the living cell ? REVIEW . *Trends in Biochemical Sciences*, 25: 631-637

Coordenadas: Protein Data Bank: <http://www.rcsb.org/pdb> BioMagResBank: <http://www.brmb.wisc.edu> Cambridge Crystall Data Centre: <http://www.ccdc.cam.ac.uk> Molecular Modelling DataBase: <http://www.ncbi.nlm.nih.gov/structure> Nucleic Acid Database: <http://ndbserver.rutgers.edu:80/> MOOSE: <http://db2.sdsc.edu/moose> Molecules To Go (R US): <http://molbio.info.nih.gov/cgi-bin/pdb> Enzyme Structures Database: <http://www.ebi.ac.uk/thornton-srv/databases/enzymes> Clasificación estructural CATH <http://www.biochem.ucl.ac.uk/bsm/cath> SCOP <http://scop.mrc-lmb.cam.ac.uk/scop> FSSP <http://www2.embl-ebi.ac.uk/dali/fssp> Programas de visualización molecular: Rasmol: <http://www.umass.edu/microbio/rasmol> Swiss-PdbViewer: <http://www.expasy.ch/spdbv/> MOLMOL <http://www.mol.biol.ethz.ch/wuthrich/software/molmol> Cn3D <http://www.ncbi.nlm.nih.gov/Structure/CN3D/cn3d.shtml> Chime <http://www.umass.edu/microbio/chime> Servidores de alineamientos de secuencias: BLAST <http://www.ncbi.nlm.nih.gov/BLAST> FASTA <http://www.ebi.ac.uk/fasta33> Servidores de predicción y modelización: SWISS-MODEL <http://expasy.ch/swissmod/> The PredictProtein Server <http://www.embl-heidelberg.de/predictprotein/predictprotein.html> Center for Molecular Modeling: <http://cmm.info.nih.gov/modeling/> GRAMM: <http://reco3.musc.edu/gramm/> PQS (Probable Quat. Structure): <http://msd.ebi.ac.uk/services/quaternary/quaternary.html>



## Recommendations

### Subjects that it is recommended to have taken before

Molecular Techniques/610441002  
Advanced Cellular Biology/610441003

### Subjects that are recommended to be taken simultaneously

Recombinant proteins and protein Engineering /610441013  
Proteomics/610441014  
Bioinformatics and Biomolecular models /610441021

### Subjects that continue the syllabus

Project/610441023

### Other comments

Green  
Campus Faculty of Sciences Program To help  
achieve a sustainable immediate environment and comply with point 6 of the  
"Environmental Declaration of the Faculty of Sciences (2020)", the  
documentary works to be carried out in this subject will be requested in  
virtual format and computer support.

(\*)The teaching guide is the document in which the URV publishes the information about all its courses. It is a public document and cannot be modified. Only in exceptional cases can it be revised by the competent agent or duly revised so that it is in line with current legislation.