Teaching Guide				
Identifying Data				**2019/20**
Subject (*)	Protein Structure and Dynamics		**Code**	610441011
Study programme	Mestrado Universitario en Bioloxía Molecular , Celular e Xenética			
Descriptors				
Cycle	**Period**	**Year**	**Type**	**Credits**
Official Master's Degree	2nd four-month period	First	Optional	3
Language	SpanishEnglish			
Teaching method	Face-to-face			
Prerequisites				
Department	Bioloxía			
Coordinador	Becerra Fernandez, Manuel	**E-mail**	manuel.becerra@udc.es	
Lecturers	Becerra Fernandez, Manuel Cerdan Villanueva, Maria Esperanza Lamas Maceiras, Mónica Vizoso Vázquez, Ángel José	**E-mail**	manuel.becerra@udc.es esper.cerdan@udc.es monica.lamas@udc.es a.vizoso@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.
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	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	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	14	28	42
Laboratory practice	A9 B3 B2 B4 C8	4	6	10
ICT practicals	A3 C3	2	3	5
Mixed objective/subjective test	A9	1	15.5	16.5
Personalized attention		1.5	0	1.5
(*)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	Oral presentation complemented with the use of audiovisual media in order to pass on knowledge and facilitate learning.
Laboratory practice	Methodology that enables students to learn effectively, through practical activities (demonstrations, simulations, etc.) the theory of a field of knowledge, through the use of communications and information technologies.
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**

Laboratory practice 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 by involving a compulsory student participation. Students with part-time dedication or waiver of presence should contact the teachers of the subject in the early going to establish a schedule of activities to acquire and evaluate in a complementary way the competences.

Assessment

Methodologies	Competencies / Results	Description	**Qualification**
Laboratory practice	A9 B3 B2 B4 C8	Regular attendance and active participation at the laboratory practices will be evaluated.	15
Mixed objective/subjective test	A9	Test relating to knowledge and skills	75
ICT practicals	A3 C3	Attendance and active participation will be valued	10

Assessment comments

To get honours preference will be given to the students evaluated at the
first opportunity in June.

Sources of information

Basic	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. & 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 & Company, New York.Gómez-Moreno, C. & 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.

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: continuos automatic evaluation of protein structure prediction servers. 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Protein dynamics using NMR relaxation. World Scientific, Nueva Jersey.§ McEwen, B. F. y Marcko, M. (2001). The emergente of electrón tomography as an important tool for investigating cellular ultrastructure. J. Histochem. Cytochem. Vol 49, 553563.§ Mc Pherson, 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 electrón cryomicroscopy: towards atomic resolution. Q. Rev. Byophis. 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://ww.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 /610441012 Proteomics/610441013 Bioinformatics and Biomolecular models /610441020
Subjects that continue the syllabus
Project/610441022
Other comments