UNIVERSIDADE DA CORUÑA

Teaching Guide					
Identifying Data					2016/17
Subject (*)	Química Médica			Code	610509015
Study programme	Mestrado en Investigación Química e Química Industrial (plan 2016)				
Descriptors					
Cycle	Period	Year		Type	Credits
Official Master's Degree	Yearly	First		Optativa	3
Language	SpanishEnglish				
Teaching method	Face-to-face				
Prerequisites					
Department	Química Fundamental				
Coordinador	Riveiros Santiago, Ricardo		E-mail	ricardo.riveiros@udc.es	
Lecturers	Riveiros Santiago, Ricardo		E-mail	ricardo.riveiros@udc.es	
Web					
General description	This subject aims that the students to acquire the basic concepts in the field of medicinal chemistry and drug design, and also to know the required steps for drug development, ranging from the discovery of an active compound in the laboratory to its integration into the market. The subject will also address the major current methodologies in finding lead compounds that are employed in both industrial and academic level, and its optimization for the development of a drug. This includes from structure-based desigh, virtual screening, to fragment-based design of compounds. The most relevant aspects in the quantification oof the structure-relationships (QSAR) will be also described. Each of the contents of this subject will be illustrated by representative examples.				

Study programme competences / results	
Code	Study programme competences / results
A1	Define concepts, principles, theories and specialized facts of different areas of chemistry.
A2	Suggest alternatives for solving complex chemical problems related to the different areas of chemistry.
A3	Apply materials and biomolecules in innovative fields of industry and chemical engineering.
A4	Innovate in the methods of synthesis and chemical analysis related to the different areas of chemistry
B1	Possess knowledge and understanding to provide a basis or opportunity for originality in developing and / or applying ideas, often within a research context
B2	Students should apply their knowledge and ability to solve problems in new or unfamiliar environments within broader (or multidisciplinary) contexts related to their field of study.
B4	Students should be able to communicate their conclusions, and the knowledge and the reasons that support them to specialists and non-specialists in a clear and unambiguous manner
B7	Identify information from scientific literature by using appropriate channels and integrate such information to raise and contextualize a research topic
B10	Use of scientific terminology in English to explain the experimental results in the context of the chemical profession
B11	Apply correctly the new technologies to gather and organize the information to solve problems in the professional activity.

Learning outcomes			
Learning outcomes	Study programme competences / results		
Acquisition of advanced knowledge in medicinal chemistry and its most important applications in drug discovery.	AC1 AC2 AC3 AC4	BC1 BC2 BC4 BC7 BC10 BC11	

Understanding the required steps for drug development, ranging from the discovery of an active compound in the laboratory to its integration into the market.	AC1 AC2 AC3 AC4	BC1 BC2 BC4 BC7 BC10 BC11	
To know the main therapeutic targets used in drug discovery.	AC1 AC2 AC3 AC4	BC1 BC2 BC4 BC7 BC10 BC11	
To know the principal tolos used in the identification and the design of hit compounds.	AC1 AC2 AC3 AC4	BC1 BC2 BC4 BC7 BC10 BC11	
Understanding the chemical basis for optimizing the activity of a hit compound.	AC1 AC2 AC3 AC4	BC1 BC2 BC4 BC7 BC10 BC11	

Contents	
Topic	**Sub-topic**
Chapter 1. General aspects, definitions and concepts	Drug discovery: historical perspective. Drug activity phases. Enzymatic catalysis. Definitions and concepts: agonist, antagonist, transition state analogs, reversible inhibition (competitive, non-competitive), irreversible inhibition, suicide substrates. Examples.
Chapter 2. Therapeutic targets	Therapeutic targets: classification and their main characteristics. Enzymes. Membrane transporters. Voltage-gated ion channels. Non-selective cation channels. Receptors with intrinsic ion channels. Receptors with intrinsic enzymatic activity. Receptors coupled to various cytosolic proteins. G-protein-coupled receptors. Nuclear receptors.
Chapter 3. Strategies for drug discovery I. Structure-based design	Evolution of the structure-based design in drug discovery. Practical aspects of the determination of the three dimensional structure of a target-X-ray crystallography for the structure-based design. Applications of NMR spectroscopy in the rational design. Docking. Molecular dynamics simulations. QM/MM. Examples.
Chapter 4. Strategies for drug discovery II. Virtual screening and fragment-based design	Basics of the virtual screening candidates. Available databases. Applications: identifying ligands for a target or potential targets of a ligand. Basics of the fragment-based design. Screening of candidates by X-ray crystallography. Other biophysical screening methods. Examples.
Chapter 5. Hit Compound optimization. QSAR studies	Molecular modifications based on isosteric replacement. Conformational restriction and steric hindrance in medicinal chemistry. Homo and heterodimeric ligands. Prodrugs. Quantification of Structure-Activity Relationship (QSAR).

Planning				
Methodologies / tests	**Competencies / Results**	**Teaching hours (in-person & virtual)**	**Student?s personal work hours**	**Total hours**

Guest lecture / keynote speech	A1 A2 A3 A4 B1 B2 B4 B7 B10 B11	12	29	41
Seminar	A1 A2 A3 A4 B1 B2 B4 B7 B10 B11	7	14	21
Supervised projects	A1 A2 A3 A4 B1 B2 B4 B7 B10 B11	2	4	6
Objective test	A1 A2 A3 A4 B1 B2 B4	3	3	6
Personalized attention		1	0	1
(*)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	It will be held 12 sessions of lectures in one group where the theoretical contents of the course will be associated with illustrative examples. It will consist mainly in PowerPoint presentations. Copies of these presentations will be available for the students in advance via the Moodle platform of the course. This will allow the students to study ahead the contents of the course and to facilitate the monitoring of explanations.
Seminar	7 sessions in small group seminars where students will present the work proposed by the profesor followed by a discussion section. Students will have in advance the proposed exercises and papers via the Moodle platform of the course. Attendance at these clases is mandatory.
Supervised projects	Tutoring scheduled by the profesor and coordinated by the Centre. It will be 2 hours per student and will involve the supervision of proposed work, clarifying doubts, etc. Attendance at these clases is mandatory.
Objective test	It will be an objective test that will cover the entire contents of the subject.

Personalized attention	
Methodologies	**Description**
Supervised projects Seminar	The students should review the theoretical concepts introduced in each chapter using the reference manual and the material provided by the profesor. Those students, which have significant difficulties when working the proposed activities, should contact with the profesor during the tutorials, in order to analyze the problema and to receive the necessary support. The profesor will analyze with those students who do not successfully pass the evaluation, and so wish, their difficulties in learning the course content. Additional material (questions, exercises, tests, etc.) to strenghen the learning of the course migh also provided.

Assessment			
Methodologies	**Competencies / Results**	**Description**	**Qualification**
Supervised projects	A1 A2 A3 A4 B1 B2 B4 B7 B10 B11	The work done during the supervised projects will be taken into account. The following factors will be assessed: resolution of exercises and practical cases (4%), realization of homework and reports (2%), oral presentations [(paperes, reviews and practical cases), 2%] and oral questions during the course (1%).	10
Seminar	A1 A2 A3 A4 B1 B2 B4 B7 B10 B11	The work done during the seminars will be taken into account. The following factors will be assessed: resolution of exercises and practical cases (11%), realization of homework and reports (7,5%), oral presentations [(paperes, reviews and practical cases), 7,5%] and oral questions during the course (4%).	30
Objective test	A1 A2 A3 A4 B1 B2 B4	The objective test will consist of theoretical questions, practical and/or theoretical-practical over the entire course content.	60

Assessment comments
Access to the objective test will be conditioned on the participation in at least 80% of the mandatory classroom teaching activities (seminars and supervised projects). The repeaters will have the same system of class attendance tan those who study the course for first time.

Sources of information	
Basic	- Camille Georges Wermuth (2008). The practice of medicinal chemistry, 3rd Ed. Amsterdam: Elsevier - Graham L. Patrick (2013). An introduction to medicinal chemistry, 5th Ed. Oxford: Oxford University Press - Donald J. Abraham & David P. Rotella, Eds. (2010). Burger's medicinal chemistry, drug discovery and development, 7th Ed. Wiley
Complementary	- E. J. Corey, B, Czakó, L. Kürti (2007). Molecules and medicine. New Jersey: John Wiley and Sons - K. C. Nicolaou, T. Montagnon, Eds. (2008). Molecules that changed the world. Weinheim: Wiley-VCH - Edward R. Zartler & Michael J. Shapiro, Eds. (2008). Fragment-based drug discovery, a practical approach. Chichester: John Wiley & Sons - Roderick, E. Hubbard Ed (2006). Structure-based drug discovery, an overview. Cambridge: RSC-Publishing - Robert A. Copeland (2005). Evaluation of enzyme inhibitors in drug discovery. New Jersey: Wiley-Interscience - Celerino Abad-Zapatero (2013). Ligand efficiency indices for drug discovery. Amsterdam: Elsevier

Recommendations
Subjects that it is recommended to have taken before
Química de Biomoléculas/610509014
Subjects that are recommended to be taken simultaneously
Subjects that continue the syllabus
Other comments
Basic knowledge in the visiualization of the three dimensional structure of biomolecules using visualization programs such as Pymol, Mercury, etc. Management of databases such as Protein Data Bank (PDB), Expasy, etc. is also recommended.