Teaching Guide				
Identifying Data				2021/22
Subject (*)	Medicinal Chemistry		Code	610509116
Study programme	Mestrado Universitario en Investigación Química e Química Industrial (Plan 2020)			
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	Departamento profesorado másterQuímica			
Coordinador	Riveiros Santiago, Ricardo	E-mail	ricardo.riveiros@udc.es	
Lecturers	Brea Fernández, Roberto Javier Criado Fernández, Alejandro Riveiros Santiago, Ricardo	E-mail	roberto.brea@udc.es a.criado@udc.es ricardo.riveiros@udc.es	
Web	http://www.usc.es/gl/centros/quimica/curso/master.html			
General description	This subject aims that the students acquire the basic concepts in the field of medicinal chemistry and drug design, and also 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.			
Contingency plan	1. Modifications to the contents - There are no modifications. 2. Methodologies *Teaching methodologies that are maintained - All teaching methodologies are maintained (magisterial session, seminars and objective test). *Teaching methodologies that are modified The teaching methodologies will be adapted to the hybrid modality: - The master sessions and seminars will be held synchronously at the time established in the calendar of activities, through the Teams platform. -The objective test will be carried out through the Moodle and Teams platforms at the time established in the activity calendar. 3. Mechanisms for personalized attention to students 4. Modifications in the evaluation *Evaluation observations: 5. Modifications to the bibliography or webgraphy			

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	Innovate in the methods of synthesis and chemical analysis related to the different areas of chemistry
A4	Apply materials and biomolecules in innovative fields of industry and chemical engineering.

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.
C1	CT1 - Elaborar, escribir e defender publicamente informes de carácter científico e técnico
C3	CT3 - Traballar con autonomía e eficiencia na práctica diaria da investigación ou da actividade profesional.
C4	CT4 - Apreciar o valor da calidade e mellora continua, actuando con rigor, responsabilidade e ética profesional.

Learning outcomes			
Learning outcomes	Study programme competences / results		
To know the main concepts in medicinal chemistry and drug design: therapeutic targets, enzimatic inhibitors, agonists, antagonists, optimal pharmacological properties, etc.	AC1 AC2 AC3 AC4	BC1 BC2 BC4 BC7 BC10 BC11	CC1 CC3 CC4
To know the required steps for drug development, starting from the discovery of an active compound in the laboratory till its integration into the market.	AC1 AC2 AC3 AC4	BC1 BC2 BC4 BC7 BC10 BC11	CC1 CC3 CC4
To know the main methodologies for the seaching of active molecules (hits) and their optimization for the development of a new drug. Since the design based on the 3D structure of the therapeutic target, the real and virtual screening of libraries or the fragment based design.	AC1 AC2 AC3 AC4	BC1 BC2 BC4 BC7 BC10 BC11	CC1 CC3 CC4

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 A4 A3 B1 B2 B4 B7 B10 B11	12	29	41
Seminar	A1 A2 A4 A3 B1 B2 B4 B7 B10 B11	7	18	25
Objective test	A1 A4 A3 B1 B10	2	5	7
Personalized attention		2	0	2
(*)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 by videoconference 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	Seven sessions in small group seminars are scheduled. In these seminars, students will solve practical exercises (interpretation and processing information using specialized software and internet, evaluation of scientific papers, etc.), will prepare reports related to the different subjects and will present them during the class, followed by a discussion section with the professor and the rest of students. Students will have in advance the information they need via the Moodle platform. Attendance at these classes is mandatory.
Objective test	It will be an objective test that will cover the entire contents of the subject.

Personalized attention	
Methodologies	Description

Seminar	Students must review the theoretical concepts introduced in each chapter using the reference manual and the material provided by the professor. Those students, which have significant difficulties to do the proposed activities, should contact with the professor during the tutorials, in order to analyze the problems and to receive the necessary support. The professor 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 strengthen the learning of the course might also provided. Students with appreciation a part-time academic and attendance waiver of exemption may complete the seminars in individual and/or group tutoring schedule to be agreed with the teachers. The activities undertaken in these tutorials will be similar to those of students in ordinary regime and consideration for the final assessment.

Assessment			
Methodologies	Competencies / Results	Description	Qualification
Seminar	A1 A2 A4 A3 B1 B2 B4 B7 B10 B11	Continuous assessment will be the 40% of the final assessment of the subject. It will have two components: interactive classes in small group (seminars) and interactive classes in very small group (tutorials). Seminars and tutorials will include solving of proposed exercises and practical cases (10%), writing reports (10%), oral presentations [(works, reports, problems, practical cases), 10%] and oral questions along the course (10%).	40
Objective test	A1 A4 A3 B1 B10	The objective test will focus on the entire contents of the subject.	60

Assessment comments
The student's final qualification will be calculated applying this formula: Final qualification = 0.4 x N1 + 0.6 x N2 N1 is the numeric qualification corresponding to the continuous assessment (scale 0-10) and N2 is the numeric qualification corresponding to the objective test (scale 0-10). To access to the objective test the student must assist in, at least, 80% of the mandatory classroom teaching activities (seminars and tutorials). Students who study the subject for a second time will have the same system of class attendance and assestment than those who study the course for first time. In the case of students with recognition of part-time dedication and academic assistance waiver, the qualification of the continuous assessment will be replaced by that obtained in the personal tutorials. Students who attend fewer than 25% of planned academic activities and do not assist to the objective test, will be qualified as "Not presented".

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

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 - Celerino Abad Zapatero (2013). Ligand efficiency indices for drug discovery. Amsterdam: Elsevier

Recommendations
Subjects that it is recommended to have taken before
/
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.

(*)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.