Teaching Guide				
Identifying Data				2021/22
Subject (*)	Medicinal Chemistry		Code	610G01040
Study programme	Grao en Química			
Descriptors				
Cycle	Period	Year	Type	Credits
Graduate	2nd four-month period	Fourth	Optional	4.5
Language	Spanish			
Teaching method	Hybrid			
Prerequisites				
Department	Química			
Coordinador	García Romero, Marcos Daniel	E-mail	marcos.garcia1@udc.es	
Lecturers	Brea Fernández, Roberto Javier Criado Fernández, Alejandro García Romero, Marcos Daniel	E-mail	roberto.brea@udc.es a.criado@udc.es marcos.garcia1@udc.es	
Web				
General description	An introductory course in Medicinal Chemistry is offered. Basic concepts related to the structure and activity of drugs, mechanisms of action and metabolism are covered. Main strategies in the design and synthesis of drugs are also analyzed.			
Contingency plan	1. Modifications to the contents 2. Methodologies *Teaching methodologies that are maintained *Teaching methodologies that are modified 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	Ability to use chemistry terminology, nomenclature, conventions and units
A9	Knowledge of structural characteristics of chemical and stereochemical compounds, and basic methods of structural analysis and research
A10	Knowledge of chemical kinetics, catalysis and reaction mechanisms
A13	Understanding of chemistry of main biological processes
A14	Ability to demonstrate knowledge and understanding of concepts, principles and theories in chemistry
A15	Ability to recognise and analyse new problems and develop solution strategies
A16	Ability to source, assess and apply technical bibliographical information and data relating to chemistry
A17	Ability to work safely in a chemistry laboratory (handling of materials, disposal of waste)
A18	Risk management in relation to use of chemical substances and laboratory procedures
A19	Ability to follow standard procedures and handle scientific equipment
A20	Ability to interpret data resulting from laboratory observation and measurement
A21	Understanding of qualitative and quantitative aspects of chemical problems
A22	Ability to plan, design and develop projects and experiments

A23	Critical standards of excellence in experimental technique and analysis
A24	Ability to explain chemical processes and phenomena clearly and simply
A25	Ability to recognise and analyse link between chemistry and other disciplines, and presence of chemical processes in everyday life
A26	Ability to follow standard laboratory procedures in relation to analysis and synthesis of organic and inorganic systems
B1	Learning to learn
B2	Effective problem solving
B3	Application of logical, critical, creative thinking
B4	Working independently on own initiative
B6	Ethical, responsible, civic-minded professionalism
B7	Effective workplace communication
C1	Ability to express oneself accurately in the official languages of Galicia (oral and in written)
C2	Oral and written proficiency in a foreign language
C3	Ability to use basic information and communications technology (ICT) tools for professional purposes and learning throughout life
C4	Self-development as an open, educated, critical, engaged, democratic, socially responsible citizen, equipped to analyse reality, diagnose problems, and formulate and implement informed solutions for the common good
C6	Ability to assess critically the knowledge, technology and information available for problem solving
C7	Acceptance as a professional and as a citizen of importance of lifelong learning
C8	Understanding role of research, innovation and technology in socio-economic and cultural development

Learning outcomes			
Learning outcomes	Study programme competences / results		
Know the structure and mode of action of drugs and the relationship with biological activity	A1 A9 A10 A13 A14 A15 A16 A21 A24 A25	B1 B2 B3 B4 B6 B7	C1 C2 C3 C4 C6 C7 C8
Know basic principles and strategies used to design and synthesized drugs.	A1 A9 A10 A13 A14 A15 A16 A17 A18 A19 A20 A21 A22 A23 A24 A25 A26	B1 B2 B3 B4 B6 B7	C1 C2 C3 C4 C6 C7 C8

Know the impact of drugs and the pharmaceutical companies in the society.	A13 A14 A16 A24 A25	B1 B3 B4 B6 B7	C1 C3 C6 C7 C8
The students should be able to identify apropriate information on the scientific literature, assess their responsibility in the management of information and knowledge in the field of Industrial Chemistry and the Chemical Research, use scientific terminology and appreciate the value of quality and continuous improvement	A14 A15 A16 A22 A24 A25	B1 B2 B3 B4 B6	C1 C2 C3 C4 C6 C7 C8

Contents	
Topic	**Sub-topic**
Chapter 1. Basic principles in Medicinal Chemistry	1.1 Medicinal Chemistry : definition and basic concepts 1.2 Historical Perspective . 1.3 Pharmacokinetics and Pharmacodynamics 1.4 Drug Discovery 1.5 Drugs: nomenclature and classification
Chapter 2. Molecular basis on pharmacological activity: Pharmacodynamics	2.1 Drug-receptor interactions . Molecular topology and biological activity 2.2 Proteins: structure and function. Protein Interactions 2.3 Enzymes: enzymatic catalysis. Michaelis - Menten equation . Enzyme inhibition : Types 2.5 Cell receptors: structure and classification . 2.6 Nucleic Acids . Structure and functions. Drug interactions with nucleic acids 2.7 Interactions with lipid and carbohydrate
Chapter 3. Phramacokinetics	3.1 ADME processes. 3.2 Absorption of drugs. Modes of administration . Physicochemical properties of drugs : Lipinsky rules . Bioavailability . 3.3 Distribution of drugs. Blood : composition and properties. Removal rate . Mid life. Volume of distribution 3.4 Drug metabolism : metabolism in phase I and phase II 3.5 Elimination of drugs.
Chapter 5. Drug discovery	4.1 Steps in drug discovery. Biological target vs Phenotypic approach. Structural diversity. Chemical space. Drug binding energy. High Throughput Screening (HTS). Chemical libraries: combinatorial chemistry , parallel synthesis , solid phase synthesis 4.2 Strategies in drug discovery (lead discovery) . Screening modes . Drug screening methods . Drug Design 4.3 Optimization of drugs (lead optimization) . Structure- actividadIdentificación pharmacophore . Pharmacomodulation : modification of functional groups. Optimization receptor binding and pharmacokinetics .

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

Guest lecture / keynote speech	A1 A9 A10 A13 A14 A15 A16 A21 A24 A25 B1 B2 B3 B4 B6 B7 C1 C3 C4 C6 C7 C8	16	16	32
Seminar	A1 A9 A10 A13 A14 A15 A16 A21 A24 A25 B1 B2 B3 B4 B6 B7 C1 C3 C4 C6 C7 C8	7	28	35
Laboratory practice	A9 A13 A14 A15 A16 A17 A18 A19 A20 A22 A23 A25 A26 B1 B2 B3 B4 B6 B7 C1 C2 C3 C4 C6 C7 C8	10	10.5	20.5
Mixed objective/subjective test	A1 A9 A13 A14 A15 B2 B3 B6 C1 C6	4	20	24
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	The contents will be presented. During the presentations the teacher can provide supplementary material to the literature with the aim that the explanations can be tracked effectively. The ability to create notes and search for information will also be developed. The understanding of the most relevant aspects of each subject will be assessed by taking asynchronous tests available on the subject's Moodle or Teams platforms
Seminar	The contents of each chapter will be discussed in seminars by solving exercises and analysis of practical cases. Students will have early enough problem sets through the Moodle platform. We may request delivery of solved exercises.
Laboratory practice	Different practicals related to the subject will be conducted, using free distribution software and web applications aimed to rational drug design. In particular, the estimation of pharmacokinetic parameters for small organic molecules is proposed, in addition to the study of the target-molecule pharmacological interaction using molecular docking.
Mixed objective/subjective test	A test with questions related to the contents of the subject will be asked.

Personalized attention	
Methodologies	**Description**
Guest lecture / keynote speech Laboratory practice Seminar	This activity will be headed to the individual assistance for explanations, doubts, as well as to the resolution of the exercises. Part-time students and those with special academic leave permission could ask for presential or email tutorials when necessary.

Assessment			
Methodologies	**Competencies / Results**	**Description**	**Qualification**
Mixed objective/subjective test	A1 A9 A13 A14 A15 B2 B3 B6 C1 C6	The responses in the written exam will be evaluated.	40

Guest lecture / keynote speech	A1 A9 A10 A13 A14 A15 A16 A21 A24 A25 B1 B2 B3 B4 B6 B7 C1 C3 C4 C6 C7 C8	Attendance to the classes will be assessed, as well as participation and correction in the asynchronous evaluation tests proposed for each topic.	10
Laboratory practice	A9 A13 A14 A15 A16 A17 A18 A19 A20 A22 A23 A25 A26 B1 B2 B3 B4 B6 B7 C1 C2 C3 C4 C6 C7 C8	Attendance and correction in the development of the different practical activities proposed will be assessed, as well as a final report.	30
Seminar	A1 A9 A10 A13 A14 A15 A16 A21 A24 A25 B1 B2 B3 B4 B6 B7 C1 C3 C4 C6 C7 C8	The active participation of students in solving the problems of the problem sets will be assessed, as well as the correction on the solving of the exercises submitted.	20

Assessment comments
The attendance to the lectures, seminars and practicals is mandatory. A student can obtain the qualification of "Not presented" if do not realise activities with an upper computation to 50% in the evaluation or not to present to the mixed test.The students will have two opportunities, and those that do not surpass the subject in the first opportunity will conserve the qualification obtained in the seminars and laboratory practicals, and will realise a second mixed test in the determinate dates by the calendar fixed by the Board of Faculty. The students that are evaluated in the second opportunity only will be able to opt to the "matrícula de honor" (highest qualification) if these have not been covered at the first opportunity. Part-time students or students with special academic permission (according to the rules of the UDC): The same evaluation criteria listed above would be applied, but being not mandatory to attend classroom lectures and seminars. Nevertheless, It is compulsory to attend practical sessions, but itwill be tried to fit the dates to the student's availability. When not possible otherwise, these students should exchange the practical activities by tasks related that not require attendance. The final grade will be the sum of 60% of the mark obtained in the lab practice and 40% of the mark obtained in the mixed test. The same criteria will be applied to both opportunities. Students who has not attended the final exam will be assessed as "non attendance". For all the students, the education-learning process, included the evaluation, refers to an academic course and starts every new academic course, including all the activities and procedures of evaluation programed.

Sources of information	
Basic	- Delgado, A.; Minguillón, C.; Joglar, J. (2002). Introducción a la síntesis de fármacos. Madrid: Síntesis - Avendaño, C (2001). Introducción a la Química Farmacéutica. Madrid: McGraw-Hill - Delgado, A.; Minguillón, C.; Joglar, J. (2003). Introducción a la Química Terapéutica. Madrid: Díaz de Santos - Patrick, G. L (2013). An Introduction to Medicinal Chemistry. 5th ed.. New York: Oxford University Press - Thomas, Gareth (2007). Medicinal Chemistry: An introduction. Wiley - Stevens, E. (2014). Medicinal Chemistry, an Introduction.. Pearson Education. New York.
Complementary	

Recommendations
Subjects that it is recommended to have taken before

Organic Chemistry 1/610G01026
Organic Chemistry 2/610G01027
Intermediate Organic Chemistry/610G01028
Advanced Organic Chemistry/610G01030
Subjects that are recommended to be taken simultaneously
Final Dissertation/610G01043
Subjects that continue the syllabus
Other comments

(*)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.