



## IDENTIFYING DATA

### Therapeutic Chemistry

Subject	Therapeutic Chemistry			
Code	V11G201V01413			
Study programme	Grado en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	6	Optional	4th	2nd
Teaching language	#EnglishFriendly Spanish			
Department				
Coordinator	Terán Moldes, María del Carmen			
Lecturers	Teijeira Bautista, Marta Terán Moldes, María del Carmen			
E-mail	mcteran@uvigo.es			
Web				
General description	<p>It is an introductory course in therapeutic chemistry, in which as drugs work at molecular level and processes involved in their in vivo effects will be studied. Drug discovery and design strategies, as well as stages prior to their commercialization will also be discussed.</p> <p>English Friendly subject. International students may request from the teachers: a) Materials and bibliographic references in English, b) tutoring sessions in English, c) exams and assessments in English.</p>			

## Training and Learning Results

Code	
A3	Students have the ability to gather and interpret relevant data (usually within their field of study) to inform judgments that include reflection on relevant social, scientific or ethical issues
A4	Students can communicate information, ideas, problems and solutions to both specialist and non-specialist audiences
B3	Ability to manage information
B4	Ability for analysis and synthesis
C43	Know the chemical compounds with therapeutic application
D3	Ability to communicate in both oral and written form in Spanish and / or Galician and / or English

## Expected results from this subject

Expected results from this subject	Training and Learning Results			
	A4	B4	C43	D3
Familiarize yourself with fundamental concepts of Therapeutic Chemistry	A4	B4		D3
Know the different types of pharmacological targets	A4	B3 B4		D3
Understand and be able to predict drug-target interactions	A3	B3	C43	D3
Know the different types of receptors and understand the signal transduction mechanisms.	A3 A4	B3 B4		D3
Differentiate a chemotherapeutic from a pharmacodynamic agent	A4	B4	C43	D3
Differentiate an agonist drug from an antagonist and from an inverse agonist	A4	B4	C43	D3
Relate the physicochemical properties of drugs with their pharmacokinetics.	A3	B3	C43	D3
Understand and be able to predict metabolic transformations	A3	B3	C43	D3
Know the different stages of drug development	A4	B3	C43	D3
Know and understand the strategies involved in discovering and optimizing leads	A4	B4	C43	D3
Know and understand the computational techniques of molecular modeling: docking strategies, QSAR and pharmacophore design	A4	B3	C43	D3

## Contents

Topic	
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Subject 1. General aspects of Therapeutic Chemistry	1.1. Concept and objectives of Therapeutic Chemistry. 1.2. Drug nomenclature systems. 1.3. Drug classification systems.
Subject 2. Drug targets: proteins	2.1. Types of drug targets and location. 2.2. Drug-target interactions. 2.3. Transport proteins as drug targets. 2.4. Structural proteins as drug targets.
Subject 3. Drug targets: enzymes	3.1. Enzyme inhibition mechanisms. 3.2. Design of enzyme inhibitors and types of enzyme inhibitors with therapeutic application. 3.3. Isoenzymes as drug targets. 3.4. Measurement and expression of enzyme inhibition.
Subject 4. Receptors	4.1. Structure and function of receptors. 4.2. Receptor types and signal transduction mechanisms. 4.3. Agonist, antagonist and inverse agonist drugs. 4.4. Measurement and expression of pharmacological effect.
Subject 5. Drug targets: nucleic acids and other biomolecules	5.1. Nucleic acids as drug targets 5.2. Lipids and carbohydrates as drug targets
Subject 5. Nucleic acids and other biomolecules as drug targets	5.1. Mechanisms of interaction between drugs and nucleic acids. 5.2. Lipids and carbohydrates as drug targets.
Subject 6. Pharmacokinetics and related topics	6.1. Absorption and distribution: mechanisms of transport across biological membranes. 6.2. Drug administration ways. 6.3. Drug metabolism. 6.4. Drug excretion.
Subject 7. Drug discovery and development	7.1. The process of obtaining and getting new drugs to the market. 7.2. Lead discovery and optimization strategies.
Subject 8. Rational drug design	8.1. Biochemical based drug design approaches. 8.2. Computational aided drug design: docking and QSAR strategies, pharmacophore based drug design approach.

## Planning

	Class hours	Hours outside the classroom	Total hours
Lecturing	24	48	72
Seminars	12	18	30
Laboratory practical	14	14	28
Objective questions exam	0	6	6
Essay questions exam	2	12	14

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

## Methodologies

	Description
Lecturing	In these sessions the professor will present in a structured form the general contents of the program, doing emphasis in important or difficult aspects of the subject. In addition, the professor, in advance and through the Moovi platform, will make available to the student the material that will be used in these sessions. In order to better understand the content explanations, students should previously check and complete this material by using the recommended literature.
Seminars	They will devote time to discuss the most complicated aspects of the treated subjects by solving exercises and questions, using molecular modeling programs, as well as presenting review works related with the content of the subject.
Laboratory practical	Laboratory practices will be developed in 4 sessions of 3.5 h each. one session will consist of visiting a pharmaceutical company to learn about their facilities and products.  Three sessions will be devoted to the synthesis and study of different peptidomimetics.

## Personalized assistance

Methodologies	Description
Lecturing	The teachers will be available to have tutoring sessions with the students, which will be arranged in advance. In the tutoring sessions, either in person or online, such as email or the virtual campus, all queries related to the study of the contents of the subject will be answered.
Seminars	The teachers will be available to have tutoring sessions with the students, which will be arranged in advance. In the tutoring sessions, either in person or online, such as email or the virtual campus, all queries related to the study of the contents of the subject will be answered.

Laboratory practical The teachers will be available to have tutoring sessions with the students, which will be arranged in advance. In the tutoring sessions, either in person or online, such as email or the virtual campus, all queries related to the study of the contents of the subject will be answered.

Tests	Description
Objective questions exam	The teachers will be available to have tutoring sessions with the students, which will be arranged in advance. In the tutoring sessions, either in person or online, such as email or the virtual campus, all queries related to the study of the contents of the subject will be answered.
Essay questions exam	The teachers will be available to have tutoring sessions with the students, which will be arranged in advance. In the tutoring sessions, either in person or online, such as email or the virtual campus, all queries related to the study of the contents of the subject will be answered.

## Assessment

	Description	Qualification	Training and Learning Results			
Seminars	The participation and resolution of all the tasks proposed by the teacher for the seminar classes will be qualified.	25	A3	B3	C43	D3
Laboratory practical	Attendance at the laboratory practical sessions will be mandatory. The laboratory work will be evaluated with a APT or NO APT. For this evaluation, compliance with the safety regulations related to the handling of chemical substances and waste removal, planning and development of proposed experiments, analysis of results and the laboratory notebook quality will be taken into account. The evaluation will be done through the systematic observation of student work. The mark of the laboratory practices will be obtained from the resolution of the tasks and works proposed by the teachers in relation to the experiments performed and the visit to the industry.  To pass the subject it is essential to obtain APT at work from laboratory.	15	A3	B4	C43	D3
Objective questions exam	A short exam (one hour long) will be carried out at week five. In this exam will enter the subject explained until that moment.	20	A3	B3	C43	A4 B4
Essay questions exam	A global exam will be carried on closing date of evaluation in order to analyze the adquired competencies.	40	A3	B3	C43	A4 B4

## Other comments on the Evaluation

Participation of students in any of the evaluation parts will involve the condition of presented and therefore the obtaining of a qualification. The presentation of some work in seminars, the attendance to laboratory practical (two or more sessions) or the performance of some written exams will be considered evaluation acts.

Students should have a minimum mark in some of the evaluation parts in order to pass the subject (5 or more points). This minimum mark should be of 4 points over 10 in the global exam, as well as in seminars and laboratory practicals.

If the required minimums are not obtained, the final mark will be the weighted mark of the highest-scoring failed part (seminars, laboratory practicals or global exam).

### Evaluation in the July Call

The mark achieved in seminars and laboratory practical will be maintained (maximum 40%). A written global exam about all theoretical contents of the subject will be performed (60%). In order to pass the subject (global score equal to or greater than 5) in this call, students must achieve a minimum mark of 5 points out of 10 in the written exam.

### Students of subsequent enrollment

Those students who were previously evaluated as APT will be awarded the APT mention for the monitoring of the laboratory practical, not being necessary the completion of the experimental work again. However, they must perform the tasks or works proposed by the teachers in relation to the laboratory practices in order to achieve the mark for the Laboratory practical (15%).

### Non-continuous evaluation option

Students who do not wish to opt for continuous assessment must request it from the subject coordinator. This request will be made during the first three weeks of the course. To pass the subject they will have to do the work of laboratory, obtain the APT qualification, and perform a global test in which all the subject contents will be evaluated, including the laboratory practical. The minimum mark of this exam must be 5 points over 10.

## Sources of information

### Basic Bibliography

G. L. Patrick, **An introduction to Medicinal Chemistry**, 7th, Oxford University Press, 2023

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N. K. Dunlap, **Medicinal Chemistry**, 1st, Garland Science, 2018

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C. Rostron, **Drug Design and Development**, Oxford University Press, 2020

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A. Delgado, C. Minguillón, J. Juglar, **Introducción a la Química Terapéutica**, 2ª, Diaz de Santos, 2003

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E. Stevens, **Medicinal Chemistry: The Modern Drug Discovery Process**, 1st, Pearson Advanced Chemistry, 2013

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**Complementary Bibliography**

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C. Avendaño, **Introducción a la Química Farmacéutica**,

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C. G. Wermuth, D. Aldous, P. Raboisson, D. Rogman, **The practice of Medicinal Chemistry**, 4th, Elsevier, 2015

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J. M. Beale Jr, J. H. Block, **Wilson and Gisvold's textbook of organic medicinal and pharmaceutical chemistry**, 12th, Wolters Kluwer, 2011

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## **Recommendations**

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

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Biology: Biology/V11G201V01101

Biochemistry/V11G201V01201

Organic chemistry I/V11G201V01205

Organic chemistry II/V11G201V01210

Organic Chemistry III: Concerted, Radical and Photochemical Reactions/V11G201V01305

Organic Chemistry IV: Design of Organic Synthesis/V11G201V01310

Stereoselective Synthesis of Bioactive Compounds/V11G201V01405

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