COURSE DATA

DATA SUBJECT

Code: 34066
Name: Pharmaceutical Chemistry
Cycle: Undergraduate Studies
ECTS Credits: 12
Academic year: 2025-26

STUDY (S)

Degree	Center	Acad. year	Period
1201 - Degree in Pharmacy	Facultat de Farmàcia i Ciències de L'alimentació	3	Annual
1211 - Double Degree in Pharmacy and Human Nutrition and Dietetics	Facultat de Farmàcia i Ciències de L'alimentació	3	Annual

SUBJECT-MATTER

Degree	Subject-matter	Character
1201 - Degree in Pharmacy	Pharmaceutical chemistry	COMPULSORY
1211 - Double Degree in Pharmacy and Human Nutrition and Dietetics	Asignaturas obligatorias del PDG Farmacia-Nutrición Humana y Dietética	COMPULSORY

COORDINATION

GONZALEZ NUÑEZ MARIA ELENA

SUMMARY

Pharmaceutical Chemistry (also known as Medicinal Chemistry) is an annual subject taught in the third year of the Degree in Pharmacy and it is worth 12 ECTS credits (including 2.5 credits of laboratory practicals).

The aim of Pharmaceutical Chemistry is to study the chemistry of the active ingredients of drugs in order to determine the relationship between their chemical structure, physicochemical properties, reactivity and biological response, with the ultimate goal of providing the knowledge required for the creation of new drugs.

Since most drugs are organic molecules, Pharmaceutical Chemistry is mainly based on the knowledge of organic chemistry, although it also requires a solid foundation in biochemistry. On the other hand, it also draws on other subjects, such as Pharmacognosy (the study of natural products as a source of new active

compounds), Pharmacology (which uses experimental models for the evaluation of new active compounds), and Molecular Pharmacology, which explains the biological effects at molecular level by interpreting the phenomena related to the association between drugs and the biomolecules triggering their action, from the standpoint of both structural and physicochemical properties.

Although the design of drugs – the ultimate objective of Pharmaceutical Chemistry – originally focused mainly on simple chemical modifications of the molecules of natural origin, current design trends are based on the study of the interactions of drugs with their target structures at molecular level. The development experienced by molecular biology and genetic engineering in the last few decades has allowed reaching a detailed knowledge of many target molecules in drug action, such as enzymes, membrane receptors and nucleic acids. Therefore, part of the design of new drugs is currently based on **drug-target interactions**.

The **synthesis** of designed compounds is another aspect to consider in the study of pharmaceutical chemistry.

The content of the theory classes has been organized into three parts. The first one deals with the drugs' origin, development and design, as well as with the study of the factors to be considered as regards their action. The second part focuses on the study of some representative families of drugs, classified by a criterion based on the molecular mechanism rather than on the more traditional pharmacological activity. In these topics, for each group of drugs, the study of the general structure, properties, chemical structure-pharmacological activity relationships, and general synthesis methods are addressed. To address this last aspect, an introductory topic on synthesis has been included, based on the reactivity studied in Organic Chemistry, paying special attention to basic aspects of heterocyclic chemistry, asymmetric synthesis, and sustainable development in chemical synthesis. Finally, a unit dedicated to the characterization of drugs by spectroscopic methods corresponds to the third part of the subject.

These units are supplemented by laboratory practicals. In the lab, students should acquire the basic skills in the experimental techniques and methodology of basic organic synthesis, and also in the isolation and characterization of organic compounds with biological activity.

PREVIOUS KNOWLEDGE

RELATIONSHIP TO OTHER SUBJECTS OF THE SAME DEGREE

There are no specified enrollment restrictions with other subjects of the curriculum.

OTHER REQUIREMENTS

Basic knowledge of organic chemistry, both theoretical (chemical structure, reactivity of functional groups and synthetic methodology) and practical (laboratory techniques in organic chemistry) is required. Basic knowledge of structural biochemistry and physiology is also recommended.

COMPETENCES / LEARNING OUTCOMES

-

Act with autonomy in learning, making informed decisions in different contexts, issuing judgements based on experimentation and analysis, and transferring knowledge to new situations.

Collaborate effectively in work teams, assuming responsibilities and leadership roles and contributing to collective improvement and development.

Contribute to the design, development and implementation of solutions that respond to social demands, taking into account the Sustainable Development Goals as a reference.

Demonstrate critical and self-critical thinking in the field of the degree programme, considering aspects such as professional ethics, moral values and the social implications of the different activities carried out.

Design, identify, obtain and analyse drugs and active ingredients.

Develop synthetic processes of drugs using appropriate scientific instruments and equipment.

Gather and transmit information in English at a level of proficiency equivalent to B1 of the Council of Europe.

Know and understand, within the field of the degree programme, gender inequalities in society; integrate different needs and preferences based on sex and gender into the design of solutions and problem solving.

Know how to communicate effectively, both orally and in writing, adapting to the characteristics of the situation and the audience.

Know how to interpret, evaluate and communicate relevant data in the different areas of pharmaceutical activity, using information and communication technologies.

Know the different functional groups present in organic molecules and relate the presence of functional groups to the physicochemical properties of organic molecules.

Module: Chemistry. Estimate the risks associated with the use of chemical substances and laboratory processes.

Module: Chemistry. Know and understand the characteristic properties of elements and their compounds, as well as their application in the pharmaceutical field.

Module: Chemistry. Know and understand the nature and behaviour of functional groups in organic molecules.

Module: Chemistry. Know the physicochemical characteristics of the substances used for the manufacture of medicines.

Obtain and analyse information to address scientific problems.

Propose creative and innovative solutions to complex situations or problems within the field of knowledge, to respond to diverse professional and social needs.

Pursue continuous education in professional development.

Recognise one's own limitations and the need to maintain and update professional competence, placing particular emphasis on self-learning of new knowledge based on available scientific evidence.

Transmit ideas, analyse problems and solve them with critical spirit, acquiring teamwork skills and assuming leadership when appropriate.

Use medicines safely, taking into account their physical and chemical properties.

Use spectroscopic techniques in the structural characterisation of drugs and active principles.

DESCRIPTION OF CONTENTS

1. Introduction

Definitions: pharmaceutical chemistry, drug and medicine. Relationship between pharmaceutical chemistry and other sciences. Drug classification criteria. Drug nomenclature. The pharmaceutical industry.

2. Drug targets

Concept of drug target. Drug-target interactions. Chemical nature of the targets: proteins (enzymes and receptors), lipids, nucleic acids and carbohydrates. Examples of drugs that interact with them. Activation and/or blockade of receptors (agonists and antagonists). Enzyme inhibition: Enzyme inhibitors by structural analogy with the substrate: antimetabolites; irreversible enzyme inhibition directed at the active region; enzyme inhibition catalysed by the inhibited enzyme itself: suicide inhibitors

3. Basic concepts in the drug action

Membranes. Physicochemical models that explain the transport across membranes. Physicochemical properties and pharmacological activity: solubility in water, ionization degree, lipid solubility and partition coefficient. Molecular topology and biological activity. Concept of structure, constitution, configuration and conformation: implications in pharmacological activity. Stereoselectivity in drug activity and pharmacokinetics.

4. Drug metabolism

Phase I: Transformation reactions (oxidation, reduction and hydrolysis reactions). Phase II: Conjugation reactions. Bioreversible derivatives: Prodrugs and bioprecursors. "Soft" drugs and "hard" drugs.

5. Design and development of new drugs

Evolution of research and drug discovery methods. Current methods for discovering lead compounds. Qualitative relationships chemical structure-biological activity. Concept of pharmacophore and auxophoric group. Pharmacomodulation: objectives. Pharmacomodulation techniques. Modulative variations: homology, vinylogy, introduction of multiple bonds, bulky groups, opening and closing rings, bioisosterism. Disjunctive variations. Conjunctive variations. Siamese compounds. Examples. Biochemical strategies in drug design. Drug design based on molecular modelling.

6. Quantitative structure-biological activity relationships(QSAR)

Physicochemical parameters. Hammett equation (electronic effects). Taft equation (steric factors). QSAR Hansch equation. Examples. Methods used to correlate physical and chemical parameters with biological activity. Examples.

7. Introduction to drug synthesis

General strategies for C-C and C-heteroatom bond formation. Synthesis and reactivity of simple heterocycles. Fundamentals of asymmetric synthesis.

8. Antibacterial drugs that act by inhibiting enzymes

Inhibitors of the synthesis of tetrahydrofolic acid. Sulfonamides. Inhibitors of bacterial cell wall biosynthesis: penicillins. Production of penicillins. Modifications of penicillins. Semisynthetic penicillins. Production of 6-aminopenicillanic acid. Penicillins resistant to acids: ampicillin and amoxicillin. Penicillins resistant to b-lactamases. Prodrugs of penicillins.
Cephalosporins. Structure. Structure-activity relationship.7-Aminocephalosporanic acid synthesis. Pharmacomodulation of cephalosporins. Synthesis from 7-ACA and from penicillins. Inhibitors of b-

lactamase: clavulanic acid. Sulbactam. Others: phosphomicyn. Inhibitors of replication and transcription of nucleic acids: quinolones and fluoroquinolones.

9. Acetylcholine modulating drugs

Cholinergic synapses. Acetylcholine: structure, biosynthesis, metabolism. Cholinergic receptors. Design and synthesis of acetylcholine agonists. Design and synthesis of muscarinic and nicotinic antagonists. Design and synthesis of acetylcholinesterase inhibitors.

10. Norepinephrine modulating drugs

Adrenergic synapse. Noradrenaline and adrenaline: structure, biosynthesis and catecholamine metabolism. Pre-and post-synaptic adrenergic receptors.
Adrenergic agonists: Arylethanolamines: design and synthesis of representative drugs. Indirect adrenergic agonists. Arylethylamines: design and synthesis of representative drugs. Adrenergic antagonists. b-blockers. Aryloxypropanolamines: design and synthesis. Other drugs that affect adrenergic transmission. Inhibitors of the synthesis of NA. Inhibitors of storage release and reuptake of NA.

11. Modulating drugs neurotransmitter in the CNS

Presynaptic and postsynaptic modulators of the g-aminobutyric acid (GABA).
Benzodiazepines and barbiturates. MAO Inhibitors. Selective biogenic amines reuptake inhibitors.

12. Modulating drugs of enkephalins and opioid receptors

Morphine. Structure and properties. Development and semisynthesis of morphine analogues. Modulative variations: drug extension and variation of substituents on N atom, rigidification. Disjunctive variations: morphinans, benzomorphans, phenylpiperidines, phenylpropylamines. Endogenous opioid peptides: endorphins and enkephalins.

13. Introduction to spectroscopic analysis

General principles. Spectroscopic applications for determining organic structures: infrared spectroscopy, nuclear magnetic resonance spectroscopy, mass spectrometry.

14. Laboratory Practices

Drug synthesis and structural characterization. Sequential synthesis. Separation of the active ingredients in medicines. Use of drawing programs and geometry optimization of organic structures. Application in the determination of the pharmacophore group of a group of drugs.

WORKLOAD

PRESENCIAL ACTIVITIES

Activity	Hours
Tutorials	6,00
Theory	64,00
Seminar	25,00
Laboratory	25,00
Total hours	**120,00**

NON PRESENCIAL ACTIVITIES

Activity	Hours
Attendance at other activities	0,00
Individual or group project	10,00
Independent study and work	65,00
Preparation of lessons	70,00
Preparation for assessment activities	32,00
Resolution of case studies	0,00
Total hours	**177,00**

TEACHING METHODOLOGY

Theory classes. Students must acquire the basic knowledge included in the list of units through self-study and by attending the lectures. In those lectures, the lecturer will give an overview of the topic under study with special emphasis on the most relevant aspects and on those of particular complexity. In order to encourage the active participation of students, the expositive method (lecture) will alternate with case studies and related problems. For individual work and further preparation of the units, proper references

and the necessary supporting material will be provided to the students.

Seminars. The group of students could be divided into subgroups for seminars, so each student must attend 1 session per week. These seminars are aimed at solving problems, exercises and questions related to pharmaceutical chemistry, and at introducing complementary topics. In addition to this type of problem-solving seminar, the lecturer may propose that students, in groups of 4-5 members, prepare and present selected topics on pharmaceutical chemistry to their colleagues. The reduced number of students in these small groups facilitates an active participation in these seminars, aimed to provide information search skills, the ability to schematise, summarise, and to prepare oral presentations, as well as to promote teamwork. Complementary activities may also be carried out (debates, analyses of readings, press releases) on topical issues related to the subject, or they may also delve into some specific aspects of more complex units.

Laboratory. Students must attend a mandatory introductory seminar prior to the practical sessions. In addition, each student has to complete prior tasks before attending the laboratory, involving the understanding of the experiment, the review of the theoretical concepts involved and the preparation of a scheme of the work process. At the beginning of each session, the lecturer will insist on the most important aspects of the experimental work and will assist the student during the session. The importance of generating the minimum amount of waste and disposing of it in an appropriate manner will be emphasised, with the aim of making the experiment as sustainable as possible. Once the experiment is completed, the student will analyse the results and will solve the questions posed by the lecturer at the beginning or during the course of the session. All this should be reflected in the lab notebook, which will be systematically reviewed by the lecturer.

Tutorials. Students will attend the tutorial sessions in small groups, according to the timetable set. In these sessions, the lecturer will evaluate their learning process in a globalised manner. To do so, he or she may present the students with specific problems to be solved either individually or collectively and which may be more complex than those presented in seminars, according to the needs of students. Tutorials will also be used to solve the queries raised by students during the lectures and to advise them on the strategies to follow in order to avoid the learning difficulties that they may have.

EVALUATION

Evidence of copying or plagiarism in any of the assessable tasks will result in failure to pass the subject and in appropriate disciplinary action being taken. Please note that, in accordance with article 13. d) of the Statute of the University Student (RD 1791/2010, of 30 December), it is the duty of students to refrain from using or participating in dishonest means in assessment tests, assignments or university official documents. In the event of fraudulent practices, the "**Action Protocol for fraudulent practices at the University of Valencia**" will be applied (ACGUV 123/2020):

https://www.uv.es/sgeneral/Protocols/C83sp.pdf

The assessment of the student's learning takes into consideration all the elements outlined in the methodology section included in this guide. **To pass** the course***, a minimum score of 5 out of 10*** must be achieved.

70% of the mark (7 points out of 10)

It will be calculated on the basis of the results obtained in the exams corresponding to the contents covered in lectures and problem-based seminars. At the end of the first term, a partial exam will be administered dealing with the contents given up to that moment. Students who obtained a mark equal or higher than **4.5** will only examine on the contents developed during the second semester in the official first-call exam, which will also have to be passed with a minimum of **4.5** points. In this case, the mark will be the average of the two exams. Students who have not passed the midterm exam will take the subjects developed throughout the entire course, and the grade corresponding to this section will be the one obtained in this exam. Students who do not pass the subject in the first call will have a second one in which they will examine all the content taught throughout the course.

The exams will consist of short questions and or test questions related to the subject and questions that require connecting aspects of the subject that appear in different units or that are complemented with other subjects. Written examinations will be held on the dates determined by the faculty.

15% of the mark (1.5 points out of 10)

It will come from the mark of practices, which will be of MANDATORY ATTENDANCE, therefore, NOT RECOVERABLE, according to the established in the article 6.5 of the Regulation of Evaluation and Qualification of the UV for Degrees and Master's Degrees. If, for **justified reasons**, a student cannot attend a session, he/she must inform the person in charge of the subject so that he/she can assign the student the possibility of recovering the session in another group.

70% of the mark will be based on the assessment of practical sessions taking into account elements such as the preparation of the laboratory sessions, the updating of the laboratory notebook and the experimental work carried out. The remaining 30% will correspond to the mark obtained by the student in a written exam on questions related to practical issues. When the total mark will be less than **5**, students will have a second practical and/or written call.

The lab mark can be carried forward for the **two** subsequent academic years although students who repeat the subject have the right to attend lab sessions again, if they wish to do so.

15% of the mark (1.5 points out of 10):

Will correspond to a continuous assessment, taking into account different aspects such as follow-up examinations, participatory class attendance, progress in the use of subject-specific terminology, critical thinking, ability to work with the rest of the group, participation in seminars and tutorials, etc.

This mark will be considered only if the student has passed the exams with a minimum mark of **4.5 points out of 10** and the laboratory practices with 5 points out of 10 or more. The scores obtained in this section will not be recoverable, except in duly justified cases. Therefore, tests not carried out do not count in the final grade and in no case will the percentages assigned to the continuous assessment tests be transferred to the percentage of the final exam.

Students who do not sit the exam in the first examination session, but have been given a mark for the other elements of assessment, will be marked as ABSENT in the first examination session. However, in the second examination session, the marks from the different elements of assessment will be weighted as explained above in this section, so not sitting the exam in this second attempt will imply a mark of FAIL.

REFERENCES

- - G. L. Patrick. An Introduction to Medicinal Chemistry. Oxford Univ. Press., 5ª Ed. 2013 y 6ª Ed. 2016. - A. Delgado, E. Minguillon, J. Joglar. Introducción a la Química Terapéutica. Díaz de Santos, 2ª Ed. 2004. - C. Avendaño. Introducción a la Química Farmacéutica. Ed. Interamericana - McGraw-Hill, 2ª edición 2001. - G. L. Patrick. An Introduction to Drug Synthesis. Oxford University Press, 2014. - P. Camps, A. Vázquez, C. Escolano. Química Farmacéutica I. Tomos 1 y 2. Publicacions i Edicions Universitat de Barcelona, 2009 y 2010. - P. Camps, S. Vázquez, C. Escolano. Fundamentos de Química Farmacéutica Publicacions i edicions Universitat de Barcelona, 2017. - ChemBioOffice Ultra, PerkinElmer (CambridgeSoft). (Aplicacions que permeten estudiar, dibuixar, formular, modelar i editar estructures moleculars químiques i biològiques. // Aplicaciones que permiten estudiar, dibujar, formular, modelar y editar estructuras moleculares químicas y biológicas.// Applications that allow to study, draw, formulate, model and edit chemical and biological molecular structures.)

- - A. Delgado, E. Minguillon, J. Joglar. Introducción a la síntesis de fármacos. Ed. Síntesis, 2002. - Enrique Raviña. Medicamentos. Un viaje a lo largo de la evolución histórica del descubrimiento de fármacos. Editorial: Universidad de de Santiago de Compostela, 2008. - C. Avendaño. Ejercicios de Química Farmacéutica. Ed. Interamericana. Mc. Graw-Hill, 1997. - R. B. Silverman, M.H. Holladay. The Organic Chemistry of Drug Design and Drug Action, Elsevier/Academic Press, 3rd Ed. 2014. - T. L. Lemke, D. A. Williams, V.F. Roche, S. W. Zito, Foyes Principles of Medicinal Chemistry, 7th ed., Wolters Kluwer, Lippincott, Williams & Wilkins, 2013. - R. J. Anderson, D. J. Bendell, P. W. Groundwater, Organic Spectroscopic Analysis, Tutorial Chemistry Texts, Royal Society of Chemistry, 2004.