VNIVERSITAT DE VALÈNCIA

Course Guide
34100 New Perspectives in Pharmaceutical Design and Synthesis

COURSE DATA

DATA SUBJECT

Code: 34100
Name: New Perspectives in Pharmaceutical Design and Synthesis
Cycle: Undergraduate Studies
ECTS Credits: 4.5
Academic year: 2026-27

STUDY (S)

Degree	Center	Acad. year	Period
1201 - Degree in Pharmacy	Facultat de Farmàcia i Ciències de l'alimentació	5	First quarter

SUBJECT-MATTER

Degree	Subject-matter	Character
1201 - Degree in Pharmacy	New perspectives in drug design and synthesis	ELECTIVES

COORDINATION

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SUMMARY

The subject "New perspectives in drug synthesis and design" is a six-month optative subject formed by 4.5 credits within the new Syllabus for the degree of Pharmacy.

The main objective is acquiring the knowledge of the usual methodology employed in the design and synthesis of drugs in enantiomerically pure form. Therefore, a sound background in the distinct methodologies that give access to chiral drugs is required for a good comprehension. Those initial ideas will later be applied to industrial drug synthesis, focusing specifically in the most often used methodologies, together with the problems encountered and the way to overcome them. A second aspect to consider is peptide chemistry, since these molecules are essential from both, a biological and a chemical point of view. In this context, the problems associated with peptide synthesis, such as the use of protecting groups are important points to consider. Nowadays, one of the main topics related to peptide chemistry is solid phase synthesis, together with the biological-mediated procedures to access them. The most important features of this methodology will be discussed in detail. Thus, in this section significant examples in the synthesis of peptides and peptidomimetics will be employed to describe the current strategies in peptide synthesis.

An alternative approach to the synthesis of chiral drugs, is based in transition metal-mediated

enantioselective catalysis. Although the principles that govern this type of catalysis are beyond the scope of this subject, the exposition of the basic principles and the study of representative examples involving both homogeneous and heterogeneous catalysis will be discussed. In this sense, the catalytic cycle of the most common cross-coupling reactions will be treated in detail. Another important aspect in the industrial production of drugs is their environmental impact, so the basic principles of the so-called 'green chemistry' will be discussed and practical examples of its implementation will be analysed, as well as its relationship with some of the United Nations Sustainable Development Goals (SDGs). In the last part of the subject several practical examples of the synthesis of drugs on an industrial scale, the basic principles of molecular modeling and the spectroscopic methods currently employed in the synthesis and identification of drugs will be described.

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 (knowledge of laboratory techniques of organic chemistry). Basic knowledge of structural Biochemistry.

COMPETENCES / LEARNING OUTCOMES

1201 - Degree in Pharmacy

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

Carry out molecular modelling of simple organic structures using appropriate software.

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.

Know advanced spectroscopic techniques and their application in the investigation of drugs and active principles.

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 propose synthetic sequences for obtaining certain active ingredients using the methodology learned.

Know the characteristics of the pharmaceutical industry and the most relevant aspects of large-scale synthesis.

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.

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

DESCRIPTION OF CONTENTS

1. Research and development in pharmaceutical industry processes

1. Introduction: Characteristics of the current pharmaceutical industry. Study methods of drug interactions with biomolecules (NMR, X-rays, computational methods, ...). 2. Asymmetric synthesis: Synthesis of enantiomerically pure drugs. Strategies and examples. 3. Metal-catalysed cross-coupling reactions. 4. Synthesis of peptides and protecting groups: Design of a synthesis. Retrosynthetic analysis. Synthesis in homogeneous and heterogeneous phase. 5. Green chemistry: Aspects to consider when selecting a synthetic route. Equipment and process safety. Reagents of choice and solvents. The presence of water in the processes. Online detection. 6. Process development: From small-scale production to industrial synthesis. Examples.

2. Informatic Workshop

Computer tools in drug design: Molecular modeling. Introduction and examples. Use of suitable software.

WORKLOAD

PRESENCIAL ACTIVITIES

Activity	Hours
Tutorials	2,00
Theory	30,00
Seminar	7,00
Computer classroom practice	6,00
Total hours	**45,00**

NON PRESENCIAL ACTIVITIES

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

TEACHING METHODOLOGY

Theoretical Lectures- Students must acquire basic knowledge included in the syllabus through self-study and attendance at the lectures. In those lectures, the teacher will give an overview of the topic under study with special emphasis on the most relevant aspects and in those of special complexity. To encourage the active participation of student the Professor will alternate the expositive method (lecture), case study and the posing of problems. For individual study and preparation of the issues in depth, students will be provided with the appropriate bibliography and the necessary support material.

Seminars and Problems .- In it mainly take place resolution of problems before known to be prepared and presented by the students themselves. The small number of students in each subgroup will facilitate more active participation.

In addition to this type of problem-solving seminar, complementary activities on topical issues related to the subject may carry out (debates, analysis of readings, press releases), or delve into some specific aspect of the topics whose understanding it more difficult, if this is required by students.

Tutorials.- The tutorials are organized in small groups of students, according to the timetable set (2 in total throughout the term). In them, the teacher will evaluate the process of student learning in a globalized manner . To do so may raise individually or collectively more complex specific issues to that resolved in the seminars, according to the needs of students. Tutorials also be used to resolve the doubts that have arisen over the lectures and advising students on strategies to follow to avoid the difficulties that they may have.

Practical classes (chemoinformatics).- in this section students will learn to use IT programs related with the contents of the subject as well as gathering relevant information by means of access to the internet.

EVALUATION

In the evaluation of student learning all aspects outlined in the methodology section of this guide will be considered and assessed continuously by the teacher.

10% of the score (1 point) come from the direct evaluation by the teacher, the result of contact with the student in the various forms of programmed learning. Various aspects such as participatory attendance, progress in the use of language characteristic of matter, critical thinking, ability to work with the rest of the

group, and participation in seminars will be taken into account. It will also be possible to carry out some voluntary tutoring activity for students from previous courses, on organic chemistry issues and its relationship with the Sustainable Development Goals (SDGs), which will be valued positively in the grade.

10% of the grade (1 point) for the seminar- presentation. This mark will be considered only if the student has passed the theoretical exam and laboratory practices.

80% of the grade (8 points) is derived from the results obtained in the written tests and examinations. It will be possible to carry out some written test on computer science practices, approximately towards the end of November. There will be one written exam to be held on the dates established by the Faculty. The exam will consist of material issues and questions that require students to relate aspects of the subject appearing in the various sections or, complementing those previously studied in other subjects. Students who do not pass the first examination session will have a second opportunity in the same academic year.

To pass the subject is required to obtain a rating of at least 5 out of 10.

REFERENCES

- Practical Process Research & Development. A Guide for organic chemists. 2nd Edition. Neal G. Anderson, Academic Press, 2012
- Introducción a la síntesis de fármacos. A. Delgado, C. Minguillón, J. Joglar Editorial Síntesis
- Introducción a la Química Farmacéutica. C. Avendaño. 2ª Edición Mc Graw Hill
- Transition metals in the synthesis of complex organic molecules, 2nd Ed., L. S. Hegedus, University Science Books, 1999
- Process Development, Fine Chemicals from Grams to Kilograms, S. Lee y G. Robinson, Oxford Science Publications, OUP 1995
- From Bench to Market, W. Cabri, R. Di Fabio, OUP 2000
- Chirality in Industry I and II, A.N. Collins, G.N. Sheldrake y J. Crosby, John Wiley & Sons Ltd. 1994, 1997
- Organic Synthesis, C. Willis y M. Willis, Oxford Science Publications, OUP 1997
- Green Chemistry in the Pharmaceutical Industry. Edited by P.J. Dunn, A.S. Wells and M.T. Williams. WILEY-VCH, Weinheim, 2010

- The Art of Drug Synthesis. Edited by D.S. Jhohnson and J.J. Li. John Wiley & Sons, Inc., 2007