VNIVERSITAT DE VALÈNCIA

Course Guide
44710 Medicinal chemistry

COURSE DATA

Data Subject	
Code	44710
Name	Medicinal chemistry
Cycle	Master's degree
ECTS Credits	4.0
Academic year	2022 - 2023

Study (s)

Degree	Center	Acad. year	Period
2226 - M.D. in Organic Chemistry	Faculty of Chemistry	1	Annual

Subject-matter

Degree	Subject-matter	Character
2226 - M.D. in Organic Chemistry	6 - Medicinal chemistry	Obligatory

Coordination

Name	Department
DEL POZO LOSADA, CARLOS	325 - Organic Chemistry

SUMMARY

Both medicinal chemistry and biological chemistry represent two of the recent areas of research more dynamics in the applied organic chemistry to the biomedicine area, to the understanding of the biological systems and to the development of new therapeutic strategies.

Obtaining new drugs, which is the final goal of medicinal chemistry, is complement nowadays with the identification of new therapeutic targets, and the identification of the action mechanism of the molecules of farmacological interest. Those contributions could be included in the frame of biological chemistry.

Therefore, this subject shows the students the most novel and relevant aspects of the present with the aim to provide a formation from a multidisciplinary point of view, in a topic that join concepts from organic chemistry, biochemistry and computational chemistry.

In this subject, we intent to give the students a general vision of the most novel technologies and strategies where the chemistry is applied to obtain information and modify biological systems. Additionally, we intent to provide the students the general bases of the new techniques and methodological tools for the rational design of drugs

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

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

Other requirements

A solid background in Organic Chemistry is required

OUTCOMES

2226 - M.D. in Organic Chemistry

- Students should apply acquired knowledge to solve problems in unfamiliar contexts within their field of study, including multidisciplinary scenarios.
- Students should be able to integrate knowledge and address the complexity of making informed judgments based on incomplete or limited information, including reflections on the social and ethical responsibilities associated with the application of their knowledge and judgments.
- Students should communicate conclusions and underlying knowledge clearly and unambiguously to both specialized and non-specialized audiences.
- Students should demonstrate self-directed learning skills for continued academic growth.
- Students should possess and understand foundational knowledge that enables original thinking and research in the field.
- Use different presentation formats (oral, written, slide presentations, boards, etc.) to communicate knowledge, proposals and positions.
- Be able to access to information tools in other areas of knowledge and use them properly.
- Saber participar en debates y discusiones, dirigirlos y coordinarlos y ser capaces de resumirlos y extraer de ellos las conclusiones más relevantes y aceptadas por la mayoría.
- Competencias de gestión tales como la capacidad para la planificación y gestión de tiempo y recursos, así como para dirigir y tomar decisiones.
- Ser capaces de valorar la necesidad de completar su formación científica, en lenguas, en informática, asistiendo a conferencias o cursos y/o realizando actividades complementarias, autoevaluando la aportación que la realización de estas actividades supone para su formación integral.
- Comprensión de la relación entre la estructura de los fármacos y su actividad.
- Conocer las principales herramientas metodológicas que se aplican en el área de la química biológica y de la química médica y saber cuál es su utilidad, aplicaciones y limitaciones.

LEARNING OUTCOMES

The final goal of this subject is to reach the chemical knowledge of the drugs in order to understand the relationship between chemical structure, physicochemical properties, reactivity and biological response. Understanding the bases of the design and drug development using different tools, being bioinformatics among them.

Design, selection and/or development products and chemical processes efficiently (ODS 7) that minimize their impact in the environment (ODS 14 and 15), taking advantage of the alternative row materials and generating the minor amount of residues possible (ODS 11)

DESCRIPTION OF CONTENTS

1. Medicinal Chemistry and pharmaceutic R&D

Development of basic concepts in medicinal- and biological chemistry. Therapeutic targets: definition, classification and validation. Identification and optimization of lead compounds. ADME properties. Preclinical trials: security and efficacy. Different transgenic and occasional animal models. Clinical trials: objectives and classification. Different stages at drug development. Costs of the process. Key points and risks in the development

2. Molecular basis of drug action.

Drugs classification. Mechanism of action of drugs. Pharmacokinetic properties. Pharmacodinamic properties

3. Discovery, design and develpment of new drugs

Natural products in medicinal chemistry. Serendipity and strengthening of unexpected properties. Chemoteques and HTS. Rational approaches. Vaccines

4. Advances in neurodrugs

Application of the medicinal- and biological chemistry strategies to drug discovery and development of neurodrugs. Definition of neurodrugs. Neurodegenerative diseases. Alzheimer disease (practical case: tideglusib. Practical case: NP-61). Parkinson disease (practical case: S14). Lateral amyotrophic sclerosis (practical case: kinase inhibitors). Multiple sclerosis (practical case: TC3.6).

5. From structure to fucntion

Introduction to the tridimensional structure of macromolecules. Macromolecular interactions. Structure activity relationship. Data bases. Workshops and practices: building a tridimensional structure of ligands. Study of physicochemical properties, drug-like and visualization prediction properties and handling of drug-receptor complexes. Data base PDB. Ligand-receptor interaction analysis.

6. Computer assisted drug design

Protein modeling. Automatic coupling methods. Docking. Virtual screening. De novo design. Pharmacophore definition. Pharmacophore search. Quantitative structure activity relationship (QSAR ad QSAR3D).
Workshops and practice: Modeling by homology. Obtaining a model. Binding mode study of diverse ligands by means of Docking techniques.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	20,00	100
Seminars	20,00	100
TOTAL	**40,00**	

TEACHING METHODOLOGY

The subject is formulated in a manner that the student is the principal actor of its own learning. From the beginning of the course, students will have the whole didactic material necessary and the teaching will be structured in the following manner:

• Master classes (in person): In those classes basic concepts of the subject will be introduced. Active participation of the students will be encouraged by means of question proposal related to the application of previously acquired concepts.

• Seminars.- This teaching assignment will be dedicated to problem resolution and questions with the active participation of students.

• Written assignment.- Additionally, when the teacher will consider it, some assignments will be proposed, normally related to the study of a practical case, connected with one of the themes of the program, that will be detailed in a scientific publication.

• Workshops and practice: Those classes will be imparted in and informatics laboratory where each student will take place its own experiences, setting the acquired knowledge in the master classes and seminars through its practical application. Those workshops will be performed individually preferentially

EVALUATION

The assessment of student learning will be performed in a continuous manner for the teacher throughout the course, and it will contain the following points:

● **Direct assessment of the professor:** 15% of the final grade will come from the direct evaluation of the professor both in theoretical and practical classes. In this evaluation, some different aspects will be considered. Among them, we outlined the following:

- Attendance and participation in the discussions.

- Progress in the use of the proper language of the field.

- Problem resolution and question proposal

- Critic spirit

- presentation of the exercices.

● **Assessment of the word performed by the student.** The contents and the form will be considered at this stage. The weighting of this part will be 25% of the total grade.

● **Written exams.** 60% of the final grade will come from the grades obtained in those written exams.

- in person examination (traditional style) with both theoretical and practical questions of contents related to the subject. The nature of those questions and problems will force the students to connect several aspects that come from different themes of the subject, or if the teacher considers it convenient, from different subjects.

- Not in person exams. The teacher will give to the students directly or by electronic mail, a series of questions that the students have to complete, either individually or in groups, depending on the decision of the teacher. In any case, the answers will be sent to the teacher again in person or by electronic mail, in the period previously stipulated

REFERENCES

Basic

- An Introduction to Medicinal Chemistry. 4ª Ed., (Oxford University Press. Oxford). By PATRICK G. L. (2009).
- Computational Drug Design (Wiley) by DAVID C. YOUNG, (2009)

Additional

- Physico-Chemical and Computational Approaches to Drug Discovery (RSC Drug Discovery) by Royal Society of Chemistry, Javier Luque, Xavier Barril and David E Thurston, 2012.
- Chemogenomics In Drug Discovery: A Medicinal Chemistry Perspective, (Wiley-VCH), Weinheim, Germany, KUBINYI, H., MULLER, G.,, 2004.