COURSE DATA

Data Subject	
Code	44711
Name	Advanced nuclear magnetic resonance
Cycle	Master's degree
ECTS Credits	3.0
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	7 - Advanced nuclear magnetic resonance	Obligatory

Coordination

Name	Department
DEL POZO LOSADA, CARLOS	325 - Organic Chemistry

SUMMARY

The evaluation of the course will be conducted by the teacher throughout the course and will consist of the following sections.

● **Continuous evaluation**. 10% of the grade will come from direct assessment of the teacher in theoretical and problem classes and tutorials. In this assessment various aspects are taken into account, among which include:

- Assistance and reasoned and clear participation in the discussions raised.

- Progress in the use of language of the subject.

- Troubleshooting and raising doubts.

- Critical spirit.

- Delivery of exercises.

● **Oral expositions and debates.** It will take into account both content and form. This section will correspond to 30% of the final grade.

● **Exams and written tests.** 60% of the mark will be obtained from the results of the written tests.

- Exams of both theoretical issues and problems of the content related to the subject. These issues and problems will be such that will require the student to relate different aspects that appear on different topics of the subject or, if the teacher considers it appropriate, in different subject matter.

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

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

Other requirements

Although spectroscopic techniques are not directly related with the reactivity of organic molecules, the understanding of the relationships between the chemical decoration of the nuclei, crucial for the interpretation of their spectral properties and its spatial location inside a molecule is only possible with a good background in organic chemistry. Therefore, is mandatory for a good follow up of the subject.
-Fundamental knowledge of organic chemistry.

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.
- Poseer habilidades sociales, un buen nivel de comunicación oral y escrita, así como capacidad para trabajar en equipo y con personas de diferentes procedencias.
- Competencias de gestión tales como la capacidad para la planificación y gestión de tiempo y recursos, así como para dirigir y tomar decisiones.
- Utilización de los datos proporcionados por la espectroscopia de RMN para profundizar en el conocimiento de las estructuras de moléculas, biomoléculas y de las interacciones de las últimas con los fármacos, y su aplicación para el diseño de fármacos.

LEARNING OUTCOMES

Final aims of this subject are summarized in the following points:

The students should go in depth in the fundamental principles of the NMR, regarding the structural determination of organic compounds.

The students should have clear concepts of the modern NMR language and an ample perception of this technique as tool for structural elucidation, applicable in a wide range of fields.

The students should be able to obtain structural information, not only regarding the atom connectivity but also the stereochemical relationships, specially in biomolecules, and the interactions of them with drugs, with capacity to transfer this knowledge to drug design.

The students should be able to combine NMR data with the ones obtained by means of other techniques such as computational chemistry and molecular modeling, in order to understand, at the atomic level, structural requirements of the molecular recognition processes of ligand-receptor with biomedical interest, and in this manner, make progress in the drug design and the understanding of biological processes.

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. NMR in the determination of tridimensional structures of biomolecules

Strategies for protein spectra assignment using labelled samples with natural abundance. Structures based in NoE experiments. NoE effect quantification. Spin diffusion. Assignment of ambiguous NoEs. Residual dipolar couplings (RDC). Partial orientation methods. RDC measurements. RDC analysis.

2. NMR, interactions and molecular recognition.

Ligand-based approaches. Interactions between molecules with different correlation time. Transferred NoE. Saturation transfer. Ligand screening. Waterlogsy. Diffusion and gradients. Receptor-based approaches. SAR by NMR.

3. NMR and drug design

Beyond SAR by NMR. SHAPES method. The use of fragments. Selected examples.

4. NMR of other nuclei of interest (15N, 19F, 31P)

Use of labelled samples with stable isotopes to deduce the presence of interactions with receptors.

5. Methodological and instrumental aspects of NMR

NMR spectrometer, measurement probes, hyperpolarization. Coupled techniques. Unique sweeping techniques, simultaneous acquisition of different NMR spectra combinations, NMR Hadamard.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	23,00	100
Seminars	14,00	100
TOTAL	**37,00**	

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.

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.

Those exams will consist in theoretic and practical questions related to the contents of 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. In this manner, the teacher will have the elements to evaluate both global knowledge and written skills of the students.

REFERENCES

Basic

- Croasmun, W. R.; Carlson, R. M. K. (Eds.), Two-Dimensional NMR Spectroscopy. Applications for Chemists and Biochemists. 2nd Edition, VCH: New York, 1994.
- Chary, K. V. R.; Govil, G., NMR in Biological Systems: From Molecules to Human, Springer: Berlin, 2008.

- De Graaf, R. A., In Vivo NMR Spectroscopy: Principles and Techniques, John Wiley: Chichester, 2007.

Additional

- Harren, J. H.; Leach, A. (Eds.), Structure-based Drug Discovery, Springer: Berlin, 2007.
- Lees, M. (Ed.), Food Authenticity and Traceability, Woodhead Publishing: Cambridge, 2003
- Shulman, R. G.; Rothman, D. L., Metabolomics by In Vivo NMR, John Wiley: Chichester, 2005.
- Waver, I.; Holzgrabe, U.; Diehl, B., NMR Spectroscopy in Pharmaceutical Analysis, Elsevier: Oxford, 2008.
- Wüthrich, K., NMR of Proteins and Nucleic Acids, John Wiley: New York, 2005.