# COURSE DATA

## DATA SUBJECT

**Code:** 44711
**Name:** Advanced nuclear magnetic resonance
**Cycle:** Master's Degree
**ECTS Credits:** 3
**Academic year:** 2025-26

## STUDY (S)

| Degree | Center | Acad. year | Period |
|---|---|---|---|
| 2226 - Master's degree in Organic Chemistry | Facultat de Química | 1 | Annual |

## SUBJECT-MATTER

| Degree | Subject-matter | Character |
|---|---|---|
| 2226 - Master's degree in Organic Chemistry | Advanced nuclear magnetic resonance | COMPULSORY |

## COORDINATION

VILA DESCALS CARLOS

# SUMMARY

This course, along with *Spectroscopic Techniques in Organic Chemistry*, aims to equip students with the ability to determine the structure of molecules of various sizes through the measurement and analysis of their spectral data from different techniques.

The relevance, breadth, and complexity of nuclear magnetic resonance (NMR) spectroscopy, as well as the density of structural information it provides, give it a special role among analytical techniques. For this reason, it has been considered appropriate to dedicate a four-credit course specifically to this subject. In the course *Advanced Nuclear Magnetic Resonance*, modern developments and applications of the technique are studied with the aim of deepening the understanding of biomolecular structures and their interactions with drugs, and subsequently using this information for drug design.

# 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.

## COMPETENCES / LEARNING OUTCOMES

**-**

Be able to access to information tools in other areas of knowledge and use them properly.

Competencias de gestión tales como la capacidad para la planificación y gestión de tiempo y recursos, así como para dirigir y tomar decisiones.

Poseer habilidades sociales, un buen nivel de comunicación oral y escrita, así como capacidad para trabajar en equipo y con personas de diferentes procedencias.

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.

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.

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.

## 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

### PRESENCIAL ACTIVITIES

| Activity | Hours |
|---|---|
| Theory | 16,00 |
| Seminar | 14,00 |
| **Total hours** | **30,00** |

### NON PRESENCIAL ACTIVITIES

| Activity | Hours |
|---|---|
| Attendance at other activities | 0,00 |
| Individual or group project | 0,00 |
| Independent study and work | 30,00 |
| Preparation of lessons | 0,00 |
| Preparation for assessment activities | 15,00 |

| | |
|---|---|
| Resolution of case studies | 0,00 |
| **Total hours** | **45,00** |

## 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:** 10% 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 20% of the total grade.

**¿ Written exams. 7**0% 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


- 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.
- 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.