

**COURSE DATA****DATA SUBJECT****Code:** 42933**Name:** Structural determination by RMN**Cycle:** Master's Degree**ECTS Credits:** 2**Academic year:** 2025-26**STUDY (S)**

Degree	Center	Acad. year	Period
2109 - Master's Degree in Experimental Techniques in Chemistry	Facultat de Química	1	First quarter

**SUBJECT-MATTER**

Degree	Subject-matter	Character
2109 - Master's Degree in Experimental Techniques in Chemistry	Advanced laboratory of experimental techniques in chemistry	COMPULSORY

**COORDINATION**

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**SUMMARY**

Laboratory Subject dedicated to the learning of advanced work methodologies used in the structural determination, based on the use of nuclear magnetic resonance and the interpretation of spectra.

Regarding the Sustainable Development Goals (SDGs), it is expected that students will be able to know in this subject how to apply the knowledge learned to guarantee an inclusive, equitable, and quality education and promote learning opportunities for everyone (SDG 4), to acquire a special sensitivity for sustainable management of water (SDG 6), raw materials and energy sources (SDG 7), as well as for an environmentally friendly and sustainable development (SDGs 11, 12, 13, 14 and 15), in addition to being able to design, select and/or develop efficient products, chemical processes, and analytical methodologies (SDG 7) that minimize their impact on the environment (SDGs 14 and 15), using alternative raw materials and reducing wastes (SDG 11).

**PREVIOUS KNOWLEDGE****RELATIONSHIP TO OTHER SUBJECTS OF THE SAME DEGREE**



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

## OTHER REQUIREMENTS

Prior knowledge of chemistry and experimental work in the laboratory of chemistry taught in the degrees indicated in the recommended income profile for the student of the master's degree are required.

## COMPETENCES / LEARNING OUTCOMES

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Be able to access the information required (databases, scientific articles, etc.) and to interpret and use it sensibly.

Realizar estudios relacionados con el análisis y/o la caracterización de sustancias químicas tales como: control de calidad, diseño de protocolos de trabajo para laboratorios, diseño e implementación de procesos de acreditación y validación, diseño y desarrollo de proyectos I+D+I, emisión de informes, certificaciones y/o dictámenes, etc.

Seleccionar la instrumentación química comercializada apropiada para el estudio a realizar y de aplicar sus conocimientos para utilizarla de manera correcta.

Ser capaces de emplear las herramientas básicas para el tratamiento de datos experimentales en el laboratorio.

Ser capaces de planificar y gestionar los recursos disponibles de un laboratorio químico, teniendo en cuenta los principios básicos de la calidad, prevención de riesgos, seguridad y sostenibilidad.

Ser capaces de seleccionar y optimizar las variables instrumentales para obtener los mejores parámetros analíticos en las técnicas experimentales estudiadas.

To acquire basic skills to develop laboratory work in biomedical research.

To prepare a clear and concise memory of the results of your work and the conclusions obtained.

## DESCRIPTION OF CONTENTS

### 1. Experimental aspects of NMR

- Choice of solvent(s) and working conditions.

- Obtainment of monodimensional spectra of samples, covering different centres of interest (1H, 13C, 19F, 31P).

- Obtainment of two-dimensional homonuclear spectra (COSY). Obtainment of heteronuclear two-dimensional



## 2. Acquisition and interpretation of spectra

- Obtainment of monodimensional spectra of samples, covering different centres of interest (1H, 13C, 19F, 31P).spectra (HSQC, HMBC).
- Obtainment of spectra at different temperatures.
- Obtainment of spectra of solid samples (as 11B, 27, 29Si nuclei).
- Interpretation of the obtained spectra.

### WORKLOAD

#### PRESENCIAL ACTIVITIES

Activity	Hours
Seminar	4,00
Laboratory	16,00
<b>Total hours</b>	<b>20,00</b>

#### NON PRESENCIAL ACTIVITIES

Activity	Hours
Attendance at other activities	0,00
Individual or group project	5,00
Independent study and work	14,00
Preparation of lessons	0,00
Preparation for assessment activities	5,00
Resolution of case studies	6,00
<b>Total hours</b>	<b>30,00</b>

### TEACHING METHODOLOGY

#### Presential Activities

Laboratory classes will begin with seminars in which Professor will perform a brief introduction of the objective, fundamentals and experimental practices methodology to perform.

The teacher will held in the laboratory the necessary explanations on operation of the instruments to be used in each practice prior to their use by students and will supervise its use during practices, to enhance knowledge on the techniques used.

Students will carry out the practice following the corresponding protocols or manual of practices.

Classroom activities performed in the laboratory, presentations and exhibitions of works will be part of the ongoing evaluation of the student (formative activities AF2 of verifica and teaching methodology MD1 of verifica)



Written examinations of the subject will be carried out on the date specified in the programming of the assessment tests (formative activities AF4 of verifica and teaching methodology MD1 of verifica).

The competences to acquire from the presential activities will be:

- Generals: CG1 and CG3
- Specific: CE2, CE3, CE4, CE5 y CE6

### **Non-presential activities**

Students will conduct the non-presential activities requested by the teacher (memoirs, reports of practices, etc.) and they will deliver them on the specified date.

The competences to acquire from the presential activities will be:

- Specific: CE7

## **EVALUATION**

La información está en un formato que no se puede convertir

## **REFERENCES**

- Bakhmutov V.I., Practical NMR relaxation for chemists, Wiley, 2004. - Duer, M.J., Introduction to solid state NMR spectroscopy, Wiley 2004.4 - Hore P.J., Nuclear Magnetic Resonance. Oxford Science Publication, 1995. - Hennel, J.W. y Klinowski, J. Fundamentals of Nuclear Magnetic Resonance Longman. - Keeler J., Understanding NMR Spectroscopy, Wiley, 2005. - Morris, G. y Emsley, J. Multidimensional NMR methods for the solution state, Wiley 2010. - Günther, H., NMR spectroscopy: Basic principles, concepts and applications in chemistry, 3rd ed. Wiley-VCH, 2013 - Pregosin, P.S., NMR in Organometallic Chemistry, Wiley-VCH, Weinheim, 2012. - Mitchell, T.N., Costisella, B., NMR- from spectra to structures, Heidelberg, Springer-Verlag, 2007.