COURSE DATA

DATA SUBJECT

Code: 44997
Name: Resolución de problemas mediante técnicas espectroscópicas
Cycle: Master's Degree
ECTS Credits: 5
Academic year: 2026-27

STUDY (S)

Degree	Center	Acad. year	Period
2249 - Master's Degree in Chemistry	Facultat de Química	1	First quarter

SUBJECT-MATTER

Degree	Subject-matter	Character
2249 - Master's Degree in Chemistry	Aplicaciones de la Química Orgánica	COMPULSORY

COORDINATION

SAEZ CASES JOSE ANTONIO

SUMMARY

In this subject, students will expand the knowledge acquired on the fundamentals of the different spectroscopic tec

PREVIOUS KNOWLEDGE

RELATIONSHIP TO OTHER SUBJECTS OF THE SAME DEGREE

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

OTHER REQUIREMENTS

Chemistry knowledge acquired during the Chemistry or recommended entry degree are required.

COMPETENCES / LEARNING OUTCOMES

2249 - Master's Degree in Chemistry

Apply the advanced theoretical and practical knowledge gained in the different specialties of chemistry to R&D and innovation.

Be able to conduct any type of research in the field of chemistry and/or the chemical industry, as a specialist.

Be able to defend positions in debates and colloquia in a rigorous and reasoned manner.

Be able to design, conduct, analyse and interpret complex experiments and data, as a specialist.

Be able to present and defend publicly the results obtained in scientific research or as a result of work in a chemical industry.

Be able to solve complex chemistry problems, whether in the academic, research or industrial application areas at a specialization or masters-level.

Gain experience in the use of information tools and in the management of the information obtained.

Have the ability to plan and to manage time and resources and gain experience in decision-making.

Possess the ability to plan and manage time and resources and gain experience in decision-making.

Students should apply acquired knowledge to solve problems in unfamiliar contexts within their field of study, including multidisciplinary scenarios.

Widen and deepen understanding of spectroscopy, NMR and MS and their applications to solve problems of industrial interest.

DESCRIPTION OF CONTENTS

1. Introduction

Review and extension of the principles of the different spectroscopic techniques. The electromagnetic spectrum and its interaction with matter. Introduction to Nuclear Magnetic Resonance Spectroscopy. Infrared and Raman spectroscopy. Raman spectroscopy: dispersive and Fourier transform. Electronic absorption spectroscopy. Mass spectrometry. Applications of the different spectroscopies to the resolution of practical cases.

2. Application in kinetic studies

Study of the kinetics of a reaction using IR, UV or NMR. Quantitative aspects of IR, UV and NMR spectroscopies. Applications of spectroscopic techniques in practical cases. Study of coalescence processes in NMR. Application to the determination of complex chemical equilibria

3. Advanced structural determination

Determination of the conformation or configuration of a compound by NMR. NOE effect. NOESY and ROESY experiments. Determination of the absolute configuration of a stereocenter. Application in practical cases: pharmaceutical industry.

4. Studies of molecular recognition processes

Techniques for the study of molecular recognition processes. Diffusion experiments. Application to practical cases.

5. Solid magnetic resonance

Principles of solid NMR. Application to practical cases.

6. NMR and Mass Spectrometry and its application in medicine

Metabolomics. Application to practical cases.

WORKLOAD

PRESENCIAL ACTIVITIES

Activity	Hours
Tutorials	10,00
Theory	40,00
Total hours	**50,00**

NON PRESENCIAL ACTIVITIES

Activity	Hours
Attendance at other activities	0,00
Individual or group project	0,00
Independent study and work	75,00
Preparation of lessons	0,00
Preparation for assessment activities	0,00
Resolution of case studies	0,00
Total hours	**75,00**

TEACHING METHODOLOGY

The course will be taught in asynchronous online mode. Among other training activities, applied practical problems

EVALUATION

First call:

-Oral and/or presential written tests (exams) based on the learning outcomes and objectives of each subject, in their theoretical and/or practical part. They will account for 60% of the grade. A minimum mark of 4.5 (out of 10) in this section is required to pass the course.

-Continuous evaluation of the activity carried out by the student through the presentation of work, problem solving, etc... This section will account for 40% of the overall mark.

Second call:

The grade of the subject, in second call will be that of the corresponding exam.

REFERENCES

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- Randazzo, Antonio. Guía Práctica para la Interpretación de Espectros de RMN. Editorial Loghía: 2018.
- Ekman R., J. Silberring, A. Westman-Brinkmalm i A. Kraj. Mass spectrometry (Instrumentation, Interpretation, and Applications. Editorial John Wiley & Sons: 2009
- Apperley, D.C., R.K. Harris i P. Hodgkinson. Solid State NMR: Basic Principles & Practice Solid State NMR. Editorial Momentum Press: 2012.
- Duer, M.J. Solid-State NMR Spectroscopy Principles and Applications. Editorial Blackwell Science Ltd: 2002.
- Pretsch, E.; Clerc, T.; Seibl, J.; Simon, W. Tablas para la determinación estructural por métodos espectroscópicos, Editorial Springer, Barcelona, 1998.
- Claridge, T. D. W. High-Resolution NMR Techniques in Organic Chemistry. 2ª edición, Editorial

Pergamon, 2009.

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- Dass, C. Fundamentals of Contemporary Mass Spectrometry. Editorial John Wiley & Sons, 2007.
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