VNIVERSITAT DE VALÈNCIA

Course Guide
44997 Resolución de problemas mediante técnicas espectroscópicas

COURSE DATA

Data Subject	
Code	44997
Name	Resolución de problemas mediante técnicas espectroscópicas
Cycle	Master's degree
ECTS Credits	5.0
Academic year	2022 - 2023

Study (s)

Degree	Center	Acad. year	Period
2249 - Master's Degree in Chemistry	Faculty of Chemistry	1	First term

Subject-matter

Degree	Subject-matter	Character
2249 - Master's Degree in Chemistry	4 - Aplicaciones de la Química Orgánica	Obligatory

Coordination

Name	Department
SAEZ CASES, JOSE ANTONIO	325 - Organic Chemistry

SUMMARY

In this subject, students will expand the knowledge acquired on the fundamentals of the different spectroscopic techniques (IR, UV, NMR, EM) to be able to apply them to practical cases of kinetic studies, to determine the structure of compounds of pharmaceutical interest or to study of heterogeneous catalysts. The medical applications of some of these techniques are also studied.

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 (RD 1393/2007) // LEARNING OUTCOMES (RD 822/2021)

2249 - Master's Degree in Chemistry

- Students should apply acquired knowledge to solve problems in unfamiliar contexts within their field of study, including multidisciplinary scenarios.
- Be able to solve complex chemistry problems, whether in the academic, research or industrial application areas at a specialization or masters-level.
- Possess the ability to plan and manage time and resources and gain experience in decision-making.
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- Gain experience in the use of information tools and in the management of the information obtained.
- 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.
- Widen and deepen understanding of spectroscopy, NMR and MS and their applications to solve problems of industrial interest.
- 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 present and defend publicly the results obtained in scientific research or as a result of work in a chemical industry.

LEARNING OUTCOMES (RD 1393/2007) // NO CONTENT (RD 822/2021)

- Expand the knowledge acquired on the fundamentals of the different spectroscopic techniques (IR, UV, NMR, MS).
- Study the kinetics of a reaction using different spectroscopic techniques.
- Study chemical equilibrium and the effect of temperature on it.
- Determine the configuration or conformation of a molecule by NMR.
- Check the existence of molecular association and recognition processes through diffusion experiments.
- Know the basic aspects of solid NMR and its applications.
- Understand some medical applications of NMR and Mass Spectrometry.
- Knowing how to apply the knowledge acquired to contribute to the Sustainable Development Goals (SDGs), such as the sustainable management of water, raw materials and energy sources (SDGs 6 and 7) and to develop a professional work with the least environmental impact and using alternative

raw materials (SDGs 11, 14 and 15)

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

ACTIVITY	Hours	% To be attended
Theory classes	40,00	100
Tutorials	10,00	100
Study and independent work	75,00	0
TOTAL	**125,00**	

TEACHING METHODOLOGY

The subject will be taught through participatory lectures, classes with directed practical activity, seminars and workshops where, among other training activities, applied practical problems will be solved aimed at evaluating the student's understanding of the subject. In addition, use will be made of the Virtual Classroom platform, a virtual space where all the information deemed appropriate for the development of teaching and the control of student participation in the proposed activities is deposited.

Due to organizational reasons, during the 2022-2023 academic year, attendance has been reduced to 80%.

EVALUATION

First call:

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

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

Second call:

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

REFERENCES

Basic

- Lambert, J.B., H.E. Shurvell, D.A. Ligther, R. Graham Cooks. Organic Structural Spectroscopy. 2a. edició. Editorial Prentice Hall: 2010
- Hesse M., H. Meier I B. Zeeh. Métodos espectroscópicos en Química Orgánica. 2ª edició. Editorial Síntesis: Madrid, 2005.

- 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.

Additional

- 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.
- Simpson J. Organic Structure Determination Using 2-D NMR Spectroscopy. 2ª edición, Editorial Academic Press, 2012.
- Dass, C. Fundamentals of Contemporary Mass Spectrometry. Editorial John Wiley & Sons, 2007.
- Field L.D., S. Sternhell, J.R. Kalman. Organic Structures from Spectra. 3ª edición, Editorial John Wiley & Sons, 2002
- Colección de publicaciones seleccionadas para el estudio de casos prácticos