COURSE DATA

DATA SUBJECT

Code: 36469
Name: Structural Determination in Organic Chemistry
Cycle: Undergraduate Studies
ECTS Credits: 6
Academic year: 2026-27

STUDY (S)

Degree	Center	Acad. year	Period
1110 - Degree in Chemistry	Facultat de Química	4	First quarter

SUBJECT-MATTER

Degree	Subject-matter	Character
1110 - Degree in Chemistry	Organic Chemistry Applied	ELECTIVES

COORDINATION

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SUMMARY

The course \"Structure Determination in Organic Chemistry\" is part of the subject \"Applied Organic Chemistry\" of 22.5 ECTS that is part of the Chemistry, Industry and Society Module. This is an optional subject of 6.0 ECTS credits taught in the 7th semester of fourth grade.

The basic objective of this course is to deepen and broaden the knowledge acquired in the Organic Chemistry courses. Its approach is fundamentally practical and its aim is to provide students with an overview of the main currently available spectroscopic techniques (UV-visible, infrared and nuclear magnetic resonance) as well as mass spectrometry, and its practical application to obtain information and structure determination of organic compounds. In addition, it is aimed for the students to acquire sufficient knowledge to design the best way to approach a given structure determination problem from the information provided by each type of spectrum, as well as be familiar with the applications and limitations of each of the spectroscopic techniques.

Today most of the structural elucidation problems, both in the research and industrial fields, are solved in an easy, fast and secure way with the use of the techniques that are studied in this course. It provides students and future chemists with sufficient resources for the application of spectroscopic methods to the resolution of the less complex structural problems.

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 the subject has a basic training character, it is essential that the student possesses a solid background in terminology, nomenclature and structural properties of the functional groups of organic molecules. The student should get acquainted with the previously gained concepts of stereochemistry and spectroscopy of organic molecules as well as the theoretical fundamentals required to understand the physical and chemical principles related to absorption spectroscopy and spin nuclear magnetic resona

COMPETENCES / LEARNING OUTCOMES

1110 - Degree in Chemistry

At the end of the course, the student will be able to address new problems and develop strategies to solve them.

At the end of the course, the student will be able to identify chemical elements and compounds, including their production, structure, reactivity, properties and applications.

At the end of the course, the student will be able to identify chemical processes in everyday life.

At the end of the course, the student will be able to identify the structure and reactivity of the main classes of biomolecules and the chemistry of key biological processes.

At the end of the course, the student will be able to implement sustainable and environmentally friendly methodologies.

At the end of the course, the student will be able to relate theory and experimentation.

At the end of the course, the student will be able to solve problems effectively.

At the end of the course, the student will demonstrate inductive and deductive reasoning skills.

At the end of the course, the student will demonstrate the ability to analyse, synthesise and apply critical reasoning.

At the end of the subject, the student will evaluate, interpret and synthesize the chemical data and information correctly.

Capacidad de análisis, síntesis y razonamiento crítico en la aplicación del método científico.

Collaborate effectively in teams, assuming responsibilities and leadership roles and contributing to collective improvement and development.

Communicate effectively, both orally and in writing, adapting to the characteristics of the situation and the audience.

Contribute to the design, development and implementation of solutions that address social needs, taking the Sustainable Development Goals as a reference.

Demonstrate critical and self-critical reasoning within the field of study, considering aspects such as professional ethics, moral values and the social implications of the different activities undertaken.

Express oneself correctly, both orally and in writing, in any of the official languages of the Valencian Community.

Ser capaces de analizar la influencia que sobre el diseño del sistema de información de costes, ejercen, tanto la actividad concreta desarrollada por la entidad como la tecnología utilizada, la estructura organizativa y el estilo de dirección. Calcular costes preestablecidos y relacionarlos con la planificación y el control de la actividad interna. Seleccionar aquellos indicadores de gestión que faciliten el desempeño personal, estableciendo la frecuencia y el formato en función del usuario de destino.

Understand and recognise, from within the discipline, inequalities based on sex and gender in society; integrate different needs and preferences related to sex and gender into problem-solving and solution design.

DESCRIPTION OF CONTENTS

1. Physical methods of structural determination. UV-visible spectroscopy (UV-Vis).

The electromagnetic spectrum. Types of radiation/matter interactions. Absorption spectroscopy: transitions between energy levels. Ultraviolet (UV) -visible spectroscopy. Electronic transitions. Fundamental concepts. The UV-VIS spectrophotometer. Sample preparation. Characteristic absorptions of organic molecules. Chromophores: olefins, polyenes, benzene and derivatives, carbonyl compounds. Effects of solvent and pH.

2. Infrared Spectroscopy (IR)

The Fundamentals of Infrared Spectroscopy. Molecular Vibrations. Hooke's law. Types of vibrations. Factors that influence the position and shape of the bands: bands coupling, hydrogen bonding, conjugation, electronic effects and ring strain. The infrared spectrophotometer. Sample preparation. Characteristic absorptions of the functional groups of organic molecules. IR spectra interpretation.

Nuclear spins. Nuclei in an external magnetic field. Energy levels population. Description of the phenomenon of nuclear magnetic resonance: resonance conditions. Macroscopic magnetization. The relaxation processes. Simplification of the analysis of the resonance process. Shielding. The NMR spectrum: Resolution. Continuous Wave NMR Spectrometers. Pulse method and Fourier transform. Angle of a pulse Width of a pulse. Induction Free Decay (FID). Fourier transform. Spectra accumulation. Pulse

3. Fundamentals of Nuclear Magnetic Resonance spectroscopy

spectrometer and Fourier transform.

4. Proton Nuclear Magnetic Resonance

Resonance frequencies for the different nuclei. Chemical shift. The δ scale. Shielding and decoupling. Sample preparation for NMR. NMR spectra analysis. Types of protons in NMR. Integration of the signals area. Signal splitting: spin-spin coupling. Types of spin-spin coupling. Multiplicity. First order couplings. More complex couplings. Chemical shift values. Factors that affect chemical displacement: Inductive effect, Magnetic anisotropy, Van der Waals repulsions, Existence of hydrogen bonds, Conjugative effects. Tables for estimating the chemical shift.

5. Analysis of proton NMR spectra

Complex spin-spin coupling systems. Second-order approximation. Examples of coupling systems. Special effects in NMR: Chemical exchange processes (intermolecular, with the solvent, Intramolecular). Spin-spin decoupling: double resonance. Introduction to the Nuclear Overhauser Effect (NOE). Two-dimensional experiments 1H 1H (COSY).

6. 13-Carbon Nuclear Magnetic Resonance

Analysis of a 13C NMR spectrum. 13C- 1H Couplings. Decoupling: Broad Band BB, Off-resonance, DEPT (Distortionless Enhancement by Polarization Transfer). Chemical shifts of 13C nuclei. Number of signals. Solvent signals. Factors influencing the displacement (δ). Empirical correlations. Two-dimensional experiments 1H 13C: HETCOR and HSQC.

7. Mass Spectrometry

Introduction. The mass spectrometer. Types of mass spectrometers. Most relevant ionization methods. Electron impact mass spectrometry. The molecular ion and isotopic peaks. Recognition of the molecular ion. Deduction of the molecular formula. Factors that control the modes of fragmentation. Main types of fragmentation. Fragmentation in α. Benzyl fragmentation. Allylic fragmentation. Fragmentation of not activated bonds. Fragmentation of mono-halogenated derivatives. Retro Diels-Alderreaction. McLafferty transpositions. Onium reactions. Loss of CO. Elimination of water. Fragmentations into bi- and poly-functionalized compounds. Other ionization methods for analysis of bioorganic molecules. MALDI-TOF-MS.

Solution of problems by the combined application of the different techniques discussed in previous themes in order to determine the structure of simple organic compounds. Use of software as aid to structural

8. Application of spectroscopic techniques to the determination of structures of organic compounds

assignment based on spectroscopic techniques.

WORKLOAD

PRESENCIAL ACTIVITIES

Activity	Hours
Tutorials	9,00
Theory	51,00
Total hours	**60,00**

NON PRESENCIAL ACTIVITIES

Activity	Hours
Attendance at other activities	0,00
Individual or group project	10,00
Independent study and work	30,00
Preparation of lessons	50,00
Preparation for assessment activities	0,00
Resolution of case studies	0,00
Total hours	**90,00**

TEACHING METHODOLOGY

The subject has been conceived to give to the student the role of principal actor of its own learning and is organized in the following manner:

• **In-person theoretical classes.**

These classes will be dedicated to the exposition to the students of the fundamental aspects of the subject. Thus, the different topics found in the program will be discussed in detail in an orally form. In this way, the student will obtain a global and comprehensive view of the subject. Both, the blackboard and power point presentations will be used during this time. Previously to the classes, the educational material needed for an easy follow-up of the subject will be introduced in the "Virtual Lecture Room". These classes will be complemented with the personal work of the student.

• **Practical classes and seminars**.

In these classes, the application of the concepts introduced in the theoretical classes will be performed for the students. Previously to the attendance of the practical classes, the students must have worked the problems proposed by the professor. The resolution of these problems will be carried out either by the

professor or by the students, in an individual form or in a team-work.

• **Tutorial classes.** There in all will be 9 sessions uniformly distributed along the course. Each session will last for one hour. During these sessions, the professor will evaluate the learning process of the students, who will be previously organized in small work-groups. Homework previously settled by the professor will be collected in the tutorials. In the same token, the tutorial classes will be used to solve the questions that could have come up along the course, together with the guidance about the selection of the most appropriate methods for the resolution of possible future problems.

EVALUATION

The evaluation of the student's academic performance and the final grade of the subject will be carried out, in a weighted manner, according to the percentages shown in each of the sections evaluated. All grades will be based on the absolute score out of 10 points, and in accordance with the scale established in RD 1125/2003. This criterion will be maintained in all calls.

The different sections that will be evaluated are the following:

1- Direct evaluation of the teacher (1 point): In this evaluation, different aspects will be considered, among which it is worth highlighting:

• Reasoned and clear attendance and participation in the discussions raised.

• Progress in the use of the language characteristic of organic chemistry.

• Problem solving and raising doubts.

• Critical spirit.

2.-Tutorials, questionnaires and tasks (overall 2 points): The grade of each student in this section will take into consideration:

•Attendance.

• Grades of the questionnaires.

• Grades of the tasks assigned by the teacher in each subgroup of work. The grade of the tasks will be an overall grade for the subgroup and will be calculated equally for each member of it.

To receive a grade in this section, you must have completed all the questionnaires and have attended a minimum of 7 tutorials.

3.- Exams (7 points): it will be held on the date indicated by the faculty and will be common to all the groups of the subject. This test will consist of questions, problems and exercises that allow the student's acquisition of the skills included in the teaching guide to be assessed. It will consist of two parts, in accordance with the double purpose of the subject: i) questions in which certain spectroscopic characteristics of known organic compounds will be established and/or justified and ii) the reasoned determination of the structure of two organic compounds through the joint analysis of their spectra.

An overall pass in the subject will necessarily imply having obtained a minimum score of 4.5 points out of 10 in the exam. In the evaluation of the second call, the grade obtained in the continuous evaluation (point 1 - "Direct evaluation of the teacher" and Point 2 - "Seminars, Questionnaires and Assignments") of the first call will be maintained and the part corresponding to Point 3 - "Exams" will be evaluated again.

Final Warning

The copying or manifest plagiarism of any task that is part of the evaluation will make it impossible to pass the subject, then submit to the appropriate disciplinary procedures. It should be noted that, in accordance with article 13 d) of the University Student Statute (RD 1791/2010, of 30 December), "*it is the duty of a student to refrain from using or cooperating in fraudulent procedures in assessment tests, in the work carried out or in official documents of the University*".

REFERENCES

- KEMP, W. Organic Spectroscopy 3ª edición, Polgrave Publishers LTD, 2002
- HESSE, M.; MEIER, H.; ZEEH, B. Métodos espectroscópicos en Química Orgánica, 2ª edición, Madrid: Editorial Síntesis, 2005.
- PAVIA, D. L.; LAMPMAN, G. M., KRIZ G. S., VYVYAN, J. A. Introduction to Spectroscopy, 5ª edición, Cengage Learning, 2015.
- PRETSCH, E.; MARTINEZ, R.; HERRERA, A.; BÜHLMANN, P. AFFOLTER, C. Determinación estructural de compuestos orgánicos + CD-ROM, Barcelona: Elsevier España, 2002
- PEDRO, J. R.; BLAY, G. 200 problemas de determinación estructural de compuestos orgánicos. Madrid: Vision Libros, 2010.
- FIELD, L. D.; STERNHELL, S.; KALMAN, J. R Organic Structures from Spectra, 4ª edición, Chichester: Wiley, 2008.
- ChemBioOffice Ultra, PerkinElmer (CambridgeSoft) Amplia selección de aplicaciones y funcionalidades que permite a químicos y biólogos dibujar, formular, modelar y editar

estructuras moleculares químicas y biológicas así como simular espectros de RMN de protón y carbono.

- PRETSCH, E.; BÜHLMANN, P.; AFFOLTER, C.; HERRERA, A.; MARTINEZ, R. Determinación estructural de compuestos orgánicos, Amsterdam: Elsevier-Masson. 2005.

- SILVERSTEIN, R. M.; WEBSTER, F. X.; KIEMLE, D. J. Spectrometric Identification of Organic Compounds, New Jersey: Wiley, 2005.

- DUDDECK, H.; DIETRICH, W.; TOTH, G. Elucidación Estructural por RMN. (Traducción de la 3ª Ed. Revisada y actualizada), Springer-Verlag Ibérica, 2000.

- EKMAN, R.; SILBERRING, J.; WESTAMN-BRINKMALM, A.; KRAJ, A. Mass spectrometry (Instrumentation, Interpretation, and Applications), Chichester: John Wiley & Sons, 2009.

- RANDAZZO, A.; Guía práctica para la interpretación de espectros de RMN. Loghia Publ., 2018