ANEXO I

Faculty of Experimental Sciences

GENERAL SPECIFICATIONS

ACADEMIC YEAR 2022-23

BACHELOR'S DEGREE IN CHEMISTRY

Subject Data

Name:	
DETERMINACIÓN ESTRUCTURAL DE COMPUESTOS ORGÁNICOS	
English name:	
STRUCTURAL ELUCIDATION OF ORGANIC COMPOUNDS	
Code:	**Type:**
757509210	Obligatory

Hours:

	Total	**In class**	**Out class**
Time distribution	150	60	90

ECTS:

Standard group	**Small groups**			
	Classroom	**Lab**	**Practices**	**Computer classroom**
6		0	0	0

Departments:	**Knowledge areas:**
Department of Chemistry	Organic Chemistry
Year:	**Semester**
3	1st semester

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TEACHING STAFF

Name:	E-mail:	Telephone
Prof. Dr. Jesús Fernández Arteaga	jesus.fernandez@diq.uhu.es	959219999

Other Data

***Theory classes*:** Mon and Wed 9-10 h (week 1-15); Tue and Thu 11-12 h (week 1-15).

Tutoring (office hours): Office hours: Mon and Wed 10-11 h, Tue and Thu 9-11 h; professor's office in Robert H. Grubbs building.

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SPECIFIC INFORMATION OF THE COURSE

1. Contents description:

1.1 In English:

Different functionalization of the organic molecules, as well as their reactivity and synthesis has been studied in previous subjects taught belonging to the Organic Chemistry Area. In the field of Organic Chemistry, the elucidation of the structure of organic molecules holds a vital place since it is used both for the identification of compounds isolated from natural sources, and in the field of the synthesis to check whether the obtained product has the desired structure.

1.2 In Spanish:

Las diferentes funcionalizaciones de las moléculas orgánicas, así como su reactividad y síntesis han sido estudiadas en asignaturas anteriores pertenecientes al Área de Química Orgánica. En el campo de la Química Orgánica, la elucidación de la estructura de las moléculas orgánicas ocupa un lugar vital ya que se utiliza tanto para la identificación de compuestos aislados de fuentes naturales, como en el campo de la síntesis para comprobar si el producto obtenido tiene la estructura deseada.
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2. Background:

2.1 Situation within the Degree:

The subject "Structural Elucidation of Organic Compounds" is taught in the third course (semester 5) of the chemistry degree. It is a compulsory subject of the fundamental module associated with the Organic Chemistry area that consists of 6 ECTS credits (150 hours).This course will provide basic knowledge about different instrumental techniques and their practical application to obtain information and determine the structures of organic compounds.

2.2 Recommendations

Have previously completed the the courses "Basic Concepts of Organic Chemistry" (first year) and "Organic Chemistry" (second year).

3. Objectives (as result of teaching):

The main goal of the course is that students were able to determine the structure of an unknown compound, based on the spectroscopic information obtained from the UV-Vis, IR, NMR and HR-MS spectra. Students must have sufficient knowledge of the Organic Chemistry subjects of the previous semesters as well as an adequate level of English to understand organic chemistry concepts in that language.
A. Knowledge objectives:
- Understand the essential concepts, principles and theories that relate spectroscopy with the different areas of Chemistry.
- Accurate managing of the concepts and foundations of the different techniques. - Manage specific terminology.
B. Technical objectives:
- Use IR, NMR and MS techniques to determine the structure of organic compounds.
- Know how to obtain and interpret information from tables and graphs.
- Relate the spectra of a compound with the spatial arrangement of its atoms (stereochemistry).
C. Conduct objectives:
- Maintain an attitude of permanent curiosity in learning the subject.
- Promote the critical spirit and improve the capacity for synthesis and analysis.

4. Skills to be acquired

4.1 Specific Skills:

C2: Conocer los tipos principales de reacción y las principales características asociadas a cada una de ellas.

C4: Conocer las técnicas principales de investigación estructural, incluyendo espectroscopía.

C11: Conocer las propiedades de los compuestos alifáticos, aromáticos, heterocíclicos y organometálicos.

C12: Conocer la naturaleza y el comportamiento de los grupos funcionales en moléculas orgánicas.

C13: Conocer las principales rutas sintéticas en química orgánica, incluyendo la interconversión de grupos funcionales y la formación de enlaces carbono-carbono y carbono-heteroátomo.

Q3: Competencia para evaluar, interpretar y sintetizar datos e información química.

Q4: Capacidad para reconocer y llevar a cabo buenas prácticas en el trabajo científico y profesional.

Q5: Competencia para presentar, tanto en forma escrita como oral, material y argumentación científica a una audiencia especializada.

P1 - Habilidad para manipular con seguridad materiales químicos, teniendo en cuenta sus propiedades físicas y químicas, incluyendo cualquier peligro específico asociado con su uso.

P2 - Habilidad para llevar a cabo procedimientos estándares de laboratorio implicados en trabajos analíticos y sintéticos, en relación con sistemas orgánicos e inorgánicos.

P4 - Habilidad para manejar instrumentación química estándar, como la que se utiliza para estudios estructurales y separaciones.

P6 - Capacidad para realizar valoraciones de riesgos relativos al uso de sustancias químicas y procedimientos de laboratorio.

4.2 General, Basic or Transversal Skills:

CG1 - Que los estudiantes hayan desarrollado y demostrado poseer habilidades de aprendizaje y conocimientos procedentes de su campo de estudio, siendo capaces de aplicarlos en su trabajo, interpretando datos relevantes para emitir juicios de temas de diversa índole pudiendo transmitirlos a un público tanto especializado como no especializado.

CB1 - Que los estudiantes hayan demostrado poseer y comprender conocimientos en un área de estudio que parte de la base de la educación secundaria general, y se suele encontrar a un nivel que, si bien se apoya en libros de texto avanzados, incluye también algunos aspectos que implican conocimientos procedentes de la vanguardia de su campo de estudio.

CB2 - Que los estudiantes sepan aplicar sus conocimientos a su trabajo o vocación de una forma profesional y posean las competencias que suelen demostrarse por medio de la elaboración y defensa de argumentos y la resolución de problemas dentro de su área de estudio.

CB3 - Que los estudiantes tengan la capacidad de reunir e interpretar datos relevantes (normalmente dentro de su área de estudio) para emitir juicios que incluyan una reflexión sobre temas relevantes de índole social, científica o ética.

CB4 - Que los estudiantes puedan transmitir información, ideas, problemas y soluciones a un público tanto especializado como no especializado.

CB5 - Que los estudiantes hayan desarrollado aquellas habilidades de aprendizaje necesarias para emprender estudios posteriores con un alto grado de autonomía.

B1 - Capacidad de análisis y síntesis.

B2 - Capacidad de organización y planificación.

B6 - Resolución de problemas.

B8 - Trabajo en equipo.

5. Training Activities and Teaching Methods

5.1 Training Activities:

Theory classes.

5.2 Teaching Methods:

Standard group/reduced group

Presence classes consisting of the theory related to the course. Didactic resources: PowerPoint presentations.

Seminar sessions about the problem solving related to the theory content of the course.

5.3 Development and Justification:

Magisterial classes of theory content: Will be realized with the complete group of students. The objective is to structure the concepts of the course. The professor's exposition is supported by audiovisual means.

Seminar sessions: Will be used to exercise the acquired theory knowledge in more complex inter-topic problems of theory and practical nature.

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6. Detailed Contents

Block I. Mass spectrometry. (5 hours)
- Topic 1. Introduction to the determination of structures: (2 hours).
Chemical methods and physical methods. Spectroscopic methods.
- Topic 2. Mass spectrometry: (3 hours)
Introduction. Instrumentation. Ionization methods. Types of ions. Determination of molecular masses. Fragmentation of positive ions. General rules of fragmentation of organic molecules. Analysis of the mass spectrum. Representative examples.

Block II. UV and IR spectroscopy. (7 hours)
- Topic 3. Ultraviolet Spectroscopy: (3 hours)
The electromagnetic spectrum. Absorption of light: Beer-Lambert Law. UV-Visible spectroscopy.
- Topic 4. Infrared Spectroscopy: (4 hours)
Introduction. Types of vibrations. Hydrogen bond. Polyatomic molecules. Characteristic absorption of different functional groups. FTIR spectrophotometer. Preparation of the sample. Interpretation of IR spectra.

Block III. Nuclear Magnetic Resonance. (24 hours)
- Topic 5. Nuclear Magnetism, NMR: (4 hours)
Basic principles of nuclear magnetic resonance. Spectrophotometers. Effects of chemical shift that influence NMR. Intensities of the bands. Reference substances. Solvents.
- Topic 6. 1H Nuclear Magnetic Resonance Spectroscopy: (8 hours)
Spin-spin coupling. The coupling constant. Relation between chemical shift-molecular structure. Complex spectra. Homotopic, enantiotopic and diastereotopic groups. Stereoisomery and NMR. Proton couplings with other nuclei. Double resonance experiments. Spin decoupling. NOE effect (Nuclear Overhouser Effect): Proximity in the 1H-1H space.
- Topic 7. 13C Nuclear Magnetic Resonance Spectroscopy: (6 hours)
Magnetic resonance of 13C. Decoupling techniques. 13C quantitative analysis. DEPT experiments. Spectralcorrelations.
- Topic 8. 2D Nuclear Magnetic Resonance Spectroscopy: (5 hours)
COSY, HETCOR, TOCSY, NOESY and HMBC. Magnetic resonance image.
- Topic 9. NMR with other important nuclei: (1 hour)
31P, 15N, 19F.

Block IV. Solving exercises of high complexity. (9 hours).

7. Bibliography

7.1 Basic Bibliography:

"Spectrometric identification of organic compounds" R.M. Silverstein, F.X. Webster, D.J. Kiemle. (Wiley, 7th Edition).
ISBN: 978-0-470-61637-6

7.2 Additional Bibliography:

- "**Tablas para la elucidación estructural de compuestos orgánicos por métodos espectroscópicos**", E. Pretsch, T. Clerc, J. Seibl, W. Simon (Ed.Springer-Verlag). ISBN: 84-07-00501-0.
- "**Spectroscopy"**, Lampman, Gary M. [et al.] (Belmont, CA : Brooks/Cole, 2010). ISBN: 978-0-538-73418-9
- "**Organic Structures from Spectra**" L.D. Field, S. Sternhell, J.R. Kalman (Wiley). ISBN: 978-1-118-32549-0.

Other references:
"Nuclear Magnetic Resonance and Spectroscopy" J. B. Lambert, E. P. Mazzola (Pearson).
"Spin Dynamics, Basics of Nuclear Magnetic Resonance" M. H. Levitt (Wiley, 2nd Edition 2008).
"Basic One- and Two-Dimensional NMR Spectroscopy", H. Friebolin (Ed. Wiley-VCH).

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8. Systems and Assessment Criteria

8.1 System for Assessment:

The assessment system consists of the following components:

Written exam,
Attendance at theoretical classes, attendance at programmed tutoring, periodic delivery of directed activities.

8.2 Assessment Criteria and Marks:

8.2.1 Examinations Convocatory I

The competences acquired in each thematic unit will be evaluated jointly by taking into account the different activities of the course, i.e., exam, laboratory report, guided activities.

- Final exam/quiz: The mark obtained in the final exam counts 70% of the final assessment of the course. The exam/quiz will consist of
theoretical and practical questions.
- 30% of the final assessment will be obtained by continuous evaluation: through the control of attendance at theoretical classes, attendance at programmed tutoring, periodic delivery of directed activities, together with the elaboration and / or exhibition of works carried out (bibliographic, problems, issues), individually or as a team and other, and online test type questionnaire (Moodle) to evaluate the contents of the subject.

In order to pass the course a minimum mark of 5.0 in the final exam/quiz is required. Furthermore, the global mark (consisting of the weighted contributions of exam and continuous evaluation) has to be 5.0 or higher (on a scale from 0 to 10) in order to receive approval.

Requisites for the attribution of “matrícula de honor”: Be the highest final mark(s) in the examined group of students and must be higher than 9.0 (over 10). If the number of students with highest mark exceeds the number of possible “highest honor” evaluations, the final exam mark will be used as differentiating criterion. The maximum number of “highest honor” evaluations is determined by the regulations of the University of Huelva. This evaluation can be only obtained in the first ordinary exam call.

In the final qualification the student’s compliance with the basic norms of behavior and functioning, which should be respected by the university community of the Faculty of Experimental Sciences, will be considered. These norms were approved in the Faculty Council.

There are no partial exams. There is no possibility to improve the mark after the realization of the assessment components.

8.2.2 Examinations Convocatory II

Mark obtained in the final exam of the subject. The exam will consist of theoretical questions and problems. To approve the subject, it is mandatory to obtain 5.0 points out of 10 in the exam.

No marks that were obtained in previous activities/evaluations will be considered. The attribution of “matricula de honor” is excluded in the final qualification the student’s compliance with the basic norms of behavior and functioning, which should be respected by the university community of the Faculty of Experimental Sciences, will be considered. These norms were approved in the Faculty Council.

8.2.3 Examinations Convocatory III

This evaluation will be realized in one final exam that counts for 100% of the global mark. Mark obtained in the final exam of the subject. The exam will consist of theoretical questions and exercises. To approve the subject, it is mandatory to obtain 5.0 points out of 10 in the exam.

No marks that were obtained in previous activities/evaluations will be considered. The attribution of “matricula de honor” is excluded in the final qualification the student’s compliance with the basic norms of behavior and functioning, which should be respected by the university community of the Faculty of Experimental Sciences, will be considered. These norms were approved in the Faculty Council.

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8.2.4 Extraordinary Convocatory

This evaluation will be realized in one final exam that counts for 100% of the global mark. Mark obtained in the final exam of the subject. The exam will consist of theoretical questions and exercises. To approve the subject, it is mandatory to obtain 5.0 points out of 10 in the exam.

No marks that were obtained in previous activities/evaluations will be considered. The attribution of “matricula de honor” is excluded in the final qualification the student’s compliance with the basic norms of behavior and functioning, which should be respected by the university community of the Faculty of Experimental Sciences, will be considered. These norms were approved in the Faculty Council.

8.3 Single Final Evaluation:

The “single final evaluation” modus is realized with one exam that counts for 100% of the final mark. This exam consists of theory questions and exercises related to the content of the course. For a “pass” evaluation a minimum mark of 5.0 (over 10) in the final exam is required.

To opt for this evaluation modus, the student is required to communicate this decision to the coordinating professor of the course. This should be done within the first two weeks of course activity, counted from the first day of classes in this course or, if the enrolment was effectuated after the start of the course, within two weeks counted from the date of enrolment. Opting for the “final evaluation” modus implies the definite renouncement of the possibility to be evaluated in the “continuous evaluation” modus. In accordance with the evaluation regulations of the University of Huelva (approved in the Government Council of the 13th of March 2019) this decision is final and the modus can not be changed back to “continuous evaluation” during the course 2022/23.

In the final qualification the student’s compliance with the basic norms of behavior and functioning, which should be respected by the university community of the Faculty of Experimental Sciences, will be considered. These norms were approved in the Faculty Council.

TENTATIVE SCHEDULE

	S1	**S2**	**S3**	**S4**	**S5**	**S6**	**S7**	**S8**	**S9**	**S10**	**S11**	**S12**	**S13**	**S14**	**S15**
Standard group	T1	T2	T3	T4	T4-5	T5-6	T6	T6	T6	T7	T7	T8	T8-9	T9	T9
Small group		T2	T3		T4			T6	T6		T7	T7	T9	T9	T9

T: theory topic.