ANEXO I

Faculty of Experimental Sciences

GENERAL SPECIFICATIONS

Subject Data

Name:
STRUCTURAL ELUCIDATION OF ORGANIC COMPOUNDS
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**
3.78	2.22	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:

The different functionalization of 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.

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 Degree in Chemistry. It is a obligatory subject of the fundamental module associated with the Organic Chemistry area that consists of 6.0 ECTS credits (150 hours). This course will provide basic knowledge about different instrumental techniques and their practical application to obtain information and determine/elucidate the structures of organic compounds.

2.2 Recommendations

Have previously completed 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: Know the main types of reaction and the main characteristics associated with each of them.

C4: Know the main techniques of structural research, including spectroscopy.

C11: Know the properties of aliphatic, aromatic, heterocyclic and organometallic compounds.

C12: Know the nature and behavior of functional groups in organic molecules.

C13: Know the main synthetic pathways in organic chemistry, including the interconversion of functional groups and the formation of carbon-carbon and carbon-heteroatom bonds.

Q3: Proficiency in evaluating, interpreting, and synthesizing chemical data and information.

Q4: Ability to recognize and carry out good practices in scientific and professional work.

Q5: Competence to present, both in written and oral form, scientific material, and argumentation to a specialized audience.

P1 - Ability to safely handle chemical materials, considering their physical and chemical properties, including any specific hazards associated with their use.

P2 - Ability to carry out standard laboratory procedures involved in analytical and synthetic work, in relation to organic and inorganic systems.

P4 - Ability to handle standard chemical instrumentation, such as that used for structural studies and separations.

P6 - Ability to perform risk assessments related to the use of chemical substances and laboratory procedures.

4.2 General, Basic or Transversal Skills:

CG1 - That students have developed and demonstrated to possess learning skills and knowledge from the field of study, being able to apply them in their work, interpreting relevant data to make judgments on different topics, being able to transmit them to both a specialized and non-specialized audience.

CB1 - That students have demonstrated to possess and understand knowledge in an area of study, that starts from the basis of general secondary education, and is usually found at a level that, although supported by advanced textbooks, also includes some aspects that imply knowledge from the forefront of their field of study.

CB2 - That students know how to apply their knowledge to their work or vocation in a professional way and possess the skills that are usually demonstrated through the elaboration and defense of arguments and the resolution of problems within their area of study.

CB3 - That students could gather and interpret relevant data (usually within their area of study) to make judgments that include reflection on relevant social, scientific, or ethical issues.

CB4 - That students can transmit information, ideas, problems, and solutions to both specialized and non-specialized audiences.

CB5 - That students have developed those learning skills necessary to undertake further studies with a high degree of autonomy.

B1 - Capacity for analysis and synthesis.

B2 - Capacity for organization and planning.

B6 - Problem solving.

B8 - Teamwork.

5. Training Activities and Teaching Methods

5.1 Training Activities:

Theory lessons.

5.2 Teaching Methods:

Standard group/reduced group.

Face-to-face lessons consisting of explanations about the theory of the course. Didactic resources: PowerPoint presentations, videos, specific simulations.

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

5.3 Development and Justification:

	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.

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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:

1. "**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.
2. **"Spectroscopy"**, Lampman, Gary M. [et al.] (Belmont, CA : Brooks/Cole, 2010). ISBN: 978-0-538-73418-9
3. "**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).

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 considering 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) must be 5.0 or higher (on a scale from 0 to 10) 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.

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 cannot be changed back to “continuous evaluation” during the course 2023/24.

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.