

GRADO EN QUÍMICA

DATOS DE LA ASIGNATURA

ASIGNATURA	STRUCTURAL ELUCIDATION OF ORGANIC COMPOUNDS	SUBJECT	STRUCTURAL ELUCIDATION OF ORGANIC COMPOUNDS
CÓDIGO	757509210		
MÓDULO	FUNDAMENTAL	MATERIA	Q. ORGÁNICA
CURSO	3 ^º	CUATRIMESTRE	1 ^º
DEPARTAMENTO	QUÍMICA PROFESOR JOSÉ CARLOS VÍLCHEZ MARTÍN	ÁREA DE CONOCIMIENTO	QUÍMICA ORGÁNICA
CARÁCTER	OBLIGATORIA	CAMPUS VIRTUAL	MOODLE

DISTRIBUCIÓN DE CRÉDITOS

	TOTAL	TEÓRICOS GRUPO GRANDE	TEÓRICOS GRUPO REDUCIDO	PRÁCTICAS DE INFORMÁTICA	PRÁCTICAS DE LABORATORIO	PRÁCTICAS DE CAMPO
ECTS	6	3.78	2.22	0	0	0

DATOS DEL PROFESORADO

COORDINADOR

NOMBRE JESÚS FERNÁNDEZ ARTEAGA

DEPARTAMENTO QUÍMICA PROFESOR JOSÉ CARLOS VÍLCHEZ MARTÍN

ÁREA DE CONOCIMIENTO QUÍMICA ORGÁNICA

UBICACIÓN P4-N5-06

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CAMPUS VIRTUAL MOODLE

DESCRIPCIÓN GENERAL DE LA ASIGNATURA

DESCRIPCIÓN GENERAL

- Contextualization within the Degree in Chemistry:

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.

- Information about the subject:

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.

- Impact on the professional profile:

The theoretical and practical knowledge of the different techniques used for the characterization of structures is essential for the accurate professional performance of a Chemist.

ABSTRACT

Within the field of Organic Chemistry the structural elucidation of organic molecules occupies a determining place since it is used both for the identification of compounds isolated from natural sources, and in synthetic works to check if the obtained product has the desired structure. Remarkably, in previous subjects taught in the Organic Chemistry area the different functionalization of organic molecules as well as their reactivity and synthesis have studied.

OBJETIVOS: RESULTADOS DEL APRENDIZAJE

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.

REPERCUSIÓN EN EL PERFIL PROFESIONAL

The use of the chemical instrumentation necessary for structural elucidation, as well as the preparation of samples and interpretation of spectra, together with the knowledge of the theoretical and practical basic concepts of the different techniques used for the elucidation of structures, is essential for the correct professional performance of a Chemist.

RECOMENDACIONES AL ALUMNADO

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

COMPETENCIAS

COMPETENCIAS BÁSICAS

COMPETENCIAS GENERALES

COMPETENCIAS TRANSVERSALES

COMPETENCIAS ESPECÍFICAS

TEMARIO Y DESCRIPCIÓN DE LOS CONTENIDOS

TEORÍA

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. Stereoisomerism and NMR. Proton couplings with other nuclei. Double resonance experiments. Spin decoupling. NOE effect (Nuclear Overhauser 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. Spectral correlations.

- **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)

METODOLOGÍA DOCENTE



Universidad
de Huelva

GUÍA DOCENTE

Curso 2021/2022



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|----------------|--|
| Grupo grande | <ul style="list-style-type: none"> • Clases presenciales relativas a los contenidos teóricos y prácticas (problemas) de la asignatura, utilizando recursos didácticos tales como transparencias, presentaciones informatizadas y videos. • Seminarios y conferencias sobre temas específicos de los contenidos propios de la asignatura, presentación de material de video y multimedia para ilustrar temas del programa teórico. • Utilización del aula de informática para reforzar los conocimientos teóricos y prácticos adquiridos previamente. • Seminarios tutorizados de resolución de problemas y de supuestos prácticos. • Actividades transversales. • Test y resolución de cuestiones teórico-prácticas. • Discusión de artículos científicos. • Empleo de páginas Web como apoyo a la docencia de la materia. |
| Grupo reducido | <ul style="list-style-type: none"> • Clases presenciales relativas a los contenidos teóricos y prácticas (problemas) de la asignatura, utilizando recursos didácticos tales como transparencias, presentaciones informatizadas y videos. • Seminarios y conferencias sobre temas específicos de los contenidos propios de la asignatura, presentación de material de video y multimedia para ilustrar temas del programa teórico. • Test y resolución de cuestiones teórico-prácticas. |

CRONOGRAMA ORIENTATIVO I

SEMANAS (S):	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10	S11	S12	S13	S14	S15
GRUPO GRANDE	T1	T2	T3	T4	T4-T5	T5-T6	T6	T6	T6	T7	T7	T8	T8-T9	T9	T9
GRUPO REDUCIDO		T2	T3		T4			T6	T6		T7	T7	T9	T9	T9
PRÁCTICAS DE LABORATORIO															
PRÁCTICAS DE INFORMÁTICA															
PRÁCTICAS DE CAMPO															

EVALUACIÓN DE LA ASIGNATURA

PRIMERA EVALUACIÓN ORDINARIA (FEBRERO/JUNIO)

EVALUACIÓN CONTINUA

For the final qualification the basic norms of behavior and working, which should be respected by the University community of the Faculty of Experimental Sciences and which were approved by the Faculty Council, will be taken into account.

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.

EVALUACIÓN FINAL

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.

The students accepted the final single evaluation function by formally communicating it to the teacher (a form that will be prepared for this purpose): a) during the first two weeks of teaching of the subject, or b) in the two weeks following the enrolment, if this has occurred after the beginning of the course. This is the reason why the student can modify the system evaluation selected later.

¿Contempla una evaluación parcial?

NO

SEGUNDA EVALUACIÓN ORDINARIA

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.

The students accepted the final single evaluation function by formally communicating it to the teacher (a form that will be prepared for this purpose): a) during the first two weeks of teaching of the subject, or b) in the two weeks following the enrolment, if this has occurred after the beginning of the course. This is the reason why the student can modify the system evaluation selected later.

TERCERA EVALUACIÓN ORDINARIA Y OTRAS EVALUACIONES

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.

The students accepted the final single evaluation function by formally communicating it to the teacher (a form that will be prepared for this purpose): a) during the first two weeks of teaching of the subject, or b) in the two weeks following the enrolment, if this has occurred after the beginning of the course. This is the reason why the student can modify the system evaluation selected later.

OTROS CRITERIOS DE EVALUACIÓN

¿Contempla la posibilidad de subir nota una vez realizadas las pruebas?

NO

Requisitos para la concesión de matrícula de honor

Being the higher mark of the group of students, and having the final average grade higher than 9.0 points out of 10. "Matrícula de Honor" will be granted in the first ordinary evaluation session (February or June).

REFERENCIAS

BÁSICAS

"Spectrometric identification of organic compounds" R.M. Silverstein, F.X. Webster, D.J. Kiemle. (Wiley, 7th Edition).

ISBN: 978-0-470-61637-6

ESPECÍFICAS

"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 (rústica)

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).