



## 1. General information

Course: STRUCTURAL DETERMINATION

Type: CORE COURSE

Degree: 341 - UNDERGRADUATE DEGREE PROGRAMME IN BIOCHEMISTRY

Center: 501 - FACULTY OF ENVIRONMENTAL SCIENCES AND BIOCHEMISTRY

Year: 3

Main language: Spanish

Use of additional  
languages:

Web site:

Code: 13318

ECTS credits: 6

Academic year: 2021-22

Group(s): 40

Duration: First semester

Second language: English

English Friendly: Y

Bilingual: N

Lecturer: <b>RUBEN CABALLERO BRICEÑO</b> - Group(s): 40				
Building/Office	Department	Phone number	Email	Office hours
Edificio 21/INAMOL despacho 1.03	QUÍMICA INORG., ORG., Y BIOQ.	926051833	Ruben.Caballero@uclm.es	Tuesday, Wednesday and Thursday 15.30 to 17.30 h upon request of time.
Lecturer: <b>MARIA PILAR DE CRUZ MANRIQUE</b> - Group(s): 40				
Building/Office	Department	Phone number	Email	Office hours
Sabatini, despacho 0.5	QUÍMICA INORG., ORG., Y BIOQ.		pilar.cruz@uclm.es	Tuesday, Wednesday and Thursday 15.30 to 17.30 h upon request of time.
Lecturer: <b>MARIA JOSE GOMEZ-ESCALONILLA ROMOJARO</b> - Group(s): 40				
Building/Office	Department	Phone number	Email	Office hours
Sabatini, despacho 0.5	QUÍMICA INORG., ORG., Y BIOQ.		mariajose.gomez@uclm.es	Tuesday, Wednesday and Thursday 15.30 to 17.30 h upon request of time.
Lecturer: <b>FERNANDO LANGA DE LA PUENTE</b> - Group(s): 40				
Building/Office	Department	Phone number	Email	Office hours
Sabatini/0.11	QUÍMICA INORG., ORG., Y BIOQ.		fernando.langa@uclm.es	Tuesday, Wednesday and Thursday 15.30 to 17.30 h upon request of time.

## 2. Pre-Requisites

Knowledge of Organic Chemistry and Biochemical Methodology and instrumentation are strongly recommended

## 3. Justification in the curriculum, relation to other subjects and to the profession

To introduce the student to the study of the correlation between the structure of organic compounds and spectroscopic data, as well as in the different applications of spectroscopic techniques in the characterization of compounds with interest in the field of Biochemistry.

It is also intended that the student:

- Acquire the appropriate and necessary knowledge that allows you to identify organic substances from a series of spectra or given spectroscopic data.
- Acquire sufficient knowledge to solve structural determination problems by obtaining the information that provide the spectra obtained by the different spectroscopic techniques studied.
- Learn about the applications and limitations of different spectroscopic techniques.

## 4. Degree competences achieved in this course

## Course competences

Code	Description
E01	Express themselves correctly in basic biological, physical, chemical, mathematical and computer terms.
E14	Know how to interpret the information provided by the most common structural characterization techniques in Biochemistry and Molecular Biology.
T01	Proficiency in a second foreign language, preferably English, at level B1 of the Common European Framework of Reference for Languages
T03	A correct oral and written communication
T05	Organizational and planning skills
T06	Capacity for design, analysis and synthesis
T10	Ability to self-learn and to obtain and manage bibliographic information, including Internet resources

## 5. Objectives or Learning Outcomes

## Course learning outcomes

Description

Know how to deduce the structure of macromolecules according to the information provided by the main structural determination techniques studied.

## Additional outcomes

- Correlate the UV-Vis spectrum with the structure and recognize the different chromophores. Learn and know the management of the tables.
- Correlate the IR-Raman spectrum with the different functional groups. Know the modifications in the spectrum that introduce the structural variations of the different functional groups.
- Correlating the NMR spectra of nuclei of organic interest with the structure. Interpret spectra. Learn the management of the tables.
- Correlate mass spectra and ionization systems. Recognize the molecular ion and the isotopic satellites. Know the main fragmentations.
- Interpret the experimental data obtained by circular dichroism and X-ray techniques.
- Know and use the spectroscopic databases, their management, applications and limitations. Use programs for the theoretical calculation of spectra.
- Consult and use the proposed bibliography for the development of the course.

## 6. Units / Contents

**Unit 1: Unit 1. Ultraviolet & visible spectroscopy (UV / VIS): electronic transitions, basic photophysical processes, the absorbance (Lambert-Beer's law), chromophores, examples of UV / Vis spectra.**

**Unit 2: Unit 2. Infrared spectroscopy (IR): General introduction. Physical basics. Instrumentation. Vibrations of covalent bonds in molecules (stretching and bending), the area of the functional groups and the fingerprint area, examples of the IR spectra.**

**Unit 3: Unit 3. Nuclear Magnetic Resonance (NMR). Introduction and physical basis. Magnetic properties of the nuclei: nuclear spin. Spectroscopic transits and energy absorption. Chemical shift. Origin and definition. Factors on which it depends: inductive effects, anisotropic, mesomeric, and solvent effects. Chemical shift reagents. Protons attached to heteroatoms. Spin-spin coupling. Spin-spin coupling constant. Effect of a stereogenic center. Geminal and vicinal coupling constants. Long-distance coupling constants. <sup>13</sup>C-NMR. Introduction. Spin coupling. Interpretation of spectra. Chemical equivalence.**

**Unit 4: Unit 4. Introduction. The mass spectrum. Recognition of the molecular ion. Determination of the molecular formula. Most important fragmentations and rearrangements of organic compounds. Analysis and interpretation of mass spectra**

**Unit 5: Unit 5. Determination of the structure of organic compounds based on complementary information obtained using various spectroscopic methods. Examples of determining the structure of organic compounds based on complementary information obtained using various spectroscopic methods. Analysis and interpretation of spectra.**

**Unit 6: Unit 6. Chiroptical methods: optical activity and rotation of linearly polarized light; Optical rotatory dispersion (ORD) and circular dichroism (CD). Introduction. Instruments. Applications.**

**Unit 7: Unit 7. X-Ray diffraction. Introduction. Basic principles. Instrumentation. Structural information. Applications.**

**Unit 8: Unit 8. Preparation of samples for different techniques. Simulation of spectra and fids manipulation with different software**

## 7. Activities, Units/Modules and Methodology

Training Activity	Methodology	Related Competences (only degrees before RD 822/2021)	ECTS	Hours	As	Com	Description
Class Attendance (theory) [ON-SITE]	Lectures	E01 E14	1.08	27	Y	N	The G5 competition will also be worked on as strategies and learning skills necessary for the structural determination of molecules with biochemistry interest will be developed.
Problem solving and/or case studies [ON-SITE]	Problem solving and exercises	E01 E14 T10	0.72	18	Y	N	The G5 competition will also be worked on as strategies and learning skills necessary for the structural determination of molecules with biochemistry interest will be developed.
Progress test [ON-SITE]	Problem solving and exercises	E01 E14 T10	0.08	2	Y	N	The G5 and G6 competences will be worked on since the student will be introduced in the management of databases of structural elucidation of organic molecules with biochemistry interest.
Final test [ON-SITE]	Assessment tests	E01 E14	0.12	3	Y	Y	The final tests are mandatory to pass the subject but it is not mandatory to present
Computer room practice [ON-SITE]	Case Studies	E01 E14 T10	0.32	8	Y	Y	The G5 and G6 competencies will be worked on since the student will be introduced in the management of databases of structural elucidation of organic molecules with biochemical interest. The attendance to the practices is considered as a compulsory and non-recoverable activity to be able to surpass the subject. The evaluation of the same will be recoverable in official exams.
Class Attendance (practical) [ON-SITE]	Practical or hands-on activities	E01 E14 T10	0.08	2	Y	Y	The G5 and G6 competencies will be worked on since the student will be introduced in the management of databases of structural elucidation of organic molecules with biochemical interest. The attendance to the practices is considered as a compulsory and non-recoverable activity to be able to surpass the subject. The evaluation of the same will be recoverable, either in the ordinary or extraordinary call.

Study and Exam Preparation [OFF-SITE]	Self-study	E01 E14 T10	3.6	90	N	-
Total:			6	150		
Total credits of in-class work: 2.4			Total class time hours: 60			
Total credits of out of class work: 3.6			Total hours of out of class work: 90			

As: Assessable training activity

Com: Training activity of compulsory overcoming (It will be essential to overcome both continuous and non-continuous assessment).

8. Evaluation criteria and Grading System			
Evaluation System	Continuous assessment	Non-continuous evaluation*	Description
Assessment of problem solving and/or case studies	10.00%	0.00%	In the classroom, a problem similar to those studied in the classroom applying the different techniques studied in class. It will be necessary to obtain a note greater than or equal to 4.0 so that this note can be weighted in the final qualification of the subject. Not mandatory, evaluable and recoverable by asking an extra question in the exam of the official calls
Laboratory sessions	10.00%	15.00%	This 10% will be the grade obtained in the practical credit of the subject that corresponds to the practices of computer and to the rest of the activities programmed like practices of the subject. It will be necessary a minimum grade of a 4.0 to be able to consider the approved practices and to be able to be weighted in the final grade of the subject. The attendance to the practices is considered as a compulsory and non-recoverable activity to be able to surpass the subject. The evaluation of these will be recoverable, either in the extraordinary or special call for completion.
Final test	80.00%	85.00%	A minimum score of 4.0 will be required to be able to add the grade obtained in the rest of the activities. The exams will consist of several questions of both a theoretical and practical nature, covering the subject matter explained. To average between the two parties it is necessary to have a minimum score of 4.0 in each of them Mandatory, evaluable and recoverable. In any case, the subject will only be considered surpassed if the set of all the evaluable activities results in a grade of a 5 or higher (out of 10).
<b>Total:</b>	<b>100.00%</b>	<b>100.00%</b>	

According to art. 4 of the UCLM Student Evaluation Regulations, it must be provided to students who cannot regularly attend face-to-face training activities the passing of the subject, having the right (art. 12.2) to be globally graded, in 2 annual calls per subject, an ordinary and an extraordinary one (evaluating 100% of the competences).

#### Evaluation criteria for the final exam:

##### Continuous assessment:

The grades obtained in the realization of the practices will be kept for two courses.

The grades obtained by solving problems will be taken into account both in the ordinary and in the extraordinary call of the same course. And recoverable by answering several questions that will be included in the exams of the official calls.

It will be necessary a minimum score of 4.0 in the final test to be able to add the score obtained in the rest of the activities. In any case, the subject will only be considered surpassed if the set of all the evaluable activities results in a grade of a 5 or higher (out of 10).

The exams will consist of several questions of both a theoretical and practical nature, covering the subject matter explained. To average between the two parties it is necessary to have a minimum score of 4.0 in each of them.

##### Non-continuous evaluation:

The grades obtained in the realization of the practices will be kept for two courses.

It will be necessary a minimum score of 4.0 in the final test to be able to add the qualification obtained in the practices carried out. In any case, the subject will only be considered surpassed if the set of all the evaluable activities results in a grade of a 5 or higher (out of 10).

The exams will consist of several questions of both a theoretic and practical nature, covering the subject matter explained. To average between the two parties it is necessary to have a minimum score of 4.0 in each of them.

#### Specifications for the resit/retake exam:

The grades obtained in the realization of the practices will be kept for two courses.

The grades obtained by solving problems will be taken into account both in the ordinary and in the extraordinary call of the same course.

In this call students will be given the possibility of recovering the practices if they had suspended them provided that they have attended all the sessions and only suspended the report.

It will be necessary a minimum score of 4.0 in the final test to be able to add the score obtained in the rest of the activities. The exams will consist of several questions of both a theoretic and practical nature, covering the subject matter explained.

To average between the two parties it is necessary to have a minimum score of 4.0 in each of them. In this call will not take into account the note obtained by the student in the ordinary call in any of the parts (theory and problems) having to examine the two parts in the extraordinary call.

#### Specifications for the second resit / retake exam:

Only a final test that will represent the 100% of the punctuation, as long as the student get a marke of 4.0 in the lab work, the lab sessions are mandatory

9. Assignments, course calendar and important dates	
Not related to the syllabus/contents	
Hours	hours

## 10. Bibliography and Sources

Author(s)	Title/Link	Publishing house	Citv	ISBN	Year	Description
Antonio Randazzo	Guía Práctica para la interpretación de espectros de RMN. Ejercicios para la determinación estructural de pequeñas moléculas orgánicas	Loghia		9788895122441	2018	
E. Pretsch, P. Bühlmann, C. Affolter, A. Herrera, R. Martinez	Determinación estructural de compuestos orgánicos	Springer		84-07-00526-6	2001	
H. Günzler, H.-U. Gremlich,	IR Spectroscopy	Wiley		3-527-28896-1	2002	
M. Hesse, H. Meier, H., B. Zeeh	Métodos espectroscópicos en Química Orgánica, 2 edición	Síntesis		84-7738-522-X	2005	
Miller, Andrew	Essentials of chemical biology : structure and dynamics of b	John Wiley		978-0-470-84530-1	2008	
N. E. Jacobsen	NMR Spectroscopy Explained	Wiley		978-0-471-73096-5	2007	
Pedro, José Ramón	200 problemas de determinación estructural de compuestos org	Visión Libros		978-84-9983-993-6	2010	
R. G. Linington, P. G. Williams, J. B. MacMillan	Problems in Organic Structure Determination: A Practical Approach to NMR Spectroscopy	CRC Press		9781498719629	2015	
R. M. Silverstein, F. X. Webster, D. J. Kiemle	Spectrometric Identification of Organic Compounds	Wiley		0-471-39362-2	2005	
S. Sternhell, J. R. Kalman	Organic Structures from Spectra, L. D. Field, 4ª edición	Wiley		978-0-470-31926-0	2008	
T. E. Lee,	A Beginner's guide to Mass Spectral interpretation	Wiley		0-471-97629-6	1998	
Y-C. Ning	Structural identification of Organic Compounds with Spectroscopic Techniques	wiley		3-527-31240-4	2005	
H. Friebolin	Basic One- and Two-Dimensional NMR Spectroscopy	Wiley-VCH		9783527327829	2010	
E Pretsch, P Bühlmann, M Badertscher	Structure Determination of Organic Compounds: Tables of Spectral Data (4th Edition; revised and enlarged)	Springer		9783540938095	2009	