# UNIVERSIDAD DE CASTILLA - LA MANCHA

# GUÍA DOCENTE

## 1. General information

**Course:** STRUCTURAL DETERMINATION
**Code:** 13318
**Type:** CORE COURSE
**ECTS credits:** 6
**Degree:** 341 - UNDERGRADUATE DEGREE PROGRAMME IN BIOCHEMISTRY
**Academic year:** 2023-24
**Center:** 501 - FACULTY OF ENVIRONMENTAL SCIENCES AND BIOCHEMISTRY
**Group(s):** 40
**Year:** 3
**Duration:** First semester
**Main language:** Spanish
**Second language:** English
**Use of additional languages:**
**English Friendly:** Y
**Web site:**
**Bilingual:** N

Lecturer: **RUBEN CABALLERO BRICEÑO** - 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 from 16.00 h to 18.00 h by appointment by e-mail |

Lecturer: **MARIA PILAR DE CRUZ MANRIQUE** - Group(s): **40**

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| Sabatini, despacho 0.5 | QUÍMICA INORG., ORG., Y BIOQ. | | pilar.cruz@uclm.es | Tuesday, Wednesday and Thursday from 16.00 h to 18.00 h by appointment by e-mail |

Lecturer: **MARIA JOSE GOMEZ-ESCALONILLA ROMOJARO** - Group(s): **40**

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| Sabatini, despacho 0.5 | QUÍMICA INORG., ORG., Y BIOQ. | | mariajose.gomez@uclm.es | Tuesday, Wednesday and Thursday from 16.00 h to 18.00 h by appointment by e-mail |

Lecturer: **FERNANDO LANGA DE LA PUENTE** - Group(s): **40**

| Building/Office | Department | Phone number | Email | Office hours |
|---|---|---|---|---|
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## 2. Pre-Requisites

Knowledge of Orgnanic Chemistry and Biolochemical 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. 13C-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. Chirooptical methods: optical activity and rotation of linearly polarized light; Optical rotatory dispersion (ORD) and circular dichroism (CD). Introduction. Instruments. Aplications.**

**Unit 7: Unit 7. X-Ray diffraction. Introduction. Basic principles. Istrumentation. 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 | 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 | 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 |
|---|---|---|---|
| Practicum performance | 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 | 45.00% | 50.00% | Final Examen (Exercises) - A minimum grade of 4.0 will be necessary to be able to add the grade obtained in the rest of the activities. Mandatory, assessable and recoverable. In any case, the subject will only be considered passed if the set of all evaluable activities results in a grade of 5 or higher (out of 10). |
| Final test | 35.00% | 35.00% | Final Examen (Theory) - A minimum grade of 4.0 will be necessary to be able to add the grade obtained in the rest of the activities. Mandatory, assessable and recoverable. In any case, the subject will only be considered passed if the set of all evaluable activities results in a grade of 5 or higher (out of 10). |
| Progress Tests | 10.00% | 0.00% | In the classroom, an exam-type problem will be solved that allows the application of the different techniques studied in class.<br>It will be necessary to obtain a grade greater than or equal to 4.0 so that this grade can be weighted in the final grade of the subject.<br>Not mandatory, assessable and non-recoverable because it is a voluntary activity.<br>This note is not taken into consideration in subsequent courses, it is only taken into account in the ordinary and / or extraordinary call of this course |
| **Total:** | **100.00%** | **100.00%** | |

*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 eachfinal tests 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.
The modality assigned by default to the student will be the continuous evaluation. Any student may request the change to the modality non-continuous evaluation (before the end of the class period) by emailing the teacher, provided that she/he has not completed 50% of the evaluable activities.

**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 each final tests 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 theoric and practical nature, covering the subject matter explained.

**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 each final tests to be able to add the score obtained in the rest of the activities. The exams will consist of several questions of both a theoric and practical nature, covering the subject matter explained.
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 Practíca para la interpretación de espectros de RMN. Ejercicios para la determinación estructural de pequeñas moléculas orgánicas | Loghìa | | 9788895122441 | 2018 | |
| E. Pretsch, P. BÜhlmann, C. Affolter, A. Herrera, R. Martinez | Deteminación 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 | |