

COURSE DESCRIPTION

COURSE DETAILS

Title (of the course): **DETERMINACIÓN ESTRUCTURAL ORGÁNICA Y FARMACOQUÍMICA**

Code: 100472

Degree/Master: **GRADO DE QUÍMICA**

Year: 3

Name of the module to which it belongs: APLICADO

Field: QUÍMICA (OPTATIVA 1)

Character: OPTATIVA

Duration: SECOND TERM

ECTS Credits: 6.0

Classroom hours: 60

Face-to-face classroom percentage: 40.0%

Study hours: 90

Online platform: <http://moodle.uco.es/m2021/>

LECTURER INFORMATION

Name: MARINAS ARAMENDIA, ALBERTO (Coordinador)

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PREREQUISITES AND RECOMMENDATIONS

Prerequisites established in the study plan

The student can enrol in elective subjects/courses once he/she has passed the 60 credits corresponding to basic training and at least 30 additional compulsory credits.

Recommendations

To have at least a B1 level in English.

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INTENDED LEARNING OUTCOMES

CB4	Knowledge of a foreign language.
CB6	Resolution of problems.
CB10	Capacity for independent learning for continued profesional development.
CE4	The principle techniques of structural investigation, including spectroscopy.
CE15	The structure and reactivity of the primary classes of biomolecules and the chemistry of the primary biological processes.
CE16	Study of instrumental techniques and their applications.
CE22	Capacity to apply said knowledge to the resolution of qualitative and quantitative problems according to previously developed models.
CE23	Competency to evaluate, interpret and synthesise data and chemical information.
CE24	Capacity to recognise and exercise good practices in scientific work.
CE26	Skilled in the handling and computer precessing of data and chemical information.
CE28	Ability to carry out standard laboratory procedures implicit in analytical and synthetic tasks, related to organic and inorganic systems.
CE30	Ability to handle standard chemical instrumentation, such as that which is used in structural investigations and separations.
CE31	Interpretation of data arising from observations and measurements in the laboratory in terms of its meaning and the theories which underpin it.

OBJECTIVES

This optional subject has two main goals:

On the one hand, to introduce the student to Pharmaceutical Chemistry, laying special emphasis on pharmacokinetics and metabolism (toxicology) of drugs. Moreover, the different methodologies to stablish structure-performance relationships will be covered. Finally, rational design of drugs will be studied, including some case studies for their synthesis.

On the other hand, this subject will complete the training acquired by students in "Advanced Organic Chemistry"/"Ampliación de Química Orgánica" (compulsory subject, 3rd Course in Chemistry Degree) concerning the four main spectroscopic techniques used for structure elucidation of organic compounds (UV-Vis, Infrared, Nuclear Magnetic Resonance and Mass Spectrometry spectroscopies). The student will acquire a more in-depth knowledge of IR, NMR and MS to solve some more difficult spectrometric identification problems.

CONTENT

1. Theory contents

Pharmacochemistry

Lesson 1. Introduction to Pharmacochemistry. Definitions. Origin of pharmacology. Nomenclature and classification of drugs. Current picture of Pharmaceutical industry. Commercial/Industrial Aspects of Pharmaceutical Industry.

Lesson 2. Physicochemical properties of drugs. Physicochemistry properties. Acid drugs. Basic drugs. Octanol/water partition coefficient.

Lesson 3. Pharmacokinetics and Pharmacodynamics. Processes occurring during drug activity. Pharmaceutical Phase. Pharmacokynetics Phase: drug absorption and distribution. Bioavailability. Pharmacokynetics Phase: drug receptors. Pharmaceutical agonism and antagonism. Drug classification: structurally specific and non-specific drugs.



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Lesson 4. Structural Characteristics and Pharmacological Action. Basic concepts of stereoisomerism. Optical isomerism and Pharmacological Action. Geometric isomerism and Pharmacological Action. Conformational analysis and pharmacological activity. Isosteres. Bioisosteres. Classic and non-classical bioisosteres.

Lesson 5. Drug metabolism. Definitions. Basic principles of toxicology. Historical evolution of toxicology. Synergistic potentiation and antagonism. Dose-response relationship. Xenobiotics and endogenous substances. Toxicological chemistry. Drug metabolism. Prodrugs. Phase I and Phase II reactions in drug metabolism. Metabolic pathways for common drugs.

Lesson 6. Rational design of drugs. Methods for drug design. Pharmacomodulation. QSAR methods. Hammett and Taft equations. Hansch method. Free-Wilson method. 3D QSAR methodologies.

Lesson 7. Green Chemistry in Pharmaceutical industry. Origins of Pharmaceutical Industry. Some choice criteria for synthetic methods: atom economy. Pharmaceutical industry and pollutant residues: E factor. Function-oriented synthesis (FOS). Sustainable/Green Chemistry and Pharmaceutical Industry. Catalysis in Pharmaceutical Industry. Solvents in Pharmaceutical Industry. Case studies.

Structural Determination of Organic Compounds.

Lesson 8. Infrared Spectroscopy (IR). Diffuse Reflectance Infrared Fourier Transform (DRIFT) and Attenuated Total Reflectance (ATR). Applications of IR spectroscopy in Organic Chemistry.

Lesson 9. Advanced Nuclear magnetic Resonance Techniques applied to the study of organic compounds. DEPT experiment. Introduction to 2D spectroscopic methods. COSY and HETCOR techniques. Solid-state NMR. Introduction to NMR techniques for the study of molecules adsorbed on solids.

Lesson 10. Tandem Mass spectrometry. Application of ion monitoring techniques to the analysis of families of organic compounds.

Lesson 11. Interpretation of Mass spectra of organic compounds.

2. Practical contents

Problems Seminars.

Structure elucidation of some organic compounds will be carried out from the corresponding IR, ¹H and ¹³C NMR (mono and bidimensional) and Mass Spectra.

Laboratory Practice.

Biginelli reaction. Synthesis of a dihydropyrimidinone (treatment of hypertension)

Synthesis of phenacetin (analgesic effect).

METHODOLOGY

Methodological adaptations for part-time students and students with disabilities and special educational needs

This type of methodological adaptations will be decided through meetings of students with their teachers.

Face-to-face activities

Activity	Large group	Medium group	Total
<i>Assessment activities</i>	3	-	3
<i>Lab practice</i>	-	6	6
<i>Lectures</i>	30	-	30



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Activity	Large group	Medium group	Total
Seminar	-	21	21
Total hours:	33	27	60

Off-site activities

Activity	Total
Activities	35
Information search	10
Reference search	10
Self-study	35
Total hours	90

WORK MATERIALS FOR STUDENTS

Coursebook

Dossier

Exercises and activities

Placement booklet

Clarifications

Students will have at their disposal at moodle virtual platform all the material required to follow theoretical explanations, as well as exercises, problems and laboratory practice manuals.

EVALUATION

Intended learnig	Document Analysis	Exams	Laboratory Practice	Oral Presentation	Problem solving
CB10	X	X	X	X	X
CB4	X			X	
CB6		X	X		X
CE15	X			X	
CE16		X		X	X
CE22	X	X			X
CE23	X	X	X		X
CE24	X	X	X		X

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Intended learnig	Document Analysis	Exams	Laboratory Practice	Oral Presentation	Problem solving
CE26	X	X	X		X
CE28			X		
CE30		X	X		X
CE31	X	X	X		X
CE4	X	X	X	X	X
Total (100%)	15%	30%	10%	15%	30%
Minimum grade	5	5	5	5	5

(*)Minimum grade necessary to pass the course

Method of assessment of attendance:

Attendance and students' active participation constitute 10% of the final mark.

General clarifications on instruments for evaluation:

Attendance and active participation to all face-to-face activities (lectures, seminars and practicals) will be evaluated (10% of the final mark). This percentage is considered in the table above, 5% in "exams" section and the other 5% in "problem solving".

Laboratory Practices are compulsory. Therefore, in order to pass the subject, both attendance and presentation of the final report are imperative. Their evaluation will represent 10% of final mark. Once approved, student will not have to repeat lab practices in subsequent courses.

Pharmacochemistry part means 30% of the final mark (15% document analysis + 15% oral presentation on assignments on drug description).

The part of **organic structural determination** constitutes 50% of the final mark, consisting in exams and problem/spectra solving.

Clarifications on the methodology for part-time students and students with disabilities and special educational needs:

Adaptation for part-time students and students with disabilities and special educational needs will be carried out according to the Faculty of Science Rules and considering the individual cases.

Qualifying criteria for obtaining honors:

According to article 80.3 of the Regulations of the University of Córdoba, the mention of "Matricula de Honor" may be awarded to students who have obtained a grade equal to or greater than 9.0.

BIBLIOGRAPHY

1. Basic Bibliography

- 1.- T.L. Lemke, D. A. Williams, **Foye's principles of medicinal chemistry**, 7th Edition, Wolters Kluwer and Lippincott Williams & Wilkins. Philadelphia. USA. 2013.
- 2.- D. Cairns, **Essentials of Pharmaceutical Chemistry**, 3rd Ed., Pharmaceutical Press, London, 2008.
- 3.- J.B. Taylor and P.D. Kennewell, **Modern Medicinal Chemistry**, Ellis Horwood Ltd., Chichester, 1993.
- 4.- M. Hesse, H. Meier, B. Zeeh. **Spectroscopic methods in organic chemistry**, Thieme. 2nd Edition 2007.



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- 5.- L. D. Field, S. Sternhell y J. R. Kalman, **Organic Structures from Spectra**, Wiley, 2002.
- 6.- W. Kemp, **Organic Spectroscopy**, McMillan Education Limited, London, (1992) 3th ed.
- 7.- R. M. Silverstein, G.C. Bassler and T. C. Morrill, **Spectrometric Identification of Organic Compounds**, J. Wiley, New York (1991) 5th Ed.
- 8.- C.G. Herbert and R.A. W. Johnstone, **Mass Spectrometry Basics**, CRC Press, Washinton D.C., 2003.
- 9.- S. A. Richard y J. C. Hollerton, **Essential Practical NMR for Organic Chemistry**, John Wiley & Sons, Ltd., 2011.
- 10.- M. Balci, **Basic ¹H- and ¹³C-NMR Spectroscopy**, Elsevier Science B. V., 2005.
- 11.- N. E. Jacobsen. **NMR Spectroscopy Explained. Simplified Theory, Applications and Examples for Organic Chemistry and Structural Biology**, John Wiley and Sons, New Jersey, 2007.
- 12.- E. Breitmaier, **Structure Elucidation by NMR in Organic Chemistry. A Practical Guide**, John Wiley and Sons, Ltd., Chischester, 2002.

2. Further reading

None

COORDINATION CRITERIA

Tasks deadlines

Clarifications

Lectures on Pharmacology will be all given at the beginning so that by the moment the student has to deal with the structure determination of more complex organic molecules, he/she will already know the fundamentals of spectroscopic techniques (taught on the compulsory subject "Advanced Organic Chemistry"/"Ampliación de Química Orgánica", second semester, 3rd Course, degree in Chemistry).

SCHEDULE

Period	Assessment activities	Lab practice	Lectures	Seminar
1# Week	0,0	0,0	2,0	0,0
2# Week	0,0	0,0	3,0	0,0
3# Week	0,0	0,0	3,0	0,0
4# Week	0,0	3,0	2,0	0,0
5# Week	0,0	3,0	2,0	0,0
6# Week	0,0	0,0	2,0	0,0
7# Week	0,0	0,0	2,0	3,0
8# Week	0,0	0,0	2,0	3,0
9# Week	0,0	0,0	2,0	3,0
10# Week	0,0	0,0	2,0	3,0
11# Week	0,0	0,0	2,0	3,0



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Period	Assessment activities	Lab practice	Lectures	Seminar
12# Week	0,0	0,0	2,0	3,0
13# Week	0,0	0,0	2,0	3,0
14# Week	3,0	0,0	2,0	0,0
Total hours:	3,0	6,0	30,0	21,0

The methodological strategies and the evaluation system contemplated in this Course Description will be adapted according to the needs presented by students with disabilities and special educational needs in the cases that are required.

CONTINGENCY PLAN: CASE SCENARIO A

Case scenario A will correspond to a diminished on-site academic activity due to social distancing measures affecting the permitted capacity of classrooms.

METHODOLOGY

General clarifications on the methodology on case scenario A

A multimodal (hybrid) teaching system will be adopted, combining both on-site and remote classes via videoconference (synchronous) that will be held in the timetable approved by the corresponding Faculty or School. The time distribution of teaching activities (both on-site and remote) will be decided by the aforementioned Faculties and Schools bearing in mind the permitted capacity of classrooms and social distancing measures as established at that time.

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EVALUATION

Intended learnig	Document Analysis	Exams	Laboratory Practice	Oral Presentation	Problem solving
CB10	X	X	X	X	X
CB4	X			X	
CB6		X	X		X
CE15	X			X	
CE16		X		X	X
CE22	X	X			X
CE23	X	X	X		X
CE24	X	X	X		X
CE26	X	X	X		X
CE28			X		
CE30		X	X		X
CE31	X	X	X		X
CE4	X	X	X	X	X
Total (100%)	15%	30%	10%	15%	30%
Minimum grade	4	4	4	4	4

(*)Minimum grade necessary to pass the course

Method of assessment of attendance (Scenario A):

Attendance and students' active participation constitute 10% of the final mark.

General clarifications on instruments for evaluation (Scenario A):

Attendance and active participation to all face-to-face activities (lectures, seminars and practicals) will be evaluated (10% of the final mark). This percentage is considered in the table above, 5% in "exams" section and the other 5% in "problem solving".

Laboratory Practices are compulsory. Therefore, in order to pass the subject, both attendance and presentation of the final report are imperative. Their evaluation will represent 10% of final mark. Once approved, student will not have to repeat lab practices in subsequent courses.

Pharmacochemistry part means 30% of the final mark (15% document analysis + 15% oral presentation on assignments on drug description).

The part of **organic structural determination** constitutes 50% of the final mark, consisting in exams and problem/spectra solving.

In the final exam, the students will be able to retake those continuous assessment tests not passed, as long as they

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have taken them in the school period.

Special cases:

In the extraordinary calls of the academic year 2020-2021 for students of second enrolment or higher, the student must take a written test that will consist of a theoretical part (25%) and a problem-solving part (25%). Likewise, the grades obtained in the 2019-2020 academic year in the analysis of documents (15%), oral presentation (15%), laboratory practices (10%) and class attendance (10%) will be preserved.

Clarifications on the methodology for part-time students and students with disabilities and special educational needs (Scenario A):

Adaptation for part-time students and students with disabilities and special educational needs will be carried out according to the Faculty of Science Rules and considering the individual cases.

Qualifying criteria for obtaining honors (Scenario A):

According to article 80.3 of the Regulations of the University of Córdoba, the mention of

CONTINGENCY PLAN: CASE SCENARIO B

Case scenario B will bring about a suspension of all on-site academic activities as a consequence of health measures.

METHODOLOGY

General clarifications on the methodology on case scenario B

On-site teaching activities will be held via videoconference (synchronous) in the timetable approved by the corresponding Faculty or School. Alternative activities will be proposed for reduced groups in order to guarantee the acquisition of course competences.

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Intended learning	Document Analysis	Exams	Laboratory Practice	Oral Presentation	Problem solving
CB10	X	X	X	X	X
CB4	X			X	
CB6		X	X		X
CE15	X			X	
CE16		X		X	X
CE22	X	X			X
CE23	X	X	X		X
CE24	X	X	X		X
CE26	X	X	X		X
CE28			X		
CE30		X	X		X
CE31	X	X	X		X
CE4	X	X	X	X	X
Total (100%)	15%	30%	10%	15%	30%
Minimum grade	4	4	4	4	4

(*)Minimum grade necessary to pass the course

Moodle Tools	Análisis de documentos	Exposición oral	Exámenes	Prácticas de laboratorio	Resolución de problemas
Chat	X	X	X	X	X
Cuestionario	X				
Pruebas simultáneas por videoconferencia			X		X
Tarea				X	
Videoconferencia		X			

Method of assessment of attendance (Scenario B):

Attendance and students' active participation constitute 10% of the final mark.

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General clarifications on instruments for evaluation (Scenario B):

Attendance and active participation to all face-to-face activities (lectures, seminars and practicals) will be evaluated (10% of the final mark). This percentage is considered in the table above, 5% in "exams" section and the other 5% in "problem solving".

Laboratory Practices are compulsory. Therefore, in order to pass the subject, both attendance and presentation of the final report are imperative. Their evaluation will represent 10% of final mark. Once approved, student will not have to repeat lab practices in subsequent courses. In this scenario B, not face-to-face, the teacher will make audiovisual material related to the practices to be done available to students in Moodle. The students must subsequently submit through moodle the memory of practices, in the form of "task".

Pharmacochemistry part means 30% of the final mark (15% document analysis + 15% oral presentation on assignments on drug description).

The part of **organic structural determination** constitutes 50% of the final mark, consisting in exams and problem/spectra solving.

In the final exam, the students will be able to retake those continuous assessment tests not passed, as long as they have taken them in the school period.

Special cases:

In the extraordinary calls of the academic year 2020-2021 for students of second enrolment or higher, the student must take a written test that will consist of a theoretical part (25%) and a problem-solving part (25%). Likewise, the grades obtained in the 2019-2020 academic year in the analysis of documents (15%), oral presentation (15%), laboratory practices (10%) and class attendance (10%) will be preserved.

Clarifications on the methodology for part-time students and students with disabilities and special educational needs (Scenario B):

Adaptation for part-time students and students with disabilities and special educational needs will be carried out according to the Faculty of Science Rules and considering the individual cases.

Qualifying criteria for obtaining honors (Scenario B):

According to article 80.3 of the Regulations of the University of Córdoba, the mention of