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/m2324/

LECTURER INFORMATION

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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, interprete 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

Structural Determination of Organic Compounds.

Lesson 1. Infrared Spectroscopy (IR). Diffuse Reflectance Infrared Fourier Transform (DRIFT) and Attenuated Total Reflectance (ATR). Applications of IR spectroscopy in Organic Chemistry.

Lesson 2. 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 3. Mass spectrometry applied to the study of organic compounds.

Pharmacochemistry

Lesson 4. Introduction to Pharmacochemistry. Definitions. Origin of pharmacology. Nomenclature and

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classification of drugs. Current picture of Pharmaceutical industry. Commercial/Industrial Aspects of Pharmaceutical Industry.

Lesson 5. Physicochemical properties of drugs. Physicochemistry properties. Acid drugs. Basic drugs. Octanol/water partition coefficient.

Lesson 6. 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.

Lesson 7. 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 8. 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. Metabological pathways for common drugs.

Lesson 9. Rational design of drugs. Methods for drug design. Pharmacomodulation. QSAR methods. Hammett and Taft equations. Hansch method. Free-Wilson method. 3D QSAR methodologies.

Lesson 10. 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.

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.

-Synthesis of phenacetin (analgesic effect).

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

SUSTAINABLE DEVELOPMENT GOALS RELATED TO THE CONTENT

Good health and well-being

Clean water and sanitation

Climate action

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METHODOLOGY

Methodological adaptations 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 University of Cordoba Rules and considering the individual cases, this type of adaptations will be decided through meetings of students with their teachers. Moreover, reports from the Inclusive Education Unit Will be considered.

Face-to-face activities

Activity	Large group	Medium group	Total
Assessment activities	3	-	3
Lab practice	-	6	6
Lectures	30	-	30
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.

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EVALUATION

Intended learning	Document Analysis	Exams	Laboratory Practice	Oral Presentation	Problem solving
CB10	X	X	X	X	X
CB4	X	X	X	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%)	***20%***	***25%***	***10%***	***15%***	***30%***
Minimum grade	***4***	***4***	***4***	***4***	***4***

(*)Minimum mark (out of 10) needed for the assessment tool to be weighted in the course final mark. In any case, final mark must be 5,0 or higher to pass the course.

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Method of assessment of attendance:

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

General clarifications on instruments for evaluation:

Atendance 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% of the final mark in "document analysis" section and the other 5% of the final mark 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 (25% of the final mark) and problem/spectra solving which will be carried out in seminars, of compulsory attendance (25% of the final mark).

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 University of Cordoba Rules and considering the individual cases, this type of adaptations will be decided through meetings of students with their teachers. Moreover, reports from the Inclusive Education Unit Will be considered.

Clarifications on the evaluation of the extraordinary call and extra-ordinary call for completion studies:

Only the exam will be repeated. The mark of the rest of the evaluation instruments will be the one obtained in the ordinary call and students must have compulsorily attended the practices and seminars.

Qualifying criteria for obtaining honors:

The criteria established in article 80.3 of the regulations of the academic regime of the undergraduate and master´s studies of the University of Cordoba will be applied.

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.

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.

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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

SCHEDULE

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