Teaching Guide				
Identifying Data				2021/22
Subject (*)	Structural Analysis and Synthetic Planning		Code	610500003
Study programme	Mestrado Universitario en Ciencias, Tecnoloxías e Xestión Ambiental (plan 2012)			
Descriptors				
Cycle	Period	Year	Type	Credits
Official Master's Degree	1st four-month period	First	Optional	6
Language	Spanish			
Teaching method	Face-to-face			
Prerequisites				
Department	Química			
Coordinador	Maestro Saavedra, Miguel Anxo	E-mail	miguel.maestro@udc.es	
Lecturers	Maestro Saavedra, Miguel Anxo	E-mail	miguel.maestro@udc.es	
Web	campusvirtual.udc.es			
General description	The subject is aimed at expanding the knowledge of Chemistry graduates in both Structural Determination and organic synthesis. In a first block applications of the mass spectrometry in Organic Chemistry and the two-dimensional NMR techniques are introduced. In a second block the strategies in organic synthesis and asymmetric synthesis, as well as the new methodologies are studied.			
Contingency plan	1. Changes in content There will be no modification 2. Methodologies * Teaching methodologies that are modified Initial activities, Master Session, Seminars through Teams Final written non-face-to-face test online, where students must solve in limited time, problems similar to those carried out during the seminar classes and oral presentation. The exam will be written to deliver on the same Teams platform. 3. Mechanisms for personalized attention to students Tutoring and resolution of doubts through Teams. Questions via email Assessment remarks: Exam 70%. Final written non-contact test online. Seminars and class participation (25% + 5%).			

Study programme competences / results	
Code	Study programme competences / results
A1	Coñecemento das realidades interdisciplinares da Química e do Medio Ambiente, dos temas punteiros nestas disciplinas e das perspectivas de futuro.
A2	Deseño de novas especies químicas e materiais con propiedades determinadas.
A3	Capacitar ao alumno para o desenvolvemento dun traballo de investigación nun campo da Química ou do Medio Ambiente, incluíndo os procesos de caracterización de materiais, o estudo das súas propiedades fisicoquímicas e biolóxicas e dos procesos que poden sufrir no medio natural.
A4	Coñecer en profundidade as características e fundamentos de diversos modelos químicos para o estudo de sistemas orgánicos, inorgánicos e biolóxicos, incluídos os materiais con proxección tecnológica.
A5	Capacitación para o deseño de vías de síntese e retrosíntese de novos compostos.
A22	Dominar as técnicas instrumentais de análises máis típicas no ámbito químico profesional.

B1	Posuír e comprender coñecementos que acheguen unha base ou oportunidade de ser orixinais no desenvolvemento e/ou aplicación de ideas, a miúdo nun contexto de investigación.
B2	Que os estudantes saiban aplicar os coñecementos adquiridos e a súa capacidade de resolución de problemas en contornas novas ou pouco coñecidos dentro de contextos máis amplos (ou multidisciplinares) relacionados coa súa área de estudo.
B3	Que os estudantes sexan capaces de integrar coñecementos e enfrontarse á complexidade de formular xuízos a partir dunha información que, sendo incompleta ou limitada, inclúa reflexións sobre as responsabilidades sociais e éticas vinculadas á aplicación dos seus coñecementos e suizos.
B4	Que os estudantes saiban comunicar as súas conclusións e os coñecementos e razóns últimas que as sustentan a públicos especializados e non especializados dun modo claro e sen ambigüedades.
B5	Que os estudantes posúan as habilidades de aprendizaxe que lles permitan continuar estudando dun modo que haberá de ser en gran medida autodirixido ou autónomo.
B6	Ser capaz de analizar datos e situacións, xestionar a información dispoñible e sintetizala, todo iso a un nivel especializado.
B7	Ser capaz de planificar adecuadamente desenvolvementos experimentais, a un nivel especializado.
C1	Ser capaz de traballar en equipos, especialmente nos interdisciplinares e internacionais.
C3	Ser capaz de adaptarse a situacións novas, mostrando creatividade, iniciativa, espírito emprendedor e capacidade de liderado.
C4	Expresarse correctamente, tanto de forma oral coma escrita, nas linguas oficiais da comunidade autónoma.
C5	Dominar a expresión e a comprensión de forma oral e escrita dun idioma estranxeiro.
C6	Utilizar as ferramentas básicas das tecnoloxías da información e as comunicacións (TIC) necesarias para o exercicio da súa profesión e para a aprendizaxe ao longo da súa vida.
C9	Valorar criticamente o coñecemento, a tecnoloxía e a información dispoñible para resolver os problemas cos que deben enfrontarse.
C11	Valorar a importancia que ten a investigación, a innovación e o desenvolvemento tecnolóxico no avance socioeconómico e cultural da sociedade.

Learning outcomes			
Learning outcomes	Study programme competences / results		
Knowledge of two-dimensional NMR techniques and strategies for the planning of an organic synthesis	AC1 AC2 AC3 AC4 AC5 AC22	BC1 BC2 BC3 BC4 BC5 BC6 BC7	CC1 CC3 CC4 CC5 CC6 CC9 CC11

Contents	
Topic	Sub-topic
Unit 1: Mass spectrometry.	Ionization methods: IC, FAB, APCI, ESI and MALDI. Applications for obtaining the molecular formula of a compound. Mass spectrometry of biomolecules: proteins and nucleic acids. Tandem mass spectrometry (MS / MS).
Unit 2: Multidimensional NMR technics.	The chemical shift and spin-spin coupling. Relaxation in NMR: NOE, nOediff. The polarization transfer: INEPT, DEPT and APT experiments. Two-dimensional NMR spectroscopy, basic concepts. Experiments COSY, HETCOR, NOESY, ROESY and INADEQUATE. Reverse Spectroscopy: HMQC Vs. HSQC. HMBC. Methods of J-resolved: JHH; JCH. Measurements of long-distance coupling constants, LR-COSY and J-HMBC. More complex experiments: 1H-1H TOCSY (HOHAHA), HSQC-TOCSY, HSQC-NOESY and HETLOC.
Unit 3. Structural analysis in Organic Chemistry	Strategies for solving combined problems.
Unit 4. Asymmetric synthesis	Introduction. Basic principles. Kinetic resolution. Stereoselective synthesis: chiral auxiliaries. Catalytic processes.

Unit 5. Planning and strategies in organic synthesis	Retrosynthetic analysis. Selectivity in organic synthesis. Protecting groups in organic synthesis.
Unit 6. Reduction reactions.	Reduction of alkenes: Asymmetric hydrogenation. Hydroboration reactions. Reactions of hydroformylation. Reduction of ketones and imines. Hydrogenation reactions. Reactions with oxazoborolidines. Hydrosilylation reactions.
Unit 7. Oxydation reactions.	Epoxydation of alkenes. Epoxydation of allylic alcohols. Epoxydation with salts of manganese (salen). Formation of azidirines. Dihydroxylation of alkenes. Aminohydroxylation of alkenes. Oxidation of Baeyer-Villiger and related
Unit 8. Reaction of nucleohylic addition to carbonyl compounds	Addition of organometallic zinc. Addition of cyanide ion. Alkylation of aldehydes. The aldol reaction. Addition reactions to imines. Baylis-Hillman reaction. Conjugate Addition Reactions.

Planning				
Methodologies / tests	Competencies / Results	Teaching hours (in-person & virtual)	Student?s personal work hours	Total hours
Guest lecture / keynote speech	A1 A2 A3 A4 A5 B1 B2 B3 B4 B5 B6 B7 C3 C1 C9 C11	20	40	60
Laboratory practice	A5 A22 B1 B2 B5 B6 B7 C3 C1 C4 C6	10	14.9	24.9
Supervised projects	A5 B1 B2 B3 B4 B5 B6 C3 C1 C4 C5 C6 C9	2	8	10
Objective test	A1 A2 A3 A5 A22 B1 B2 B3 B4 B6 C3 C1 C4 C5	2	8	10
Oral presentation	B4 B5 C4 C5 C6 C9 C11	1	4	5
Collaborative learning	B1 B2 B3 B4 B5 B6 B7 C3 C1	9.5	26.6	36.1
Introductory activities	A1 A2 A3 C9 C11	0.5	0.5	1
Personalized attention		3	0	3
(*)The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.				

Methodologies	
Methodologies	Description
Guest lecture / keynote speech	Development of the fundamental contents of the program through theoretical explanations and practical examples.
Laboratory practice	Analysis and resolution of the problems selected by the teacher. Structural elucidation of unknown compounds by analysis and integration of NMR and mass data. Laboratory sessions are proposed that will focus on the use of new methodologies in Organic Synthesis: Microwave, solid phase synthesis, ultrasound, etc.
Supervised projects	Elaboration of a report on the prediction and / or interpretation of the reactivity of organic compounds with special attention to the use of computational methods
Objective test	A written exam is scheduled, in order to evaluate the degree of assimilation and the ability to apply the contents of the subject by students.
Oral presentation	Exhibition of the tutored work, with support of new technologies.
Collaborative learning	Preparation of the expositive classes, resolution of exercises in groups and / or individualized.
Introductory activities	Presentation of the course and its programming of contents, activities and evaluation criteria

Personalized attention	
Methodologies	**Description**
Laboratory practice Collaborative learning	Follow-up and orientation during the drafting of the report on synthetic strategies and structural analysis, in individual sessions in the teacher's tutoring schedule.

Assessment			
Methodologies	**Competencies / Results**	**Description**	**Qualification**
Laboratory practice	A5 A22 B1 B2 B5 B6 B7 C3 C1 C4 C6	Continuous evaluation of the work in the laboratory, which will take into account the interest and attitude of the student, the skill achieved in the use of synthetic tools, as well as the resolution of problems of structural elucidation by analyzing spectroscopic data.	50
Supervised projects	A5 B1 B2 B3 B4 B5 B6 C3 C1 C4 C5 C6 C9	The preparation of a bibliographical revision work and its writing in a concise and rigorous manner, using the appropriate terminology, on some of the contents presented in the master sessions.	10
Oral presentation	B4 B5 C4 C5 C6 C9 C11	Evaluation of the oral expositions corresponding to the work of bibliographical revision and the solutions of the problems of structural elucidation	10
Objective test	A1 A2 A3 A5 A22 B1 B2 B3 B4 B6 C3 C1 C4 C5	Solving Problems of Organic Synthesis and Structural Determination.	30

Assessment comments
It is necessary to obtain 50% to pass the subject.For a methodology to be accounted for, it must exceed at least 40% of the grade.

Sources of information	
Basic	- Crews, P, Rodríguez, J., Jaspers, M. (2009). Organic Structure Analysis. 2nd Ed. Osxord University Press; New York - E. N. Jacobsen, A. Pfaltz, H. Yamamoto (1999). Comprehensive Asymmetric Catalysis . Berlin, Springer - Smith, M. B (2002). Organic Synthesis. Boston, McGraw-Hill - Gewert J. A.; Görlitzer, J.; Götze, S.; Looft, J.; Menningen, P.; Nöbel, T.; Schirock, H.; Wulff, C. (2000). Organic Synthesis Workbook. Weinheim, Wiley - Bittner, C.; Busemann, A. S.; Griesbach, U.; Haunert, F.; Krahnert, W.-R.; Modi, A.; Olschimke, J. (2000). Organic Synthesis Workbook II. Weinheim, Wiley - Tom Kinzel... [et al.] (2007). Organic synthesis workbook III. Weinheim, Wiley - Wyatt, P.; Warren, S. (2007). Organic Synthesis: Strategy and Control.. England, Wiley
Complementary	- Hesse, M. (1995). Métodos Espectroscópicos en Química Orgánica. . Madrid, Síntesis - Eliel, E. L. (1994). Stereochemistry of Organic Compounds. New York, Wiley

Recommendations
Subjects that it is recommended to have taken before
Subjects that are recommended to be taken simultaneously
Subjects that continue the syllabus
Other comments

(*)The teaching guide is the document in which the URV publishes the information about all its courses. It is a public document and cannot be modified. Only in exceptional cases can it be revised by the competent agent or duly revised so that it is in line with current legislation.