UNIVERSIDADE DA CORUÑA

Teaching Guide				
Identifying Data				2018/19
Subject (*)	Advanced Structural Determination		Code	610509103
Study programme	Mestrado Universitario en Investigación Química e Química Industrial (Plan 2017)			
Descriptors				
Cycle	Period	Year	Type	Credits
Official Master's Degree	Yearly	First	Obligatory	3
Language	SpanishGalicianEnglish			
Teaching method	Face-to-face			
Prerequisites				
Department	Química			
Coordinador	Rodriguez Gonzalez, Jaime	E-mail	jaime.rodriguez@udc.es	
Lecturers	Rodriguez Gonzalez, Jaime Sanchez Andujar, Manuel	E-mail	jaime.rodriguez@udc.es m.andujar@udc.es	
Web	http://www.usc.es/gl/centros/quimica/curso/master.html			
General description	This module is focused in the advanced aspects which are essential in subjects at highest level in Chemistry. Discussions will be focused in the most important tasks in the basic chemical research directed to own or interdisciplinary studies. The five main subjects in the module will be extended in 15 ECTS and they will be intensively given by the three associated universities during the first quarter. These subjects will be simultaneously taught by the three universities during the months of September and October of each academic year.			

Study programme competences	
Code	Study programme competences
A1	Define concepts, principles, theories and specialized facts of different areas of chemistry.
A2	Suggest alternatives for solving complex chemical problems related to the different areas of chemistry.
A3	Innovate in the methods of synthesis and chemical analysis related to the different areas of chemistry
A7	Operate with advanced instrumentation for chemical analysis and structural determination.
A8	Analyze and use the data obtained independently in complex laboratory experiments and relating them with the chemical, physical or biological appropriate techniques, including the use of primary literature sources
A9	Promote innovation and entrepreneurship in the chemical industry and in research.
B1	Possess knowledge and understanding to provide a basis or opportunity for originality in developing and / or applying ideas, often within a research context
B2	Students should apply their knowledge and ability to solve problems in new or unfamiliar environments within broader (or multidisciplinary) contexts related to their field of study.
B4	Students should be able to communicate their conclusions, and the knowledge and the reasons that support them to specialists and non-specialists in a clear and unambiguous manner
B5	Students must possess learning skills to allow them to continue studying in a way that will have to be largely self-directed or autonomous.
B7	Identify information from scientific literature by using appropriate channels and integrate such information to raise and contextualize a research topic
B10	Use of scientific terminology in English to explain the experimental results in the context of the chemical profession
B11	Apply correctly the new technologies to gather and organize the information to solve problems in the professional activity.
C1	CT1 - Elaborar, escribir e defender publicamente informes de carácter científico e técnico
C2	CT2 - Traballar en equipo e adaptarse a equipos multidisciplinares.
C3	CT3 - Traballar con autonomía e eficiencia na práctica diaria da investigación ou da actividade profesional.
C4	CT4 - Apreciar o valor da calidade e mellora continua, actuando con rigor, responsabilidade e ética profesional.

Learning outcomes	
Learning outcomes	Study programme competences

Be able to propose a molecular structure of both organic and inorganic Compostos by using spectroscopic techniques or mass spectrometry techniques.	AC1 AC2 AC3 AC7 AC8 AC9	BC1 BC2 BC4 BC5 BC10 BC11	CC1 CC2 CC3 CC4
Be able to identify in a mass spectrum the base peak, molecular ion (main peak and isotope peaks) and some peak fragmentations. Be able to identify acronyms in the different ionization techniques. Be able to manually determine isotopic compositions of molecules using isotopomers and isotopologues. Be able to identify common elements such S, Cl, Br based on isotopic patterns. Be able to estimate the maximum number of carbons based on the M+1 peak Be able to get possible molecular formulaes for a given mass using de rule of 13. Be able to use the nitrogen rule in the number of possible formulas. Be able to determine the degree of unsaturation from an empirical formula (DBE) Be able to interpret NMR magnetization through pulse sequences. Be able to interpret basic concepts as relaxation processes in NMR. Be able to describe or outline basic experiment by NMR pulses and NMR acquisition parameters (SI, O1, SW, AQ, DW, FIDRES, P1, D1 ...). Be able to interpret type of NMR data such absorption and dispersion. Be able to distinguish NMR in time scale (FID) and NMR frequency scale (NMR spectrum) and to describe the Fourier Transformation in NMR. Be able to describe the basic work-up of two-dimensional NMR experiments. Be able to identify molecular fragments by using an heteronuclear experiments (HSQC / HMQC). Use of the DEPT-135 Edited HSQC experiment. Be able to gather information from NOE experiments. Use of essential difractometric techniques for a X-RAy single crystal experiments in the structural determination of small molecules.	AC8	BC1 BC2 BC4 BC7	

Contents	
Topic	**Sub-topic**
1. The mass spectrometry	Basic principles. Ionization methods: ESI, APCI, MALDI Isotopic patterns High resolution mass spectrometry. Fragmentation in mass spectrometry
2. Monodimensional NMR experiments. Heteronuclear NMR spectroscopy.	Selective irradiation experiments, 1D-NOE and 1D-TOCSY. Edited heteronuclear experiments: INEPT and DEPT. Aplications in stereochemistry problems Other nuclei: N-15 and F-19 NMR
3. Bidimensional NMR experiments.	Heteronuclear correlation experiments. HSQC and HMBC 2D-NMR experiments: COSY basic principles; TOCSY NOE experiments. NOESY and ROESY Heteronuclear 2D-experiments
4.- Monocrystal X-Ray difraction	Basic concepts. Resolution methods and refinament of the structural models: examples. Criterios de calidad del modelo. Compuational tools for calculation and representation for structures.

Planning				
Methodologies / tests	**Competencies**	**Ordinary class hours**	**Student?s personal work hours**	**Total hours**

Seminar	A2 A3 A7 A8 A9 B2 B4 B5 B7 B11 C1 C3 C4	12	30	42
Supervised projects	A8 B1 B7 B10 C2 C3 C4	1	4	5
Mixed objective/subjective test	A1 A8 B7 B10	1	7	8
Guest lecture / keynote speech	A1 A8 B1 B11 C1	9	9	18
Personalized attention		2	0	2
(*)The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.				

Methodologies	
Methodologies	**Description**
Seminar	It is proposed to carry out 12 sessions of seminars-problems of small groups where the students will solve sets of proposed problems presented by the teacher in handouts. The students will have in advance the problem on the moodle platform, in that form student will individuially elaborate the answers before the classes. Seminars will be used also for the resolution of doubts theoretical explanations. Attendance is mandatory.
Supervised projects	This monitored activity will be directed in solving exercises, clarification of doubts about the theory or practice, readings or other proposed tasks, as well as presentations, discussions or comments made individually by students or in small groups. In many cases teachers will require from students writen answers in advance. Attendance at these classes is mandatory.
Mixed objective/subjective test	Final test will contribute to the assessment of the level of knowledge and skills acquired by students.
Guest lecture / keynote speech	In these large group sessions the theoretical contents along with relevant illustrative examples are developed. The students will have the material to be taught in advance, before conducting the activity. The active participation of students will be encouraged.

Personalized attention	
Methodologies	**Description**
Supervised projects Seminar	Students who have special difficulties with any aspects of the subjects, should contact the hours of tutoring with the teacher to receive the necessary support.

Assessment			
Methodologies	**Competencies**	**Description**	**Qualification**
Supervised projects	A8 B1 B7 B10 C2 C3 C4	The continuous grading of the student will be assessed through questions and problems, in addition to the attendance and participation in the class.	20
Mixed objective/subjective test	A1 A8 B7 B10	Exame escrito con exercicios integrados das diferentes técnicas de RMN, masas e RX expliacadas nas clases presenciais.	55
Seminar	A2 A3 A7 A8 A9 B2 B4 B5 B7 B11 C1 C3 C4	Resolution of problems, practical cases and presentations that will be delivered to the student previously. The explanations and examples explained in the class will be followed.	25

Assessment comments

The completion of the set of activities related to seminars and supervised projects by the students is fundamental to successfully overcome the subject. In the seminary classes we will mainly work on solving problems. The problems and the calendar of classes in which these problems will be solved will be available to the students in the virtual classroom of the subject. Students should try to solve them autonomously, delivering the solution in the virtual classroom in advance of the classes. Subsequently, the solutions will be analyzed in the classes. The seminars will also propose brief exercises to be solved at the moment, which will serve to focus on the topics discussed and which will be taken into account in the evaluation.
It is recommended that students use the recommended bibliography. The faculty will advise the sections of each book that are most appropriate for each topic. In case of finding difficulties, students can raise their doubts both in the classes and in the tutorials.

Sources of information	
Basic	- Gross, J. H. (2004). Mass Spectrometry. Springer - Günther, H. (1995). NMR Spectroscopy, Basic principles, concepts, and applications in Chemistry. 2nd Ed. John Wiley - Crews, P, Rodríguez, J., Jaspers, M. (2010). Organic Structure Analysis. 2nd Ed. Oxord University Press; New York - Lifshin, Eric (1999). X-ray Characterization of Materials. Wiley-VCH - Clegg, William (1998). Crystal Structure Determination. Oxford University Press
Complementary	- Glusker, Jenny P. and Trueblood, Kenneth N. (1985). Crystal Structure Analysis, a Primer. Oxford University Press, (2 ed.) - Donald E. Sands (1988). Introducción a la cristalografia. Ed. Reverté - Silvestein R. M.; Webster, F. X., Kiemle, D. J. (2005). Spectrometric Identification of Organic Compounds. 7th Ed. Wiley - Hesse, M. (1995). Métodos Espectroscópicos en Química Orgánica. Madrid, Síntesis - Smart, Lesley and Moore, Elaine A. (2012). Solid state chemistry : an introduction. CRC Press, (4 ed.).

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 accomplishment of the activities of the block a) evaluation is very important for the student to successfully overcome the Subject. In the seminar classes you will mainly work on solving problems. The problems and the calendar in which these problems will be solved will be available to students in the web site of the course (Moodle). Students should try to solve all problems autonomously, delivering the solution in the virtual classroom in advance of classes. Solutions will be analyzed in the classes. Seminars will contain short exercises to be solve in the same class. Discussion and the way to solve each problem will be taken into account in the final grade. Students are encouraged to follow the recommended literature for each chapter. In case of difficulties, the students can raise their doubts in both classes and tutorials.