UNIVERSIDADE DA CORUÑA

Teaching Guide					
Identifying Data					2016/17
Subject (*)	Análise Estrutural Avanzado			Code	610509005
Study programme	Mestrado en Investigación Química e Química Industrial (plan 2016)				
Descriptors					
Cycle	Period	Year		Type	Credits
Official Master's Degree	Yearly	First		Obligatoria	3
Language	SpanishGalicianEnglish				
Teaching method	Face-to-face				
Prerequisites					
Department	Química Fundamental				
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					
General description	This module is focused in the advanced aspects which are essential in subjects at highest level in Chemistry. Discussions will be centered 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 / results	
Code	Study programme competences / results
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.
A4	Innovate in the methods of synthesis and chemical analysis related to the different areas of chemistry
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.

Learning outcomes			
Learning outcomes	Study programme competences / results		
Be able to propose a molecular structure of both organic and inorganic Compostos by using spectroscopic techniques or mass spectrometry techniques.	AC1 AC2 AC4	BC1 BC2 BC4 BC5 BC7 BC10 BC11	

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.	AC1 AC2 AC4	BC1 BC2 BC4 BC5 BC7 BC10 BC11	

Contents	
Topic	**Sub-topic**
1. The mass spectrometry	Basic principles. Isotopic patterns High resolution mass spectrometry.
2. Monodimensional NMR experiments. Heteronuclear NMR spectroscopy.	1D-NMR: vectorial model in pulse experiments NMR spectral parameters: signal integration and chemical shifts. Doble irradiation experiments 1D-NMR pulse sequences..
3. Bidimensional NMR experiments.	Heteronuclear correlation experiments. 2D-NMR experiments:COSY basic principles NOE experiments. Heteronuclear 2D-experiments
4.- Monocrystal X-Ray difraction	
5. Another structural analysis techniques	

Planning				
Methodologies / tests	**Competencies / Results**	**Teaching hours (in-person & virtual)**	**Student?s personal work hours**	**Total hours**
Seminar	B1 B2 B4 B5 B7 B10 B11	12	30	42
Supervised projects	B1 B2 B4 B5 B7 B10 B11	1	4	5
Mixed objective/subjective test	A1 A2 A4 B1 B2 B4 B5 B7 B10 B11	1	7	8
Guest lecture / keynote speech	A1 A2 A4	10	10	20
Personalized attention		0		0
(*)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 / Results**	**Description**	**Qualification**
Supervised projects	B1 B2 B4 B5 B7 B10 B11		0
Mixed objective/subjective test	A1 A2 A4 B1 B2 B4 B5 B7 B10 B11		0
Seminar	B1 B2 B4 B5 B7 B10 B11		0

Assessment comments
The assessment of this course will be done through continuous monitoring and conducting a final test, Access to such test will be conditioned on a minimum participation of 80% of the mandatory classroom teaching activities (seminars and supervised work). Continuous assessment (N1) will count 40% of the final grade, and it will consist of two components: seminars and tutored projects. Important aspects of evaluation are: problems solving and individual cases (15%), performing work and writings (10%) reports, oral presentation (10%) and oral questions during the course (5%). The final exam (N2) will cover the entire contents of the subject. The grade will be obtained as a result of applying the following formula: Final grade = 0.4 * 0.6 * N1 + N2 N1 is the corresponding numerical grade to the continuous assessment (scale 0-10) and N2 is the numerical grade of the final examination (scale 0-10). Non-first timer students have the same system of class attendance to those studying the subject for the first time.

Sources of information

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