Teaching Guide				
Identifying Data				2021/22
Subject (*)	Analytical Mass Spectrometry of Organic Compounds		Code	610509126
Study programme	Mestrado Universitario en Investigación Química e Química Industrial (Plan 2020)			
Descriptors				
Cycle	Period	Year	Type	Credits
Official Master's Degree	Yearly	First	Optional	3
Language	Spanish			
Teaching method	Face-to-face			
Prerequisites				
Department	Departamento profesorado másterQuímica			
Coordinador		E-mail		
Lecturers		E-mail		
Web				
General description	It is a subject of the Specialty on Advanced Analytical Techniques. Mass spectrometry is an indispensable tool in any chemical analysis laboratory, particularly those that perform their activity in the areas of food safety, environment, clinic, etc.,; it is used for the identification and quantitative determination of species of interest. This subject aims to improve the student's knowledge on the instrumental techniques of analysis acquired during the degree, and to know the recent trends in relation to sources of ionization, mass analyzers and information extraction systems.			
Contingency plan	1. Modifications to the contents 2. Methodologies *Teaching methodologies that are maintained *Teaching methodologies that are modified 3. Mechanisms for personalized attention to students 4. Modifications in the evaluation *Evaluation observations: 5. Modifications to the bibliography or webgraphy			

Study programme competences	
Code	Study programme competences
A3	Innovate in the methods of synthesis and chemical analysis related to the different areas of chemistry
A6	Design processes involving the treatment or disposal of hazardous chemicals
A7	Operate with advanced instrumentation for chemical analysis and structural determination.
A9	Promote innovation and entrepreneurship in the chemical industry and in research.
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
B9	Demonstrate ability to analyze, describe, organize, plan and manage projects
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
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		
Acquisition of knowledge on aspects of analytical interest on mass spectrometry for the study of organic compounds. Acquisition of the characteristics and uses of the isotope dilution. Acquisition of knowledge related to studies of degradation and metabolomics.	AC3 AC6 AC7 AC9	BC2 BC4 BC5 BC7 BC9 BC10 BC11	CC1 CC3 CC4

Contents	
Topic	Sub-topic
1. INTRODUCTION TO ANALYTICAL MASS SPECTROMETRY.	Descrición básica da instrumentación: O espectrómetro de masas. Sistemas de vacío. Etapas na xeración dun espectro de masas. Calibración de masas e axuste do espectrómetro de masas. Conceptos básicos en espectrometría de masas: Distribucións isotópicas: masas promedio e monoisótopicas. Cálculo do defecto de masas. Avaliación da exactitude e resolución: masas nominais fronte a exactas. Cargas simples e múltiples.
2. IONIZATION TECHNIQUES. Fundamentals, operations and instrumentation	Introdución: dependencia analito-fonte de ionización-analizador de masas. Clasificación das técnicas de ionización. Ionización Electrónica (EI). Ionización Química (CI). Selección de gases reactivos e mecanismos de ionización. Ionización a P atmosférica: ESI, APCI, APPI. Desorción Láser asistida por matriz (MALDI). Outras técnicas de ionización: DESI, DART.
3. MASS ANALYZERS. Operational principles, instrumentation and basic characteristics	Principais analizadores. Cuadrupolos. Trampas de iones. Sistemas de tempo de voo (TOF). De sector magnético. Orbitrap. Analizadores en tándem. Analizadores híbridos en tándem.
4. HYBRIDIZATION WITH CHROMATOGRAPHIC TECHNIQUES	Aspectos técnicos. Obtención e tratamento de datos. Adquisición. Modos de operación. Aplicacións da hibridación GC-MS e GC-MS/MS. Aplicacións da hibridación LC-MS e LC-MS/MS. Análise cuantitativa. Dilución isotópica. Identificación de metabolitos e produtos de transformación. Deconvolución espectral.

Planning				
Methodologies / tests	Competencies	Ordinary class hours	Student?s personal work hours	Total hours
Guest lecture / keynote speech	A3 A6 A7 A9 B5 C1 C3 C4	12	36	48
Seminar	A7 B2 B4 B5 B7 B9 B10 B11 C1 C3 C4	7	18	25
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

Guest lecture / keynote speech	Clases presenciais teóricas. Clases expositivas (utilización de pizarra, computador, canón), complementadas coas ferramentas propias da docencia virtual. Estudo persoal baseado nas diferentes fontes de información Realización das diferentes probas para a verificación da obtención tanto de coñecementos teóricos como prácticos e a adquisición de habilidades e actitudes
Seminar	Seminarios realizados con profesorado propio do Máster, ou con profesionais convidados da empresa, a administración ou doutras universidades. Sesións interactivas relacionadas coas distintas materias con debates e intercambio de opinións cos alumnos. Resolución de exercicios prácticos (problemas, cuestiones tipo test, interpretación e procesamento da información, avaliación de publicacións científicas, etc.) Realización de traballos, tanto individualmente, como en grupo, sobre contidos da materia Exposición oral de traballos, informes, etc., incluíndo debate con profesores e alumnos.

Personalized attention	
Methodologies	**Description**
Seminar	Tutorías individuales o en grupo reducido.

Assessment			
Methodologies	**Competencies**	**Description**	**Qualification**
Seminar	A7 B2 B4 B5 B7 B9 B10 B11 C1 C3 C4	Resolución de problemas e casos prácticos Realización de traballos e informes escritos Avaliación continua durante o curso	25
Guest lecture / keynote speech	A3 A6 A7 A9 B5 C1 C3 C4	Examen final	75

Assessment comments

Sources of information	
Basic	Bibliografía recomendada Básica (manuais de referencia) C. Dass, Fundamentals of Contemporary Mass Spectrometry, Wiley, 2007 R. M. Smith, K.L. Busch, Understanding Mass Spectra- A basic Approach, John Wiley & Sons, 1999. R.K. Boyd, C. Basic, R.A. Behen, Trace Quantitative Analysis by Mass Spectrometry, John Wiley and Sons, 2008 Complementaria E. de Hoffmann, V. Stroobant, Mass Spectrometry: Principles and Applications, 3a ed., Wiley, 2007 A. E. Ashcroft, Ionization Methods in Organic Mass Spectrometry, Royal Society of Chemistry, 1997 J. H. Gross, Mass Spectrometry: a textbook, Springer, 2005 K. Downard, Mass Spectrometry: a Foundation Course, RSC, 2004 B. Ardrey, Liquid Chromatography-Mass spectrometry: an introduction, Wiley, 2003 R. Willoughby, E. Sheehan, S. Mitrovich, A global view of LC/MS, Global View Publishing, 2nd edition, 2002 M. C. McMaster, GC/MS, A Practical User´s Guide, John Wiley & Sons, 2008 W.M.A. Niessen, Liquid Chromatography-Mass spectrometry, Taylor and Francis, 2007
Complementary	

Recommendations
Subjects that it is recommended to have taken before
Subjects that are recommended to be taken simultaneously
Sample Preparation Techniques /610509128 Chromatography and Analytical Separation Techniques /610509125
Subjects that continue the syllabus

Other comments
The knowledge compulsory are those that are established as basic requirements for access this Master. It is advisable to have basic knowledge about Mass spectrometry, acquired in the different subjects that give access to the present Master. It is also recommended to study the subject of "Chromatography and Separation Analytical Techniques"