



| Teaching Guide           |  |        |                           |         |
|--------------------------|--|--------|---------------------------|---------|
| Identifying Data         |  |        | 2017/18                   |         |
| Subject (*)              | Analytical Mass Spectrometry of Organic Compounds  | Code   | 610509126                 |         |
| Study programme          | Mestrado Universitario en Investigación Química e Química Industrial (Plan 2017)   |        |                           |         |
| Descriptors              |  |        |                           |         |
| Cycle                    | Period   | Year   | Type                      | Credits |
| Official Master's Degree | Yearly   | First  | Optativa                  | 3       |
| Language                 | Spanish  |        |                           |         |
| Teaching method          | Face-to-face   |        |                           |         |
| Prerequisites            |  |        |                           |         |
| Department               | Química  |        |                           |         |
| Coordinador              | Muniategui Lorenzo, Soledad  | E-mail | soledad.muniategui@udc.es |         |
| Lecturers                | Muniategui Lorenzo, Soledad  | E-mail | soledad.muniategui@udc.es |         |
| 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. |        |                           |         |

| 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. | AC3 | BC2                         | CC1 |
| Acquisition of the characteristics and uses of the isotope dilution.  | AC6 | BC4                         | CC3 |
| Acquisition of knowledge related to studies of degradation and metabolomics.  | AC7 | BC5                         | CC4 |
|   | AC9 | BC7                         |     |
|   |     | BC9                         |     |
|   |     | BC10                        |     |
|   |     | BC11                        |     |



| 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 monoisotópicas. 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<br>C3 C4            | 12                   | 36                            | 48          |
| Seminar                        | A7 B2 B4 B5 B7 B9<br>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.<br>Estudo persoal baseado nas diferentes fontes de información<br>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.<br>Resolución de exercicios prácticos (problemas, cuestións tipo test, interpretación e procesamento da información, avaliación de publicacións científicas, etc.)<br>Realización de traballos, tanto individualmente, como en grupo, sobre contidos da materia<br>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<br>B10 B11 C1 C3 C4 | Resolución de problemas e casos prácticos<br>Realización de traballos e informes escritos<br>Avaliación continua durante o curso | 25            |
| Guest lecture /<br>keynote speech | A3 A6 A7 A9 B5 C1<br>C3 C4            | Examen final   | 75            |

| Assessment comments |
|---------------------|
|                     |

| Sources of information |  |
|------------------------|--|
| <b>Basic</b>           | Bibliografía recomendada<br>Básica (manuais de referencia).C. Dass, Fundamentals of Contemporary Mass Spectrometry, Wiley, 2007R. 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, 2007A. E. Ashcroft, Ionization Methods in Organic Mass Spectrometry, Royal Society of Chemistry, 1997J. H. Gross, Mass Spectrometry: a textbook, Springer, 2005K. Downard, Mass Spectrometry: a Foundation Course, RSC, 2004B. 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. |
| <b>Complementary</b>   |  |

| Recommendations  |
|--|
| <b>Subjects that it is recommended to have taken before</b>  |
|  |
| <b>Subjects that are recommended to be taken simultaneously</b>  |
| Chromatography and Analytical Separation Techniques /610509125<br>Sample Preparation Techniques /610509128   |
| <b>Subjects that continue the syllabus</b>   |
|  |
| <b>Other comments</b>  |
| Especialidade de Técnicas Analíticas Avanzadas. Os únicos coñecementos obrigatorios son aqueles que se establecen como requisitos básicos para acceder a este Máster. É recomendable dispoñer de noções básicas sobre Espectrometría de Masas, adquiridas nas diferentes materias que dan acceso ao presente Máster. Recomendase cursar tamén a Materia de "Cromatografía e Técnicas Analíticas de Separación" |

(\*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.