UNIVERSIDAD DE CASTILLA - LA MANCHA

GUÍA DOCENTE

1. General information

Course: ADVANCED TECHNIQUES OF INSTRUMENTAL ANALYSIS
Code: 310586
Type: CORE COURSE
ECTS credits: 6
Degree: 2366 - MASTER DEGREE PROGRAMME IN CHEMICAL
Academic year: 2023-24
Center: 1 - FACULTY OF SCIENCE AND CHEMICAL TECHNOLOGY
Group(s): 20
Year: 1
Duration: First semester
Main language: Spanish
Second language: English
Use of additional languages:
English Friendly: Y
Web site:
Bilingual: N

Lecturer: **ALFONSO ARANDA RUBIO** - Group(s): **20**

Building/Office	Department	Phone number	Email	Office hours
Marie Curie/2ª planta	QUÍMICA FÍSICA	926051915	alfonso.aranda@uclm.es	Tuesday, Wednesday and Thursday from 16:00 to 18:00

Lecturer: **BERNABE BALLESTEROS RUIZ** - Group(s): **20**

Building/Office	Department	Phone number	Email	Office hours
Marie Curie, primera planta	QUÍMICA FÍSICA	926052049	bernabe.ballesteros@uclm.es	L,M: 9-11h J: 17-19h

Lecturer: **JOSE ANTONIO MURILLO PULGARIN** - Group(s): **20**

Building/Office	Department	Phone number	Email	Office hours
Edificio San Alberto Magno	Q. ANALÍTICA Y TGIA. ALIMENTOS	3441	joseantonio.murillo@uclm.es	Tues., W., Thu. 17:00 to 19:00h.

2. Pre-Requisites

Not established

3. Justification in the curriculum, relation to other subjects and to the profession

Technological advances in fields such as mass spectrometry and laser technology are enabling the development of new scientific tools.

Knowledge of the principles, equipment and applications enables the use of advanced instrumental techniques in the field of chemistry research.

4. Degree competences achieved in this course

Course competences

Code	Description
CB07	Students are able to apply their acquired knowledge and problem-solving skills in new or unfamiliar environments within broader (or multidisciplinary) contexts related to their field of study.
CB10	Students possess the learning skills that will enable them to continue studying in a largely self-directed or autonomous way.
CE04	Evaluate the usefulness of separation, analysis and structural determination techniques for joint application in problem solving, and be skilled in the use of such techniques in both research and routine laboratories applying methods of organic and inorganic analysis and/or synthesis.
CE06	Assess the principles of sustainable chemistry and safety standards for the handling of known or newly synthesised chemicals.
CE07	To learn about the possibilities offered by new analytical methodologies in different fields of application, as well as the current trends in analytical chemistry of interest for the development of R+D+I or its implementation in specialised control laboratories.
CG01	Transfer the concepts and fundamentals of chemistry in the context of scientific research and/or in the specialised profession of the chemist.
CG02	To achieve advanced training in the fundamentals and potential of the instrumental techniques available in chemistry for the development of scientific research and/or application in specialised control laboratories.

5. Objectives or Learning Outcomes

Course learning outcomes

Description

Acquire knowledge of the different ionisation sources, mass analysers and interfaces used in mass spectrometry. To know the different couplings of mass spectrometry with different separation techniques and their applications.

To understand the fundamentals and applications of laser technology and laser-induced fluorescence.

Acquire scientific criteria for the selection of the most appropriate separation technique according to the requirements of the components and samples to be analysed, as well as the quality of the required results.

Acquire a critical spirit to modify and improve analytical procedures already established in the literature.

To learn about the possibilities offered by new luminescent methodologies in different fields of application such as environmental analysis, pharmacology, food safety.

To know how to select the most appropriate luminescent or voltammetric technique for the resolution of an analytical problem depending on the nature of the analyte and the complexity of the matrix, without loss of sensitivity and selectivity.

6. Units / Contents

Unit 1: Mass spectrometry. Ionisation techniques and ion discrimination.

Unit 1.1 History, evolution and fundamentals of mass spectrometry. Concepts. Mass spectra. Isotopic effects.

Unit 1.2 Vacuum technology. Vacuum and high vacuum pumping systems and instrumentation.

Unit 1.3 Ionisation methods: Volatile and low volatile substances. Electronic ionisation, chemical ionisation, field ionisation, laser desorption, fast atom bombardment, secondary ions, electrospray. Ionisation sources at atmospheric pressure.

Unit 1.4 Mass analysers. Ion separation. Sectors, quadrupole, Ion Trap, cyclotron, time of flight. Tandem mass spectrometry.

Unit 1.5 Ion detectors. SEM, Channeltron, scintillation and multichannel.

Unit 1.6 Operating modes: Scan, SIM, SRM, MRM and use of spectrum libraries.

Unit 2: Instrumental hybridisation with mass spectrometric detection.

Unit 2.1 Couplings and different sample handling and insertion systems.

Unit 2.2 Combined use with other techniques: GC-MS, LC-MS, ICP-MS, PTR-MS, Aerosol Mass Spectrometry. Sampling with SPME.

Unit 3: Laser-induced fluorescence. Fundamentals and instrumentation.

Unit 3.1 Characteristics of laser radiation. Types of lasers.

Unit 3.2 Laser spectroscopy

Unit 3.3 Kinetic and spectroscopic applications of gas-phase LIF.

Unit 4: Analytical applications of hybridisations with mass spectrometric detection. Analytical applications of laser-induced fluorescence techniques.

Unit 4.1 Mass spectrometric detection with hybridisations.

Unit 4.2 Applications of laser-induced fluorescence to the characterisation of compounds. Quantitative applications. Kinetic spectroscopic applications. Other applications.

Unit 5: Scattering techniques. Optical rotating scattering and diffuse reflectance.

Unit 5.1 Non-spectroscopic optical techniques. General characteristics.

Unit 5.2 Optical scattering. Optical rotating scattering and diffuse reflectance.

Unit 6: Electrochemical characterisation techniques by cyclic voltammetry.

Unit 6.1 Basics of voltamperometry.

Unit 6.2 Cyclic voltammetry. Comparison with linear scanning voltamperometry. Characterisation by cyclic voltamperometry

Unit 6.3 Example of applications.

7. Activities, Units/Modules and Methodology

Training Activity	Methodology	Related Competences (only degrees before RD 822/2021)	ECTS	Hours	As	Com	Description
Writing of reports or projects [OFF-SITE]	Self-study	CB07 CB10	1.52	38	N	-	
Class Attendance (theory) [ON-SITE]	Lectures	CE04 CE06 CE07	1.12	28	N	-	
Study and Exam Preparation [OFF-SITE]	Self-study	CG01 CG02	1.48	37	N	-	
Analysis of articles and reviews [OFF-SITE]	Self-study	CB10 CE04 CE06 CE07	1.28	32	N	-	
Project or Topic Presentations [ON-SITE]	Case Studies	CB07 CG01	0.08	2	Y	Y	
Other off-site activity [OFF-SITE]	Combination of methods	CB10 CE07	0.16	4	Y	Y	
Progress test [ON-SITE]	Assessment tests	CE04 CE06 CE07	0.08	2	Y	Y	
Workshops or seminars [ON-SITE]	Problem solving and exercises	CB07 CE04 CE06 CE07 CG01	0.2	5	Y	Y	
Group tutoring sessions [ON-SITE]	Cooperative / Collaborative Learning	CB07 CG01	0.08	2	N	-	
		Total:	**6**	**150**			
		Total credits of in-class work: 1.56					**Total class time hours: 39**
		Total credits of out of class work: 4.44					**Total hours of out of class work: 111**

As: Assessable training activity
Com: Training activity of compulsory overcoming (It will be essential to overcome both continuous and non-continuous assessment).

8. Evaluation criteria and Grading System

Evaluation System	Continuous assessment	Non-continuous evaluation*	Description
Final test	40.00%	100.00%	Exam with theoretical and practical contents
Assessment of problem solving and/or case studies	40.00%	0.00%	Reports or work developed during the course
Other methods of assessment	20.00%	0.00%	On line activities
Total:	**100.00%**	**100.00%**	

According to art. 4 of the UCLM Student Evaluation Regulations, it must be provided to students who cannot regularly attend face-to-face training activities the passing of the subject, having the right (art. 12.2) to be globally graded, in 2 annual calls per subject , an ordinary and an extraordinary one (evaluating 100% of the competences).

Evaluation criteria for the final exam:

Continuous assessment:

Assessment of works or reports: 40%.
Final exam: 40%
Assessment of online activities 20%.

Non-continuous evaluation:

For students who justify at the beginning of the course that they cannot follow the continuous assessment, a final test will be held with theoretical and practical questions on the subject of the course: 100%.

Specifications for the resit/retake exam:

In the case of continuous assessment, the grades obtained during the course will be taken into account:
Assessment of reports or assignments: 40%.
Final test: 40%.
Assessment of online activities: 20%.
Only the assessment blocks not passed during the course must be passed.

Specifications for the second resit / retake exam:

Final test with theoretical and practical questions on the subject matter of the course: 100%

9. Assignments, course calendar and important dates

Not related to the syllabus/contents

Hours	hours

Unit 1 (de 6): Mass spectrometry. Ionisation techniques and ion discrimination.

Activities	Hours
Writing of reports or projects [AUTÓNOMA][Self-study]	9
Class Attendance (theory) [PRESENCIAL][Lectures]	7
Study and Exam Preparation [AUTÓNOMA][Self-study]	8
Analysis of articles and reviews [AUTÓNOMA][Self-study]	8
Project or Topic Presentations [PRESENCIAL][Case Studies]	.5
Other off-site activity [AUTÓNOMA][Combination of methods]	1
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	1
Group tutoring sessions [PRESENCIAL][Cooperative / Collaborative Learning]	.5

Unit 2 (de 6): Instrumental hybridisation with mass spectrometric detection.

Activities	Hours
Writing of reports or projects [AUTÓNOMA][Self-study]	4
Class Attendance (theory) [PRESENCIAL][Lectures]	2
Study and Exam Preparation [AUTÓNOMA][Self-study]	4
Analysis of articles and reviews [AUTÓNOMA][Self-study]	3
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	1

Unit 3 (de 6): Laser-induced fluorescence. Fundamentals and instrumentation.

Activities	Hours
Writing of reports or projects [AUTÓNOMA][Self-study]	6
Class Attendance (theory) [PRESENCIAL][Lectures]	5
Study and Exam Preparation [AUTÓNOMA][Self-study]	6
Analysis of articles and reviews [AUTÓNOMA][Self-study]	5
Project or Topic Presentations [PRESENCIAL][Case Studies]	.5
Other off-site activity [AUTÓNOMA][Combination of methods]	1
Progress test [PRESENCIAL][Assessment tests]	1
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	1
Group tutoring sessions [PRESENCIAL][Cooperative / Collaborative Learning]	.5

Unit 4 (de 6): Analytical applications of hybridisations with mass spectrometric detection. Analytical applications of laser-induced fluorescence techniques.

Activities	Hours
Writing of reports or projects [AUTÓNOMA][Self-study]	6
Class Attendance (theory) [PRESENCIAL][Lectures]	4
Study and Exam Preparation [AUTÓNOMA][Self-study]	6
Analysis of articles and reviews [AUTÓNOMA][Self-study]	5

Unit 5 (de 6): Scattering techniques. Optical rotating scattering and diffuse reflectance.

Activities	Hours
Writing of reports or projects [AUTÓNOMA][Self-study]	6
Class Attendance (theory) [PRESENCIAL][Lectures]	5
Study and Exam Preparation [AUTÓNOMA][Self-study]	6
Analysis of articles and reviews [AUTÓNOMA][Self-study]	5
Other off-site activity [AUTÓNOMA][Combination of methods]	1
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	1

Unit 6 (de 6): Electrochemical characterisation techniques by cyclic voltammetry.

Activities	Hours
Writing of reports or projects [AUTÓNOMA][Self-study]	7
Class Attendance (theory) [PRESENCIAL][Lectures]	5
Study and Exam Preparation [AUTÓNOMA][Self-study]	7
Analysis of articles and reviews [AUTÓNOMA][Self-study]	6
Project or Topic Presentations [PRESENCIAL][Case Studies]	1
Other off-site activity [AUTÓNOMA][Combination of methods]	1
Progress test [PRESENCIAL][Assessment tests]	1
Workshops or seminars [PRESENCIAL][Problem solving and exercises]	1
Group tutoring sessions [PRESENCIAL][Cooperative / Collaborative Learning]	1

Global activity

Activities	hours
Analysis of articles and reviews [AUTÓNOMA][Self-study]	32

Workshops or seminars [PRESENCIAL][Problem solving and exercises]	5
Writing of reports or projects [AUTÓNOMA][Self-study]	38
Other off-site activity [AUTÓNOMA][Combination of methods]	4
Project or Topic Presentations [PRESENCIAL][Case Studies]	2
Progress test [PRESENCIAL][Assessment tests]	2
Group tutoring sessions [PRESENCIAL][Cooperative / Collaborative Learning]	2
Class Attendance (theory) [PRESENCIAL][Lectures]	28
Study and Exam Preparation [AUTÓNOMA][Self-study]	37
Total horas:	150

10. Bibliography and Sources

Author(s)	Title/Link	Publishing house	Citv	ISBN	Year	Description
-Orazio Svelto,	Principles of Lasers	Springer			2009	
-Edmond de Hoffmann y Vicent Stroobant	Mass Spectrometry. Principles and Applications	Wiley			2007	
Eric Plum, V. A. Fedotov and Nikolay I. Zheludev	Specular optical activity of achiral metasurfaces				2015	
Watson, J; Sparkman, D.	Introduction to Mass Spectrometry,	Wiley			2007	
-Helmut H. Telle, Angel González Ureña, Robert J. Donovan	Laser Chemistry	Wiley			2007	
Requena Rodríguez, A.	Espectroscopía volume II: Métodos Avanzados.	García Moroto ediciones			2020	
-Gross, J.	Mass Spectrometry: a textbook	Springer			2011	
Laane, Jaan	Frontiers and Advances in Molecular Spectroscopy	Elsevier			2017	