

**COURSE DATA****Data Subject**

<b>Code</b>	44603
<b>Name</b>	Advanced analytical chemistry
<b>Cycle</b>	Master's degree
<b>ECTS Credits</b>	5.0
<b>Academic year</b>	2021 - 2022

**Study (s)**

<b>Degree</b>	<b>Center</b>	<b>Acad. Period</b>
2218 - M.U. en Química	Faculty of Chemistry	1 First term

**Subject-matter**

<b>Degree</b>	<b>Subject-matter</b>	<b>Character</b>
2218 - M.U. en Química	1 - Advanced chemistry	Obligatory

**Coordination**

<b>Name</b>	<b>Department</b>
RUIZ ANGEL, MARIA JOSE	310 - Analytical Chemistry

**SUMMARY**

The course Advanced Analytical Chemistry is part of the Advanced Chemistry subject area. Its main objective is to expand and supplement the knowledge of analytical chemistry acquired in the degree. In particular, the course aims to deepen understanding of the stages of sample preparation and treatment as part of the analytical process, and provides an introduction to assisted systems and microextraction techniques. Among the separation analytical techniques, those based on electrophoresis and related techniques will be covered, as well as the hybridization of chromatographic systems. Vibrational spectroscopy, inductively coupled plasma spectroscopy and X-ray fluorescence spectroscopy will supplement previous knowledge of students on the use of spectroscopy in analytical chemistry. The features and applications of chemical sensors, as well as aspects related to their miniaturization, will be the main topics covered in this course in relation to electroanalytical techniques. Finally, the use of chemometrics in analytical chemistry will be dealt with, and attention will be focused on exploratory data analysis by applying linear discriminant analysis and principal component analysis, and on the use of partial least squares multivariate regression.



Not only the theoretical and methodological aspects of the different techniques will be considered but also their main applications will be covered in order to provide an overview of the different techniques for the students to get a practical and functional perspective through the topics covered.

## PREVIOUS KNOWLEDGE

### Relationship to other subjects of the same degree

There are no specified enrollment restrictions with other subjects of the curriculum.

### Other requirements

Prior knowledge of chemistry is required, at the level taught in the qualifications listed in the recommended profile for admission of candidates to the Masters Degree.

## OUTCOMES

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- Students should apply acquired knowledge to solve problems in unfamiliar contexts within their field of study, including multidisciplinary scenarios.
- Students should be able to integrate knowledge and address the complexity of making informed judgments based on incomplete or limited information, including reflections on the social and ethical responsibilities associated with the application of their knowledge and judgments.
- Students should communicate conclusions and underlying knowledge clearly and unambiguously to both specialized and non-specialized audiences.
- Be able to solve complex chemistry problems, whether in the academic, research or industrial application areas at a specialization or masters-level.
- Promote, in academic and professional contexts in the field of economic policy, ... technological, social or cultural progress within a society based on knowledge and respect for: a) fundamental rights and equal opportunities between men and women, b) the principles of equal opportunities and universal accessibility for people with disabilities and c) the values of a culture of peace and of democratic values.
- Be able to design, perform, analyse and interpret experiences and complex data in the environment of chemistry at a specialization level.
- Acquire advanced knowledge to assess the importance of chemistry in health, the environment, new materials and energy.



## LEARNING OUTCOMES

- Describe the fundamentals and methodology of the main techniques for sample treatment, and explain the effect of the different experimental variables on the outcomes.
- Select, from among the most widely used sample preparation techniques, those that are most appropriate for solving a given analytical problem considering the sample type, the analyte type and concentration and the quality parameters expected from the analysis.
- Design procedures for sample treatment taking into account the quality of the results to be obtained, safety and sustainability criteria.
- Explain the fundamentals of the main advanced analytical separation techniques (chromatographic and related techniques), electroanalytical and spectroscopic techniques, and describe their respective instrumentation.
- Specify the experimental methodology, including the selection of experimental variables, interpret the records obtained in each of the techniques studied, and describe the most relevant applications in each case.
- Select and apply, from among the main chemometric techniques, the most appropriate for the treatment of complex analytical data, and interpret the results obtained.

## DESCRIPTION OF CONTENTS

### 1. Sample preparation and treatment

Representativeness and sampling. Basic operations in sample preparation. Use of assisted systems for sample preparation. Microextraction techniques. New developments.

### 2. Analytical separation techniques

Separation techniques in analytical chemistry. Electrophoresis and related techniques. Hybridization of chromatographic techniques. Applications.

**3. Analytical spectroscopy**

Spectroscopic techniques in analytical chemistry. Vibrational spectroscopy. Inductively coupled plasma spectroscopy: ICP-OES and ICP-MS. X-ray fluorescence. Applications.

**4. Electroanalysis**

Electroanalytical techniques. Electrochemical sensors: general aspects, sensitivity and specificity. Electroanalysis and miniaturization. Applications.

**5. Chemometrics**

Chemometrics in analytical chemistry. Exploratory data analysis: PCA and LDA. Case study of PCA and LDA. Multivariate regression: partial least squares (PLS). Case study.

**WORKLOAD**

ACTIVITY	Hours	% To be attended
Theory classes	35,00	100
Tutorials	5,00	100
Seminars	5,00	100
Computer classroom practice	5,00	100
Study and independent work	75,00	0
<b>TOTAL</b>	<b>125,00</b>	

**TEACHING METHODOLOGY**

The course will be taught through participatory classes, seminars aimed at solving practical problems, and tutorials in which the ability of the students to understand the different topics covered will be evaluated. Additionally, the Aula Virtual platform will be used for communication and information exchange, and the resources in the computer room will be used for conducting practicals in chemometrics.

**EVALUATION****First examination sitting:**

In the first examination sitting, the final mark is calculated from the scores obtained in a final examination and from continuous assessment of coursework, according to the following percentages:



- (a) Final exam: 70%.
- (b) Coursework: 30%.

The score obtained in each part must be at least 4.5 for it to count towards the final mark.

The minimum overall mark to pass the course is 5.0.

### **Second examination sitting:**

In the second examination sitting, the same criteria apply.

## **REFERENCES**

### **Basic**

- Cámara C. (ed.), Fernández P., Martín Esteban A., Pérez-Conde C. i Vidal M. Toma y tratamiento de muestras. Editorial Síntesis, Madrid, 2002
- A. Ríos Castro, M. C. Moreno Bondi, B. M. Simonet Suau (coords.) Técnicas espectroscópicas en química analítica (vol. I y II). Editorial Síntesis, Madrid, 2012
- SKOOG D. A., HOLLER F. J., NIEMAN T. A. Principios de Análisis Instrumental, 5a edició, McGrawHill, Madrid, 2001
- Miller J. C. i J. N. Miller Estadística y Quimiometría para Química Analítica. Pearson Education S. A., Madrid, 2002

### **Additional**

- Mitra (ed) S. Sample preparation techniques in analytical chemistry. John Wiley and Sons. New Jersey, 2003
- Dean. J. R. Methods for environmental trace analysis. John Wiley and Sons. Chichester, 2003
- Luque de Castro M. D. i Luque García J. L. Acceleration and automation of solid sample treatment. Elsevier, Amsterdam, 2002
- Aballe, M.; López Ruiz, J.; Badía, J. M.; Adeva, P. (eds.) Microscopía Electrónica de Barrido y Microanálisis por Rayos X, CSIC i ed. Rueda, Madrid, 1996
- Bonnel, D. A. (ed.) Scanning Probe Microscopy and Spectroscopy: Theory, Techniques and Applications. 2a ed., Wiley, Nueva York, 2001



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- Goldstein, J. L.; Newbury, D. E.; Echlin, P.; Joy, D. C.; Fioril, Ch.; Lifshin, E. Scanning Electron Microscopy and X-Ray Microanalysis. Plenum Press, Nueva York, 1984
- TAYLOR H.E. Inductively Coupled Plasma-Mass Spectrometry. Practices and Techniques. Academic Press, San Diego, 2001
- MONTASER A. Inductively Coupled Plasma Mass Spectrometry. Wiley-VCH, New York, 1997
- Massart D. L., B. G. M. Vandeginste, L. M. C. Buydens, S. De Jong, P. J. Lewi i J. Smeyers-Verbeke, Handbook of Chemometrics and Qualimetrics: part A i B, Elsevier, Amsterdam, 1997
- Sagrado S., E. Bonet, M. J. Medina i Y. Martín. Manual Práctico de Calidad en los Laboratorios. Enfoque ISO 17025. AENOR 2005

## ADDENDUM COVID-19

**This addendum will only be activated if the health situation requires so and with the prior agreement of the Governing Council**

### Contents

*The contents initially indicated in the teaching guide are maintained.*

### Workload and temporary teaching planning

Regarding the workload:

*The different activities described in the Teaching Guide are maintained but the hours of dedication to each activity are changed, as shown in the following table:*

ACTIVITY	Hours	% To be attended
Theory classes	35.00	70-100
Tutorials	5.00	70-100
Seminars	5.00	70-100



Computer classroom practice	5.00	70-100
Study and independent work	75.00	0
<b>TOTAL</b>	<b>125.00</b>	

Regarding the temporary teaching planning:

*The material to follow the theory/tutoring/classroom-seminar classes allows to continue the temporary teaching planning both in days and schedule, whether the teaching is face-to-face in the classroom or not.*

### Teaching Methodology

*Theory courses:* Theory classes and classroom tutoring will tend to the maximum possible face-to-face teaching, always respecting the health restrictions that limit the capacity of the classrooms to 50% of their usual occupation. Depending on the capacity of the classroom and the number of students enrolled, some of the students may need to follow the classes synchronously in an auxiliary classroom. If this situation arises, students will attend the main classroom or auxiliary classroom for weekly rotary shifts (preferably in alphabetical order). However, the rotation system will be fixed once the actual enrollment data is known, guaranteeing, in any case, that the percentage of face-to-face teaching of all students enrolled in the subject is the same.

*Computer-classroom courses:* The occupation of computer classrooms will be 50% compared to the usual occupation. If the number of students enrolled exceeds the capacity of 50% of the classroom, students will attend the face-to-face course in weekly rotating shifts (preferably in alphabetical order). However, the rotation system will be fixed once the actual enrollment data is known, guaranteeing, in any case, that the percentage of face-to-face teaching of all students enrolled in the subject is the same.

The methodology used for non-face-to-face classes shall be:

1. Synchronously using virtual classroom tools (Teams, Blackboard ...)
2. Asynchronously using locut power-point presentations or other virtual classroom tools
3. Resolution of exercises and questionnaires

*If there is a closure of the facilities for health reasons that totally or partially affects the classes of the course, they will be replaced by non-face-to-face sessions following the established schedules and using the tools of the virtual classroom.*



## **Evaluation**

*The evaluation system described in the Teaching Guide of the subject in which the various evaluable activities have been specified as well as their contribution to the final grade of the subject is maintained.*

*If there is a closure of the facilities for health reasons affecting the development of any face-to-face evaluable activity of the subject, it will be replaced by a test of a similar nature that will be carried out in virtual mode using the computer tools licensed by the University of Valencia. The contribution of each evaluable activity to the final grade of the subject will remain unchanged, as set out in this guide.*

## **References**

*The literature recommended in the Teaching Guide is maintained since it is accessible, and it is complemented by notes, slides and problems uploaded to the Virtual Classroom as material of the course.*