

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

<b>Code</b>	34230
<b>Name</b>	Analytical Chemistry III
<b>Cycle</b>	Grade
<b>ECTS Credits</b>	6.0
<b>Academic year</b>	2023 - 2024

**Study (s)**

<b>Degree</b>	<b>Center</b>	<b>Acad. year</b>	<b>Period</b>
1110 - Degree in Chemistry	Faculty of Chemistry	3	First term
1929 - D.D. in Physics-Chemistry	Double Degree Program Physics and Chemistry	4	First term

**Subject-matter**

<b>Degree</b>	<b>Subject-matter</b>	<b>Character</b>
1110 - Degree in Chemistry	6 - Analytical Chemistry	Obligatory
1929 - D.D. in Physics-Chemistry	4 - Cuarto Curso (Obligatorio)	Obligatory

**Coordination**

<b>Name</b>	<b>Department</b>
CAMPINS FALCO, PILAR	310 - Analytical Chemistry

**SUMMARY**

On this course students complete their overview of the various types of instrumental analytical techniques by analysing separation and coupled techniques. The course provides students with a solid foundation for selecting analytical methods using the techniques they have studied both in previous academic years and in this one and for addressing univariate, bivariate and multivariate data processing with the most common statistical techniques and the independence and critical spirit that is afforded by satisfactory knowledge of the fundamentals of this sub-discipline.



## PREVIOUS KNOWLEDGE

### Relationship to other subjects of the same degree

1108 - Degree in Chemistry V1-2009 :

1110 - Degree in Chemistry V2-2018 :

1929 - Double Degree in Physics and Chemistry :

1934 - Programa de doble Grado Química-Ingeniería Química\_2023 :

### R4-OBLIGATION TO HAVE SUCCESSFULLY COMPLETED THE COURSE

34183 - General Chemistry I

34184 - General Chemistry II

34183 - General Chemistry I

34184 - General Chemistry II

34183 - General Chemistry I

34184 - General Chemistry II

34183 - General Chemistry I

34184 - General Chemistry II

### Other requirements

To successfully complete this course, students should have acquired knowledge from previous courses. In particular, they should have a basic understanding of the analytic process and analytical chemistry as well as knowledge of the chemistry of solutions, spectroscopic techniques, univariate data management (calibration), and significant features of the analytical methods.

## OUTCOMES

### 1110 - Degree in Chemistry

- Develop capacity for analysis, synthesis and critical thinking.
- Demonstrate leadership and management skills, entrepreneurship, initiative, creativity, organization, planning, control, leadership, decision making and negotiation.
- Solve problems effectively.
- Demonstrate ability to work in teams both in interdisciplinary teams and in an international context.
- Demonstrate ability to communicate information, ideas, problems and solutions to both specialist and non-specialist audiences and using information technology, as appropriate.



- Demonstrate a commitment to ethics, equality values and social responsibility as a citizen and as a professional.
- Learn autonomously.
- Acquire a permanent sensitivity to quality, the environment, sustainable development and the prevention of occupational hazards.
- Demonstrate knowledge of the main aspects of chemical terminology, nomenclature, conventions and units.
- Interpret the variation of the characteristic properties of chemical elements according to the periodic table.
- Demonstrate knowledge of the main types of chemical reaction and their main characteristics.
- Demonstrate knowledge of the principles of thermodynamics and kinetics and their applications in chemistry.
- Demonstrate knowledge of the principles, procedures and techniques for the determination, separation, identification and characterisation of chemical compounds.
- Show knowledge of the metrology of chemical processes including quality management.
- Demonstrate knowledge and understanding of essential facts, concepts, principles and theories related to the areas of chemistry.
- Solve qualitative and quantitative problems following previously developed models.
- Recognise and analyse new problems and plan strategies to solve them.
- Evaluate, interpret and synthesise chemical data and information.
- Handle chemicals safely.
- Handle the instrumentation used in the different areas of chemistry.
- Interpret data from observations and measurements in the laboratory in terms of their significance and the theories that underpin them.
- Evaluate the risks in the use of chemicals and laboratory procedures.
- Relate theory and experimentation.
- Recognise and evaluate chemical processes in daily life.
- Understand the qualitative and quantitative aspects of chemical problems.
- Develop sustainable and environmentally friendly methods.
- Relate chemistry with other disciplines.
- Students must be able to apply their knowledge to their work or vocation in a professional manner and have acquired the competences required for the preparation and defence of arguments and for problem solving in their field of study.
- Students must have the ability to gather and interpret relevant data (usually in their field of study) to make judgements that take relevant social, scientific or ethical issues into consideration.



- Students must be able to communicate information, ideas, problems and solutions to both expert and lay audiences.
- Students must have developed the learning skills needed to undertake further study with a high degree of autonomy.
- Express oneself correctly, both orally and in writing, in any of the official languages of the Valencian Community.
- Have basic skills in the use of information and communication technology and properly manage the information obtained.

## LEARNING OUTCOMES

The previous section includes the competences contained in the document VERIFICA. This subject addresses part of the learning results of the matter Analytical Chemistry that allow to acquire specific knowledge of chemistry, cognitive skills and general skills recommended by the EUROPEAN CHEMISTRY THEMATIC NETWORK (ECTN) for the Chemistry Eurobachelor® Label. The following table lists the learning outcomes acquired in the subject Analytical Chemistry III related to the competences of the degree in Chemistry.

SPECIFIC KNOWLEDGE OF CHEMISTRY	
The learning process should allow the degree graduates to demonstrate:	
	Competences of the subject Analytical Chemistry III that contemplate the learning outcomes EUROBACHELOR®
The principles and procedures used in chemical analysis and the characterisation of chemical compounds.	<p>Demonstrate knowledge of the principles, procedures and techniques for the determination, separation, identification and characterisation of chemical compounds.(CE8)</p> <p>Show knowledge of the metrology of chemical processes including quality management..(CE10)</p> <p>Handle the instrumentation used in the different areas of chemistry.(CE19).</p> <p>Understand the qualitative and quantitative aspects of chemical problems..(CE24).</p> <p>Develop sustainable and environmentally</p>



	friendly methods.(CE25)
<b>COMPETENCES AND COGNITIVE SKILLS</b>	
<b>The learning process should allow the degree graduates to demonstrate:</b>	
	<b>Competences of the subject Analytical Chemistry III that contemplate the learning outcomes EUROBACHELOR®</b>
Ability to demonstrate knowledge and understanding of the facts, concepts, principles and fundamental theories related to the topics mentioned above.	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories related to the areas of chemistry..(CE13).
Ability to apply this knowledge and understanding to the solution of common qualitative and quantitative problems.	Solve qualitative and quantitative problems following previously developed models..(CE14). Recognise and analyse new problems and plan strategies to solve them..(CE15). Understand the qualitative and quantitative aspects of chemical problems..(CE24).
Competences for the evaluation, interpretation and synthesis of information and chemical data.	Evaluate, interpret and synthesise chemical data and information..(CE16). Interpret data from observations and measurements in the laboratory in terms of their significance and the theories that underpin them..(CE20).
Competences to present and argue scientific issues orally and in writing to a specialized audience.	Relate chemistry with other disciplines.(CE26). Prepare reports, surveys and industrial and environmental projects in the field of chemistry..(CE27). Demonstrate ability to communicate information, ideas, problems and solutions to





	<p>both specialist and non-specialist audiences and using information technology, as appropriate. (CG6).</p> <p>Students must be able to communicate information, ideas, problems and solutions to both expert and lay audiences..(CB4).</p>
Ability to calculate and process data, related to information and chemistry data.	<p>Solve qualitative and quantitative problems following previously developed models..(CE14).</p> <p>Recognise and analyse new problems and plan strategies to solve them..(CE15).</p>
<b>COMPETENCES AND COGNITIVE SKILLS RELATED TO THE PRACTICE OF CHEMISTRY</b>	
<b>The learning process should allow the degree graduates to demonstrate:</b>	
	<b>Competences of the subject Analytical Chemistry III that contemplate the learning outcomes EUROBACHELOR®</b>
Ability to interpret data derived from observations and laboratory measurements in terms of their relevance, and relate them to the appropriate theory.	<p>Interpret data from observations and measurements in the laboratory in terms of their significance and the theories that underpin them..(CE20).</p> <p>Relate theory and experimentation..(CE22).</p> <p>Recognise and evaluate chemical processes in daily life..(CE23).</p> <p>Understand the qualitative and quantitative aspects of chemical problems..(CE24).</p> <p>Relate chemistry with other disciplines..(CE26).</p>
<b>GENERAL COMPETENCES</b>	
<b>The learning process should allow the degree graduates to demonstrate:</b>	



	<b>Competences of the subject Analytical Chemistry III that contemplate the learning outcomes EUROBACHELOR®</b>
Ability to apply practical knowledge to solve problems related to qualitative and quantitative information.	<p>Solve problems effectively..(CG4).</p> <p>Solve qualitative and quantitative problems following previously developed models..(CE14).</p> <p>Relate theory and experimentation..(CE22).</p> <p>Recognise and evaluate chemical processes in daily life..(CE23).</p> <p>Understand the qualitative and quantitative aspects of chemical problems..(CE24).</p>
Competences in information management, in relation to primary and secondary sources, including information retrieval through on-line searches.	<p>Demonstrate ability to communicate information, ideas, problems and solutions to both specialist and non-specialist audiences and using information technology, as appropriate..(CG6).</p> <p>Have basic skills in the use of information and communication technology and properly manage the information obtained.(CT2).</p>
Ethical commitment to the European Code of Conduct:	<p>Acquire a permanent sensitivity to quality, the environment, sustainable development and the prevention of occupational hazards.(CG10).</p> <p>Demonstrate a commitment to ethics, equality values and social responsibility as a citizen and as a professional. (CG7).</p> <p>Students must have the ability to gather and interpret relevant data (usually in their field of study) to make judgements that take relevant social, scientific or ethical issues into consideration. (CB3).</p>

[http://ec.europa.eu/research/participants/data/ref/h2020/other/hi/h2020-ethics\\_code-of-conduct\\_en.pdf](http://ec.europa.eu/research/participants/data/ref/h2020/other/hi/h2020-ethics_code-of-conduct_en.pdf)



These learning outcomes should ensure that on successful completion of Analytical Chemistry III students will be able to:

- Identify the basic criteria for choosing an instrumental analytical technique, or separation technique in this case, including selecting the working and detection conditions.
- Describe and interpret the experimental method to follow for the analysis using the analytical techniques studied.
- Identify the most common types of interference with the analytical techniques studied as well as the procedures for correcting them.
  - Provide representative examples of the applications of the analytical techniques studied.
- Given a specific example of an application or a published article on an analytical method applied to a specific sample, justify its use, discuss its analytical characteristics, reasonably explain the steps to follow, and indicate how to perform the calculations.
- Perform the calculations needed to solve analytical problems using the analytical techniques studied, correctly expressing the results and explaining the conclusions drawn.
- Treat the data using univariate, bivariate and multivariate statistical techniques, expressing the results graphically and numerically and interpreting them correctly.
- Demonstrate an ethical and responsible conduct in the exercise of their professional work, values that are transmitted by teachers and researchers of the University, as a generator and transmitter of scientific knowledge.

Regarding the Sustainable Development Goals (SDGs), it is expected that students will be able to know in this subject how to apply the knowledge learned to guarantee an inclusive, equitable, and quality education and promote learning opportunities for everyone (SDG 4), to acquire a special sensitivity for sustainable management of water (SDG 6), raw materials and energy sources (SDG 7), as well as for an environmentally friendly and sustainable development (SDGs 11, 12, 13, 14 and 15), in addition to being able to design, select and/or develop efficient chemical products, processes and/or analytical methodologies (SDG 7) that minimize their impact on the environment (SDGs 14 and 15), using alternative raw materials and reducing wastes (SDG 11).

## DESCRIPTION OF CONTENTS

### 1. Non-chromatographic separation techniques

Concept of analytical separation and classification of separation techniques. Liquid-liquid extraction. Liquid-solid extraction. Solid-liquid extraction. Gas-solid extraction. Miniaturized techniques. Active and passive samplers.

### 2. Chromatographic techniques

Concept of chromatography and classification of chromatographic techniques. Chromatography theories. Fundamental parameters in zonal elution chromatography. General characteristics of the detectors used in chromatography. Qualitative and quantitative methods.





### **3. Gas Chromatography**

Gas chromatograph schematic. Field of application, common derivatizations in GC. Injection of the sample with/without division and directly in the column. PTV injectors. usual stationary phases. Column types. Common detectors in CG. Qualitative and quantitative applications.

### **4. High-Performance Liquid Chromatography**

HPLC chromatograph. Scope. Injection systems. Pumping systems. Columns: types and selection criteria. Detectors in liquid chromatography. Partition liquid chromatography. Ion chromatography. Capillary electrophoresis.

### **5. Mass spectrometry. Coupled techniques.**

Basic components of a mass spectrometer. Sample introduction systems. Ionization sources. Analyzers. Detectors. Work modes and data characteristics. GC-MS, HPLC-MS, ICP-MS hybridization: instrumentation, common interfaces, acquisition modes and field of application.

### **6. Multivariate chemometrics.**

Objects and variables. Types of variables. The object-variable matrix and its transpose. Data preprocessing. Variance-covariance matrix. Matrix of correlations. Classification of multivariable chemometric techniques.

### **7. Unsupervised and supervised analysis techniques.**

Cluster analysis. Principal component analysis (PCA). Discriminant analysis. Classification techniques using non-parametric methods. Smooth modeling technique independent of class analogies (SIMCA).

### **8. Experimental design and multivariate optimization.**

Objectives and terminology in experimental design and multivariate optimization. sweeping designs. Evaluation of the importance of the factors and their interaction. Designs for calculating response surface. Interpretive optimization. Sequential optimization.

**WORKLOAD**

ACTIVITY	Hours	% To be attended
Theory classes	51,00	100
Tutorials	9,00	100
Development of group work	13,00	0
Development of individual work	7,00	0
Study and independent work	18,00	0
Readings supplementary material	6,00	0
Preparation of evaluation activities	21,00	0
Preparing lectures	8,00	0
Preparation of practical classes and problem	8,00	0
Resolution of case studies	9,00	0
<b>TOTAL</b>	<b>150,00</b>	

**TEACHING METHODOLOGY**

This course consists of:

- Whole-group lectures

Lectures will be combined with cooperative learning models. The instructor will provide an overview of the topic under study, explain the key concepts, and answer any questions that arise. To help students meet the learning objectives, activities to promote cooperative learning and student participation will be introduced. To encourage individual study and in-depth preparation of the topics, basic and complementary bibliographies will be provided.

The practical problem-solving sessions will apply the theoretical knowledge acquired. The lecturer will provide problem-type examples and present the information the students will need for learning to identify the essential features of the approach and the techniques needed to solve the problems.

- Tutorials with each subgroup

The lecturer will guide the student on all elements of the learning process regarding both general approaches and specific issues. In class students will solve problems, tackle other issues and conduct other work proposed by the lecturer. A selection of these activities will be corrected or presented. The lecturer will also provide other problems and issues for students to work on at home before correcting them in class.

Seminars and Conference



Seminars and Conference will focus on complementary aspects of their training in Analytical Chemistry. For this task, students attending the event and answer a questionnaire prepared by the instructor.

## EVALUATION

Learning will be evaluated by taking into account all aspects outlined in the Methodology section of this course guide. Attendance and reply to a Seminar-Conference will be equivalent to a tutorial. The student activities are not recoverable. Students may submit a request in writing to be evaluated only by examination.

### FIRST CALL

Final examination (70%) + student activities (30%)

The score on each of these two parts must be at least 4.5 in order to apply the average.

The minimum overall grade to pass the course is 5.0.

### SECOND CALL

In the second call the final grade is obtained by applying the same criteria as in the first call.

### Final warning

Copying or plagiarism of any assignment that is part of the evaluation will make it impossible to pass the course, and the student will be subject to the appropriate disciplinary procedures.

Please note that, according to Article 13 d) of the University Student Statute (RD 1791/2010, December 30), *"it is the duty of a student to refrain from using or cooperating in fraudulent procedures in evaluation tests, in the work performed or in official University documents"*.

## REFERENCES

### Basic

- SKOOG, D.A.; HOLLER, F.J. Y NIEMAN, T.A. Principios de Análisis Instrumental, 5ª Edición. Madrid: McGraw-Hill, 2001. ISBN 8448127757
- HARVEY, D. Química Analítica moderna. Madrid: McGraw-Hill, 2002. ISBN 9788448136352
- HARRIS, D.C. Análisis Químico Cuantitativo, 3ª Edición. Barcelona: Reverté, 2007. ISBN 9788429172249
- SKOOG, D.A.; WEST, D.M.; HOLLER, F.J. Y CROUCH, S.R. Fundamentos de Química Analítica, 8ª edición. Madrid: Thomson-Paraninfo, 2005. ISBN: 9788497323338



- MILLER, J.N. Y MILLER, J.C. Estadística y Quimiometría para Química Analítica. Madrid: Prentice Hall, Pearson Educación, 2002. ISBN 8420535141
- KELLNER, R.; MERMET, J.M.; OTTO, M.; VALCÁRCEL, M. Y WIDMER, H.M. Analytical Chemistry: a modern approach to analytical science, 2ª edición. Winheim: Wiley-VCH, 2004. ISBN 3527305904
- RAMIS, G. Y GARCÍA ALVAREZ-COQUE, M.C. Quimiometria. Madrid: Síntesis, 2001. ISBN 8477389047