

| Data Subject               |                          |                                  |              |
|----------------------------|--------------------------|----------------------------------|--------------|
| Code                       | 34230                    |                                  |              |
| Name                       | Analytical Chemistry III |                                  |              |
| Cycle                      | Grade                    |                                  |              |
| ECTS Credits               | 6.0                      |                                  |              |
| Academic year              | 2021 - 2022              |                                  |              |
| Study (s)                  |                          |                                  |              |
| Degree                     | . /                      | Center                           | Acad. Period |
|                            |                          |                                  | year         |
| 1110 - Degree in Chemistry |                          | Faculty of Chemistry 3 First ter |              |
| Subject-matter             |                          |                                  |              |
| Degree                     | 485 384                  | Subject-matter                   | Character    |
| 1110 - Degree in Chemistry |                          | 6 - Analytical Chemistry         | Obligatory   |
| Coordination               |                          |                                  |              |
| Name                       |                          | Department                       |              |
| CHISVERT SANIA, ALBERTO    |                          | 310 - Analytical Chemistry       |              |
|                            |                          |                                  |              |

## SUMMARY

On this course students complete their overview of the various types of instrumental analytical techniques by analysing electro-analytical, 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



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### 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.



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- 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.



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- 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.

| The learning process should al   | low the degree graduates to demonstrate:   |
|--|--|
| RA<br>I  | Competences of the subject Analytical<br>Chemistry III that contemplate the learning<br>outcomes EUROBACHELOR®   |
|  | Demonstrate knowledge of the principles,<br>procedures and techniques for the determination,<br>separation, identification and characterisation of<br>chemical compounds.(CE8) |
| The principles and procedures<br>used in chemical analysis and<br>the characterisation of chemical<br>compounds. | Show knowledge of the metrology of chemical processes including quality management(CE10)   |
|  | Handle the instrumentation used in the different areas of chemistry.(CE19).  |
|  | Understand the qualitative and quantitative aspects of chemical problems(CE24).  |
|  | Develop sustainable and environmentally friendly methods.(CE25)  |



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|  | Competences of the subject Analytical<br>Chemistry III that contemplate the learning<br>outcomes EUROBACHELOR®  |
|--|---|
| Ability to demonstrate<br>knowledge and understanding<br>of the facts, concepts, principles<br>and fundamental theories<br>related to the topics mentioned<br>above. | Demonstrate knowledge and understanding of<br>essential facts, concepts, principles and theories<br>related to the areas of chemistry(CE13).  |
| Ability to apply this knowledge<br>and understanding to the<br>solution of common qualitative<br>and quantitative problems.  | Solve qualitative and quantitative problems<br>following previously developed models(CE14)<br>Recognise and analyse new problems and plan<br>strategies to solve them(CE15).<br>Understand the qualitative and quantitative<br>aspects of chemical problems(CE24).  |
| Competences for the evaluation,<br>interpretation and synthesis of<br>information and chemical data.   | Evaluate, interpret and synthesise chemical data<br>and information(CE16).<br>Interpret data from observations and<br>measurements in the laboratory in terms of their<br>significance and the theories that underpin<br>them(CE20).  |
| Competences to present and<br>argue scientific issues orally<br>and in writing to a specialized<br>audience.   | Relate chemistry with other disciplines.(CE26).<br>Prepare reports, surveys and industrial and<br>environmental projects in the field of<br>chemistry(CE27).<br>Demonstrate ability to communicate<br>information, ideas, problems and solutions to<br>both specialist and non-specialist audiences and<br>using information technology, as appropriate.<br>(CG6).<br>Students must be able to communicate<br>information, ideas, problems and solutions to |



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|   | both expert and lay audiences(CB4).   |
|---|---|
| Ability to calculate and process<br>data, related to information and<br>chemistry data.       | Solve qualitative and quantitative problems<br>following previously developed models(CE14).<br>Recognise and analyse new problems and plan<br>strategies to solve them(CE15). |
| COMPETENCES AND COG<br>PRACTICE OF CHEMISTRY  | NITIVE SKILLS RELATED TO THE<br>Y   |
| The learning process should al  | llow the degree graduates to demonstrate:   |
| REY BE  | Competences of the subject Analytical<br>Chemistry III that contemplate the learning<br>outcomes EUROBACHELOR®  |
| Ability to interpret data derived   | Interpret data from observations and<br>measurements in the laboratory in terms of their<br>significance and the theories that underpin<br>them(CE20).                        |
| from observations and   | Relate theory and experimentation(CE22).  |
| laboratory measurements in<br>terms of their relevance, and<br>relate them to the appropriate | Recognise and evaluate chemical processes in daily life(CE23).  |
| theory.   | Understand the qualitative and quantitative aspects of chemical problems(CE24).   |
|   | Relate chemistry with other disciplines.(CE26).   |
| GENERAL COMPETENCES   | VVNIDAJ   |
| The learning process should al  | llow the degree graduates to demonstrate:   |
|   | Competences of the subject Analytical<br>Chemistry III that contemplate the learning<br>outcomes EUROBACHELOR®  |



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

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:



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- 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.

### **DESCRIPTION OF CONTENTS**

### **1. Introduction to Electroanalytical Methods**

Electrochemical cells. Potentials of cell and electrode. Electrode reactions. Polarization. Transport mechanisms. Thermodynamic and kinetic aspects. Reversibility. Classification of electroanalytical methods.

### 2. Potentiometry

Reference electrodes. Types of Indicator electrodes. Potential. Membrane electrodes. Direct potentiometric measurements. pH measurement. Measuring cell. Selective electrodes. Calibration. Potentiometric titrations.

### 3. Voltamperometry

Working electrodes. Basic instrumentation. Classification of voltammetric methods. Qualitative and quantitative aspects. Polarography. The polarographic wave, the diffusion current, the Ilkovic equation. Limitations. Pulse voltammetry. Parameters. Advantages. Stripping voltammetry. Classification. Stages. Comparison of voltammetric methods. Amperometric titrations.



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### 4. Introduction to Separation Techniques

Concept of analytical separation and classification of separation techniques. Liquid-liquid extraction. Characteristics of common solvents. Theory of liquid-liquid extraction: partition constant, capacity factor and distribution ratio. Numerical problems of extraction. Solid-phase extraction: concept and classification (liquid-solid, solid-solid and gas-solid). SPE as a preconcentration technique. Bonded phases. Common phases and phase distribution in normal, reverse and HILIC. Common phases in ion exchange and retention.

### 5. Analytical Separation Techniques

The concept of chromatography and the classification of chromatographic techniques. Elution modes. The main parameters in zonal elution chromatography: geometric, operational, and characteristic of the solutes. Introduction to two theories of chromatography. Equilibrium theory, the Craig machine. The concept of HETP. Dynamic theory and the rate equation. Experimental measurement of efficiency. Resolution and the selectivity factor. The relationship between resolution and retention. General characteristics of the detectors used in chromatography: measuring the LOD from background noise. Linear dynamic range, limits, qualitative and quantitative variables. Quantitative methods.

### 6. Gas Chromatography

Introduction and outline of the gas chromatograph. Scope and derivatizations common in GC. Sample injection with and without direct derivation and on-column injection. PTV injectors. Common stationary phases. Properties. Types of columns. Capillary columns. Selection criteria. Flame ionization detector (FID). Flame photometric detector. NPD detectors and PSD. Electron capture detector. Elution temperature. Identification in gas chromatography.

### 7. High-Performance Liquid Chromatography

HPLC chromatograph. The manual injector and the automatic injector. Dual piston pump. Mixture modules at low and high pressures. Features. Columns: types and selection criteria. Detectors in liquid chromatography. Classification. Spectrophotometric detection. Classification of liquid chromatography according to the retention mechanism. Selecting the mobile and stationary phases (I): controlling the eluotropic strength. Selecting the mobile and stationary phases (II): controlling selectivity. Isocratic and gradient elution. Ion exchange equilibrium: selectivity coefficients. Conductivity detection. Indirect photometric detection. Selectivity of the response. Anionic suppression.

### 8. GC-MS and HPLC-MS Hybridization

Basic components of mass detectors. Sample-introduction systems. Ionization sources. Analysers. Detectors. Working modes and characteristics of the data. GC-MS hybridization. HPLC-MS hybridization. Common interfaces and scope.



### 9. Introduction to Chemometrics and Multivariate Exploratory Data Analysis

Objects and variables. Types of variables. The object-variable matrix and its transpose. Pre-processed data. The variance-covariance matrix. The correlation matrix. Classification of multivariate chemometric techniques. Cluster analysis. Principal component analysis (PCA).

## 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                 |
| ΤΟΤΑ   | L 150,00 | . III <b>2</b> 78 |

## **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.

### REFERENCES

#### **Basic**

- SKOOG, D.A.; HOLLER, F.J. Y NIEMAN, T.A. Principios de Análisis Instrumental, 5<sup>a</sup> Edición. Madrid: McGraw-Hill, 2001. ISBN 8448127757
- HARVEY, D. Química Analítica moderna. Madrid: McGraw-Hill, 2002.ISBN 9788448136352
- HARRIS, D.C. Análisis Químico Cuantitativo, 3<sup>a</sup> Edición. Barcelona: Reverté, 2007. ISBN 9788429172249
- SKOOG, D.A.; WEST, D.M.; HOLLER, F.J. Y CROUCH, S.R. Fundamentos de Química Analítica, 8<sup>a</sup> 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, 2<sup>a</sup> edición. Winheim: Wiley-VCH, 2004. ISBN 3527305904



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- RAMIS, G. Y GARCÍA ALVAREZ-COQUE, M.C. Quimiometria. Madrid: Síntesis, 2001. ISBN 8477389047

## 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 with the intended dedication.

### 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**

<u>Theory courses</u>: 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.

### According to the teacher's criteria, the tools will be used based on the following considerations:

The installed cameras and the hardware and software will allow you to have a set of tools that, in addition to the filming of the teacher, will also allow other options with retransmission of what is being projected from the computer or presenting through a tablet- "electronic whiteboard", being at the discretion of the teachers of the use of any of the tools at their disposal that allow the monitoring of the class synchronously by the students in an auxiliary classroom. The follow-up of the classes will realize of synchronous form in auxiliary classrooms not contemplating the option to do them through external links



to the University of Valencia, unless it has the express authorization of the professor affected. Under no circumstances will the images and / or sound transmitted synchronously be recorded.

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

1. 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

(Indicate the option applicable to the subject)

- 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.

