UNIVERSIDADE DA CORUÑA

Teaching Guide			
Identifying Data			2016/17
Subject (*)	Química Analítica Avanzada e Quimiometría	Code	610G01015
Study programme	Grao en Química		

Descriptors				
Cycle	Period	Year	Type	Credits
Graduate	1st four-month period	Fourth	Obligatoria	6

Language	SpanishEnglish		
Teaching method	Face-to-face		
Prerequisites			
Department	Química Analítica		
Coordinador	Lopez Mahia, Purificacion	E-mail	purificacion.lopez.mahia@udc.es
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Web	http://campusvirtual.udc.es		
General description	This subject deals with quantifying substances in different types of samples at trace levels. The most common methodologies will be presented, along with their usual problems, difficulties and limitations when applying them. Major emphasis will be placed on how to plan and execute the different stages of the so-called ?analytical process?. Options to automate several working steps will be discussed. Finally, some basic tools to treat the final data sets will be studied. This is termed chemometrics and it deals with experimental design and optimization of an analytical procedure, calibration and multivariate analyses of the data (including data mining).		

Study programme competences / results	
Code	Study programme competences / results
A14	Ability to demonstrate knowledge and understanding of concepts, principles and theories in chemistry
A15	Ability to recognise and analyse new problems and develop solution strategies
A16	Ability to source, assess and apply technical bibliographical information and data relating to chemistry
A17	Ability to work safely in a chemistry laboratory (handling of materials, disposal of waste)
A19	Ability to follow standard procedures and handle scientific equipment
A20	Ability to interpret data resulting from laboratory observation and measurement
A21	Understanding of qualitative and quantitative aspects of chemical problems
A22	Ability to plan, design and develop projects and experiments
A23	Critical standards of excellence in experimental technique and analysis
A26	Ability to follow standard laboratory procedures in relation to analysis and synthesis of organic and inorganic systems
B2	Effective problem solving
B3	Application of logical, critical, creative thinking
B4	Working independently on own initiative
B5	Teamwork and collaboration
C2	Oral and written proficiency in a foreign language
C3	Ability to use basic information and communications technology (ICT) tools for professional purposes and learning throughout life
C4	Self-development as an open, educated, critical, engaged, democratic, socially responsible citizen, equipped to analyse reality, diagnose problems, and formulate and implement informed solutions for the common good
C6	Ability to assess critically the knowledge, technology and information available for problem solving
C8	Understanding role of research, innovation and technology in socio-economic and cultural development

Learning outcomes

Learning outcomes	Study programme competences / results		
To know how to select the proper analytical methodology for each particular problem.	A15 A16 A20 A22 A26	B3	C4 C6 C8
To know how to plan and execute the different stages of the analytical procedure to quantify analytes at trace levels, including the interpretation of the data.	A14 A17 A19 A20 A21 A23	B2 B4	C3
To know the main objectives of the most common chemometric techniques and to know their main application fields. To know how to extract relevant information from a multivariate study, in particular of a simplified environmental problem.	A14 A15 A16 A20 A26	B2 B4 B5	C2 C3 C4 C6

Contents	
Topic	Sub-topic
Chapter 1: Introducing trace analysis	Importance of quantifying substances at trace levels. The analytical process when determining trace amounts: special requirements. Basic requisites and importance of sampling. Sources of errors when storing and treating samples. Quality assurance in trace analyses.
Chapter 2: Analyzing inorganic substances	Introduction. Decomposition and dissolution of inorganic matrices. Separation and preconcentration. Speciation of some relevant chemical elements. Examples of analytical applications.
Chapter 3: Analyzing organic substances	Introduction. Extraction methods for solid and liquid samples. Purification, fractionation and concentration of organic extracts. Examples of analytical applications.
Chapter 4: Automation in the analytical laboratory	Objectives of laboratory automation. Pros and cons. Classification of the automated analytical systems. Robotics. Miniaturization. Analysis of industrial processes.
Chapter 5: Introducing chemometrics	Defining chemometrics and its role in the analytical process. Concept of uncertainty and basic calculations.
Chapter 6: Statistical inference and univariate calibration	Most common inference statistical tests in laboratories. Analysis of Variance. Examples of applications in laboratories and industrial process control. Classical calibration by the least squares fit. Validation. Confidence intervals.
Chapter 7: Experimental design and optimization	Basic ideas of experimental design and optimization. Factorial designs, fractional factorial designs, Plackett-Burman designs, response surfaces. Sequential optimization by Simplex.
Chapter 8: Multivariate data analyses	Introduction. Classification of the most common pattern recognition methods. Unsupervised methods: principal components analysis, clustering. Supervised methods: SIMCA, k-nearest neighbours.
Laboratory	Pupils will apply the theoretical concepts studied throughout the theoretical lessons. Laboratory problems will deal with real problems in the environmental, industrial or foodstuff fields (among others) that pupils have to solve.

Planning

Methodologies / tests	Competencies / Results	Teaching hours (in-person & virtual)	Student?s personal work hours	Total hours
Laboratory practice	A15 A16 A17 A19 A20 A21 A22 A23 A26 B3 B4 B5	20	30	50
Seminar	A15 A16 A20 A21 B2 B3 B4 C3	6	12	18
Workbook	C4 C6 C8	1	2.5	3.5
Guest lecture / keynote speech	A15 A16 A21 A22 C4	21	52.5	73.5
Mixed objective/subjective test	A14 A15 C2	3	0	3
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
Laboratory practice	They will consist on the determination of some analytes at trace levels in samples gathered from real problems (environmental samples, foodstuff, clinic mixtures, etc.). The practices emulate a comprehensive problem: from sampling to sample treatment, separation of the analyte, measurement and data interpretation. The student must deliver a laboratory notebook. In addition to laboratory practices where analytical instrumentation will be handled by students, other practices will be carried out on computers to study the chemometric concepts (mainly, the multivariate data analyses techniques). At the end of the laboratory work the student will deliver a report of the work done with a critical and detailed analysis.
Seminar	They are intended to reinforce the understanding of several concepts given at the theoretical lessons. Numerical exercises will be solved by the students. A comparison of the results generated in the laboratory practices will be made with other values gathered from other students. From the discussions, common sources of errors will be visualized. The student should perceive the difficulties inherent to the analyses of trace amounts of substances. Studies will be also made using computers to discuss a real multivariate dataset derived from environmental studies.
Workbook	Some specific, short readings will be proposed by the teacher. These will consist of reports where from the students will deliver a small report explaining some key ideas (e.g., a summary of the analytical strategy undertaken to solve the problem).
Guest lecture / keynote speech	The teacher will develop and explain the basic contents of each chapter. Some documents will be delivered to the students before the classes and they should have been reviewed before attending them. Audiovisual media will be employed throughout. Open dialogue will be empowered sometimes to solve doubts and improve the understanding of some basic issues.
Mixed objective/subjective test	Written test to be held in the official call on January / July, in which the degree of learning and the acquisition of skills by the student is evaluated. It will consist of theoretical questions and applied questions, problem solving and practical content. The completion date is indicated on the examination timetable grade.

Personalized attention	
Methodologies	Description
Workbook Seminar Laboratory practice	Close supervision here means that the teacher will monitor as close as possible the activities of the student. The personal work of the student will be required and tested. The teacher may recommend further readings, clarify wrong statements, recommend literature searches, etc. Personal attention will also include the general scheduled tutorships. Students being recognized officially as partial-time and entitled not to attend the lectures will be attended in a tutorships regime (set hour with teacher in advance).

Assessment			
Methodologies	Competencies / Results	Description	Qualification
Workbook	C4 C6 C8	The report delivered by the student will be examined. In particular, identification and justification of the analytical strategies presented into the work.	5
Seminar	A15 A16 A20 A21 B2 B3 B4 C3	Active participation of the students will be scored, as well as the correct answers to questions or numerical calculations.	10
Laboratory practice	A15 A16 A17 A19 A20 A21 A22 A23 A26 B3 B4 B5	They will be scored on a on-going basis (order into the laboratory, correctness of the calculations, good manual operations, report delivered on-time, etc.).	15
Mixed objective/subjective test	A14 A15 C2	The exam will consist of tests (with a unique true response), short questions and numerical exercises. They will be related to the theoretical aspects of the subject. Some questions on these practices will be included in the objective test.	70

Assessment comments
Students will be evaluated in a continuous way according to their attendance to the scheduled activities, their engagement in the seminars, their discussions on the questions and numerical calculations, summary of workbook, the laboratory practices and the mixed test. Laboratory practices are mandatory, otherwise the subject will not be aproved. To pass the subject, all activities must be scored as 4, at least (on a 10-points scale). All the scores will be averaged and to pass the subject the average should be 5 or higher. However, note that the subject will not be aproved (even when the overall sum exceeds 5) if a particular score does not reach 4. In this case, the final score of the subject will be "fail" (score = 4,5). The mixed test will consist of two parts: theoretical questions and exercises, each part must be passed. The studen will obtain the qualification of "Not presented" when do not perform the laboratory practices and the mixed test. The ?second opportunity? of the subject this corresponds only to the mixed mixed. This means that the scores of the other activities will be maintained. If the student fails to pass the subject, allactivities should be repeated in following academic courses. No scores will be maintained. Students being recognized officially as partial-time and/or exempted from regular attendance to the lessons, will be evaluated only according to their scores on the objective tests (80%), workbook (5%) and the laboratory practices (15%). For them, the laboratory practices will be scheduled as flexible as possible, although taking into account the regular timetables, as well as the instrumental and human resources available. This holds for both evaluation opportunities.

Sources of information	
Basic	- CAMARA, C.; FERNANDEZ, P.; MARTIN-ESTEBAN, A.; PEREZ-CONDE, C.; VIDAL, M. (2002). Toma y tratamiento de muestra. Madrid, Sintesis - MILLER, J.N.; MILLER, J.C. (2002). Estadística y quimiometría para química analítica, 4th edition. Madrid, Prentice-Hall - RAMIS, G.; GARCIA, M.C. (2001). Quimiometria. Madrid, Sintesis - CaMARA, C.; PEREZ-CONDE, C (2011). Análisis químico de trazas. Madrid, Sintesis
Complementary	- VALCARCEL, M.; CARDENAS, M.S. (2000). Automatización y miniaturización en química analítica. Barcelona, Springer-Verlag - KELLNER, R,; MERMET, J.M.; OTTO, M.; WIDMER, H.M. (1998). Analytical chemistry: a modern approach to analytical science. Winheim, Willey-VCH - OTTO, M. (2007). Chemometrics. Weingeim, Willey-VCH

Recommendations
Subjects that it is recommended to have taken before

Química Analítica 1/610G01011 Química Analítica 2/610G01012 Química Analítica Instrumental 1/610G01013 Química Analítica Instrumental 2/610G01014
Subjects that are recommended to be taken simultaneously
Medio ambiente e calidade/610G01037
Subjects that continue the syllabus
Traballo de fin de Grao/610G01043
Other comments
To keep the subject updated is highly recommended. This includes reviewing the theoretical lessons after the classes, solving the numerical exercises, studying the practical classes, etc. Students should take advantage of seminars, supervision activities, etc. to solve their doubts. They should try to generate a sense of ?analytical criterion? to solve a problem; from sampling to data treatment.Students will need knowledge of the analytical techniques studied in previous academic courses (gravimetry, titration, spectrometry, chromatography, electrochemistry, etc.)A minimum knowledge of informatics is needed (word processors, spreadsheets, searches throughout internet, etc.).