

		Teaching Guide			
Identifying Data 203				2020/21	
Subject (*)	Advanced Analytical Chemistry and	Chemometrics	Code	610G01015	
Study programme	Grao en Química				
	·	Descriptors			
Cycle	Period	Year	Туре	Credits	
Graduate	1st four-month period	Fourth	Obligatory	6	
Language	SpanishEnglish				
Teaching method	Hybrid				
Prerequisites					
Department	Química				
Coordinador	Lopez Mahia, Purificacion E-mail purificacion.lopez.mahia@udc.es			ez.mahia@udc.es	
Lecturers	Andrade Garda, Jose Manuel E-mail jose.manuel.andrade@udc.es		drade@udc.es		
	Lopez Mahia, Purificacion		purificacion.lope	ez.mahia@udc.es	
	Muniategui Lorenzo, Soledad		soledad.muniate	egui@udc.es	
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 emphasis will be placed on how to plan and execute the different stages of the so-called ?analytical process?. C automate several working steps will be discussed. Finally, some basic tools to treat the final data sets will be stuis termed chemometrics and it deals with experimental design and optimization of an analytical procedure, calibrative analyses of the data (including data mining).			ns when applying them. Major		
			?analytical process?. Options to		
			nal data sets will be studied. This		
			lytical procedure, calibration and		

Contingency plan

1. Modifications to the contents

No changes will be done

- 2. Methodologies
- *Teaching methodologies that are maintained

Readings

Seminars

Mixed Test

Personal atention

*Teaching methodologies that are modified

Laboratory practices: It will not be possible to perform them at the Faculty and, therefore, they will be substituted by a practical case-study schedulled by the teachers to groups of students. A written report has to be delivered by each student and by each group of students.

- 3. Mechanisms for personalized attention to students
- e-mail: Daily, to make answers, ask for some virtual meetting to solve doubts and monitor the case-study.
- ? Moodle: Daily, according to the needs of the students. It contains thematic forums to make questions.
- ? Teams: weekly, to advance in the theoretical contents and seminars, at the hours schedulled previously at the Faculty. One or two weekly sesions (according to the needs of the students) in small groups (< 6 persons), to monitor the progress and elaboration of the report, to prepare the presentations of the readings, numerical exercises and the study of the case-study.
- 4. Modifications in the evaluation
- *Evaluation observations:
- Solving a case-study (to substitute the laboratory practices), with the same ratio of qualification. Aspects to be considered will be: suitability of the methodological approach, details and clarity of the reports, and critical discussions related to the case-study.
- The other methodologies will be maintained. The Mixed Test will be done virtually (via Moodle and/or Teams), in both the first and second opportunity.

The same applies to part-time students, formally recognized according to the "NORMA QUE REGULA O RÉXIME DE DEDICACIÓN AL ESTUDIO DE LOS ESTUDIANTES DE GRADO EN LA UDC (Arts. 2.3; 3.b e 4.5) (29/5/212).

5. Modifications to the bibliography or webgraphy

No changes. All materials will be in digital format in Moodle.

	Study programme competences		
Code	Study programme competences		
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		
В3	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		
To know how to select the proper analytical methodology for each particular problem.	A15	В3	C4
	A16		C6
	A20		C8
	A22		
	A26		
To know how to plan and execute the different stages of the analytical procedure to quantify analytes at trace levels, including	A14	B2	СЗ
the interpretation of the data.	A17	B4	
	A19		
	A20		
	A21		
	A23		
To know the main objectives of the most common chemometric techniques and to know their main application fields. To know	A14	B2	C2
how to extract relevant information from a multivariate study, in particular of a simplified environmental problem.	A15	B4	СЗ
	A16	B5	C4
	A20		C6
	A26		

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 Students will apply the theoretical concepts studied in the theoretical lessons	
	application of the analytical methodologies necessary to solve a real problem in the
	environmental, industrial, food, clinical

	Planning			
Methodologies / tests	Competencies	Ordinary class	Student?s personal	Total hours
		hours	work hours	
Laboratory practice	A15 A16 A17 A19	20	32	52
	A20 A21 A22 A23			
	A26 B3 B4 B5			
Seminar	A15 A16 A20 A21 B2	6	7.8	13.8
	B3 B4 C3			
Workbook	C4 C6 C8	1	5	6
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		1.5	0	1.5

(*)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	Groups of students will be formed who will be assigned a reading selected by the teacher related to the trace analysis.
	Subsequently, the group must submit a short report in which it identifies and summarizes the successive strategy for solving
	the analytical problem in reading as well as the power point presentation of it.
Guest lecture /	The teacher will develop and explain the basic contents of each chapter. Some documents will be delivered to the students
keynote speech	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	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
objective/subjective	student is evaluated.
test	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	Close supervision here means that the teacher will monitor as close as possible the activities of the student. The personal
Seminar	work of the student will be required and tested. The teacher may recommend further readings, clarify wrong statements,
Laboratory practice	recommend literature searches, etc.

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	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.	15
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.	15
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.).	25
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.	45

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.

The

mixed test will consist of two parts: theoretical questions and exercises, each

part must be passed. In case of passing only part at the first opportunity, it will NOT be retained at the second opportunity.

FIRST

OPPORTUNITY

To pass the subject it is required to get, at least, 5 points (out

of 10) in the Objective test (exam) and in the laboratory practices. The final score of the subject will not be lower than that of the examen or the weighted sum of all scheduled activities.

Students will be qualified as "Not presented" whenever they do not

perform neither the laboratory practices nor the mixed test.

SECOND

OPPORTUNITY

The "second opportunity" should be understood as a

second opportunity for the mixed test (exam). All the original scores

associated to practices, seminars, readings, etc. will be maintained, only the

score of the exam made in second opportunity will substitute that of the first

opportunity. The final score of the subject will not be lower than that of the examen or the weighted sum of all scheduled activities.

Students may only obtain the qualification "with honors" whenever the total number of the assigments was not given in the first opportunity.

STUDENS WITH PARTIAL-TIME DEDICATION

The evaluation criteria applied is the same indicated previously.

STUDENTS EXEMPTED FROM REGULAR ATTENDANCE TO THE LESSONS

For the students exempted from regular attendance to the lessons, the same evaluation criteria indicated above apply (except in the part of Seminars where only the resolution of the questions / problems raised by the teacher will be taken into account). 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	
	- CaMARA, C.; PEREZ-CONDE, C (2011). Análisis químico de trazas. 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	
	- MONGAY FERNÁNDEZ, CARLOS (2005). Quimiometría. Universidad de Valencia	
	- SOGORB SANCHEZ,M.A; VILANOVA GISBERT,E. (2004). Técnicas anallíticas de contaminantes químicos. Díaz	
	de Santos, Madrid	

Complementary	- jOHN R. DEAN (2014). Environmental Trace Analysis : techniques and applications. United Kingdom, Wiley & Dean (2014).
	Sons
	- KELLNER, R,; MERMET, J.M.; OTTO, M.; WIDMER, H.M. (2004). Analytical chemistry: a modern approach to
	analytical science. Winheim, Willey-VCH
	- VALCARCEL, M.; CARDENAS, M.S. (2000). Automatización y miniaturización en química analítica. Barcelona,
	Springer-Verlag
	- OTTO, M. (2007). Chemometrics : statistics and computer application in analytical chemistry . Weingeim,
	Willey-VCH

Recommendations

Subjects that it is recommended to have taken before

Analytical Chemistry 1/610G01011

Analytical Chemistry 2/610G01012

Instrumental Analytical Chemistry 1/610G01013

Instrumental Analytical Chemistry 2/610G01014

Subjects that are recommended to be taken simultaneously

Environment and Quality/610G01037

Subjects that continue the syllabus

Final Dissertation/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.).

(*)The teaching guide is the document in which the URV publishes the information about all its courses. It is a public document and cannot be modified. Only in exceptional cases can it be revised by the competent agent or duly revised so that it is in line with current legislation.