

COURSE: CHEMOMETRICS

SUBJECT: Statistics and Experimentation

MODULE: Technological

PROGRAM: University Master's Degree in Analytical Chemistry

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GENERAL FEATURES *

Type: Basic Training Compulsory Elective

Master's thesis work, Practicum

Duration: Semester

Semester / s: 1

Number of ECTS credits: 5

Language / s: Spanish, Catalan

DESCRIPTION

BRIEF DESCRIPTION AND JUSTIFICATION (The meaning of the course in relation to the program. Between 100 and 200 words.)

Chemometrics is the science of extracting information from chemical systems by treating the data they provide. These treatments use mathematical and statistical techniques, both for the design of the experiments that will give rise to the data, and for its process with the objective of obtaining information. One of the areas where chemometrics has special application is in Analytical Chemistry, given the amount of data that is generated.

COMPETENCES (Of course you put in relation to the skills pre-assigned in the field.)

Basic competences

CB6 - Have and understand knowledge which provides the ground or opportunity to be innovative in the development and/or application of ideas, often in a research context

CB7 - Apply their knowledge and their ability to solve problems in new or unfamiliar environments within broader (or multidisciplinary) contexts related to their field of study

CB8 - Integrate knowledge and deal with the complexity of formulating judgments based on information which, being incomplete or limited, includes reflections on social and ethical responsibilities related to the application of their knowledge and judgments

CB9 - Communicate conclusions, and the reasons that sustain them, to specialized and non-specialized audiences in a clear and unambiguous way.

General competences

CG2 - Ability to perform a responsible practice of the profession

Specific competences

E7- Demonstrate advanced knowledge of statistical techniques, design of experiments and process optimization for designing and developing analytical methods.

E8 - Ability to interpret the results obtained applying statistical techniques, design of experiments and process optimization methods to experimental data obtained in an analytical chemistry laboratory

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Transversal competences

T3 - Ability to assess the impact of the use of chemistry in the sustainable development of the society

PREREQUISITES * (Modules, materials, disciplines or expertise needed to track the subject. Contain subjects that must have been completed can be made.)

Students who have accessed the master's degree from bachelor's degrees in chemistry will not need any additional training complement. For the other degrees, they must have previously studied subjects that included basic contents of instrumental analytical chemistry and structural elucidation (including mass spectrometry) and statistics.

CONTENTS (Sections that make up the syllabus, to a second level of detail.)

1. Historical evolution of Chemometrics and its applications in Analytical Chemistry.
2. Data processing in the analysis laboratories
 - a. Comparison and transfer of methods
 - b. Intermediate precision
 - c. Linearity
 - d. Control charts and trend analysis
 - e. Analysis of data of sensory origin
3. Design and optimization of methods
 - a. Experimental designs
 - b. Sequential optimization methods
 - c. Adjustment of response surfaces.
4. Multivariate Analysis:
 - a. Cluster analysis
 - b. Principal component analysis. Regression
 - c. Partial least squares.

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METHODOLOGY

TRAINING ACTIVITIES * (Complete the table relating activities, workload in ECTS credits, and skills.)

Training Activities	ECTS	Competences
Sessions of exposition of concepts	25 / 0,93	E7, E8, T3, CG2
Sessions solving exercises, problems and cases	9 / 0,33	E7, E8, T3, CG2
Seminars	3 / 0,11	
Presentations	4 / 0,15	E7, E8, T3, CG2
Activities of personal study by students	90 / 3,33	E7, E8
Evaluation activities (exams, monitoring controls ...)	4 / 0,15	E7, E8
TOTAL	135 / 5	

TEACHING METHODOLOGY (Justifying the teaching methods used in relation to the competences and contents of the course. Between 100 and 200 words.)

- Sessions of exposition of concepts: Exposition of contents through presentation or explanation (possibly including demonstrations) by a professor.
- Sessions solving exercises, problems and cases: Solving exercises, approach / problem solving and presentation / discussion of cases by a professor with the active participation of students.
- Seminars: Statement made by a teacher in order to review, discuss and answer questions about materials and topics presented in the sessions of exposure sessions concepts and solving exercises, problems and cases.
- Practical work / laboratory: Performing laboratory activities or similar (practices with computer, projects, workshops, etc.) by the student, under the direct supervision of a professor.
- Presentations: Oral presentation to a professor and possibly other students by a student. It can be a paper prepared by the student by searching the published literature or a summary of a practical or project undertaken by the student.
- Activities of personal study by students: Personal work required of the student to acquire the competences of each subject and assimilate the knowledge presented in the sessions of exposition of concepts and of solving exercises, problems and cases, using, when necessary, the consultation recommended material.
- Evaluation activities: Oral and/or written statements made during a semester or after it.

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EVALUATION

ASSESSMENT SYSTEM * (Complete the table relating evaluation methods, competences and weight in the course grade.)

Evaluation Methods	%	Competences
Final Exam	30%	E5, E6, T3, CG2
Monitoring activities	40%	E5, E6, T3, CG2
Projects and presentations	20%	E5, E6, T3, CG2
Participation	10%	E5, E6, T3, CG2

LEARNING OUTCOMES (Explanation of the embodiments that allow the student skills assessment, relating them to the skills and methods of assessment.)

- The student must demonstrate his knowledge in the application of statistical techniques in the field of Analytical Chemistry. (E7, E8)
- The student must demonstrate his knowledge to design the program of experiences that allows to extract the maximum information with the minimum number of experiments depending on the specific problem. (E7, E8)
- The student must demonstrate sufficient statistical sense in order to analyze and interpret the results obtained from a series of experiences and design complementary tests if it is necessary. (E7, E8)
- The student must demonstrate sufficient knowledge and ability to optimize an analytical procedure and characterize it by defining the appropriate parameters. (E7, E8)
- The student must demonstrate knowledge of the repercussions derived from the incorrect use of statistical techniques and the results obtained. (CG2, T3)

QUALIFICATION (Explanation of the computer system of the course grade.)

First call

If the individual qualifications of the final exam, monitoring activities and projects and presentations are equal or greater than 3.0, the grade of this course is obtained:

Final exam	30%
Monitoring activities	30%
Projects and presentations	30%
Participation	-

If the individual qualifications of the final exam, monitoring activities and projects and presentations are less than 3.0, the grade of this course will be the minimum qualification obtained in these evaluation methods.

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Second call

The grade of this course is obtained:

Final exam	60%
Monitoring activities	40%

In subsequent calls, the grade of the course will be the qualification obtained in the exam.

ASSESSMENT OF THE COMPETENCES (Define calculation expressions for each competence and the relevant evaluation methods.)

The qualification of the competences will be the same as the final exam grade.

BIBLIOGRAPHY (Recommended and accessible to students.)

Basic:

- Miller, J. N., & Miller, J. C. (2010). Statistics and chemometrics for analytical chemistry. 6/E Pearson Education. (<http://www.pearsoned.co.uk/miller>)
- Miller, J. N., & Miller, J. C. (2002). Estadística y quimiometría para química analítica. 4/E

Complementary:

- Mullins, E. (2003). Statistics for the quality control chemistry laboratory. Royal Society of Chemistry.
- Vandeginste, B. G. M., Deming, S. N., Michotte, & Kaufman, L. (1988). Chemometrics: a textbook.
- Brereton, R. G. (2003) Chemometrics. Data analysis for the laboratory and chemical plant. Wiley

DOCUMENT HISTORY

PREVIOUS CHANGES (You set the date and author / s, the most recent first)

28/02/2015 Lucinio González Sabaté

01/09/2014 Lucinio González Sabaté

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