# Bachelor's Degree in Chemistry

# **Subject Guide**

# 1. Information about the subject

SUBJECT	Numerical Calculus and Applied Statistics			GQUIMI01-1-006	
EDUCATIONAL OFFER	Bachelor's Degree in Chemistry	CENTER Facultad de Químic		d de Química	
TYPE	Core	N° TOTAL CREDITS	6.0		
PERIOD	Second Semester	LANGUAGE	Spanish English		
COORDINATORS/ES		EMAIL			
Salamanca Jurado Juan Jesus		salamancajuan@uniovi.es			
LE	EMAIL				
Salamanca Jurado Juan Jesus		salamancajuan@uniovi.es			
Salas Riesgo Antonia Josefina		antonia@uniovi.es	(English	n Group)	

#### 2. Context

Statistics is an instrumental course from the basic module corresponding to the subject of Mathematics. It allows to compile and summarize information in order to process data by means of the most adequate method so that the conclusions are acceptable in a general sense (and not only for that particular case).

Passing this course is a requirement for the Analytical Chemistry I course.

Staff belongs to the Statistics and Operational Research field from the Statistics and Operational Research and Mathematics Teaching

Department of the University of Oviedo.

#### 3. Requirements

Pupils should know and apply correctly the mathematical concepts introduced in the scientific high school. Any knowledge obtained at the Mathematics course of this first year will be helpful and appreciated for the comprehension of this course.

### 4. Competencies and learning results

General abilities (know):

- 1. Develop the ability of analysis and summary (CG-1).
- 2. Solve problems in an effective way (CG-2).
- 3. Manage information appropriately (CG-6).
- 4. Develop a critical reasoning (CG-17).
- 5. Work in group (CG-18).

These abilities turn into the following learning objectives:

- 1. To write and perform correctly the presentation of a report. During the transversal activities (OA) informative texts related to any subject of the module or to environmental activities will be read by the pupils in order to prepare a summary which will be presented orally to their mates and the teaching staff. Pupils will also prepare in group a theme posed by the teaching staff that will be summarized in a poster and presented and defended in public.
- 2. To formulate and solve problems within the area of applicability of the subjects that make up the module.
- 3. To realize the necessity of Statistics for scientifically dealing with those situations involving a large number of data in a random or uncertainty environment.
- 4. To get the skills related with critical analysis, abstraction and meticulous logic reasoning.
- 5. To apply the theoretical and practical knowledge to the statement and planning of problems and to the search of a solution both in academic and professional environments.
- 6. To address subsequent specialised studies in Statistics as well as in any other science requiring good statistical basis.
- 7. To summarize and analyze datasets in a descriptive way.
- 8. To construct and analyze linear and nonlinear methods for evaluating the possible influence between two variables, making predictions and measuring the reliability.
- 9. To know the basic models and to be able of identifying random experiments and its process.
- 10. To understand and handle the basic concepts and principles of Statistical Inference, as well as the related methods and approaches, realizing their applicability to real problems.

#### 5. Contents

- Lesson 1: Descriptive Statistics.
  - 1.1 Unidimensional statistical variables.
  - 1.2 Bidimensional statistical variables.
- Lesson 2: Function fitting.
  - 2.1 Minimum squares.
  - 2.2 Regression and correlation.
  - 2.3 Other fitting methods.
- Lesson 3: Probability.
  - 3.1 Axioms and its consequences.
  - 3.2 Discrete random variables.
  - 3.3 Continuos random variables.
  - 3.4 Limit theorems.
- Lesson 4: Statistical inference.
  - 4.1 Pointwise and interval estimation.

4.2 Hypothesis testing.

Lesson 5: Model fitting

- 5.1 Error propagation.
- 5.2 Simulation.
- 5.3 Model validation.

#### 6. Methodology and working plan

Theory class (CE; 30 hours): The theoretical contents of the lessons will be explained in these classes together with the resolution of practical cases by the teacher which will help to fix the knowledge related with the foretold skills. This will give way to the resolution of problems in the Problem classes.

Problem class (PA; 14 hours): In order to fix the concepts developed in the theory classes, problems of the same type of those already solved in them will be proposed and resolved mainly with the students involvement.

Computer class (PL; 7 hours): R statistical package (free software) will be used in the Computer classes for solving the same kind of problems already solved in CE and PA. A final evaluation of the knowledge obtained in these classes will be made.

Tutorial class (TG; 4 hours): Pupils will deliver and defend individually a work which has been previously (previously enough, not the previous day) proposed. This defense will be evaluated by the teacher. In order to do this evaluation, each pupil must go to the tutorial group assigned by the administration (the single delivery of the work will not be evaluated). Pupils can also share doubts and obtain an explanations for them. This corresponds to the agreement of the Center Council achieved on 22nd June 2015.

Other activities (OA; 3 hours): In order to get the work-in-group skill, some activities will be held with other courses of the first year.

Evaluation (2 hours): There will be a final exam (two hours at most) in every official round of exams.

In order to acquire the proposed learning skills pupils' personal work is essential for fixing the knowledge exposed in the classroom.

		NON PRESENTIAL WORK								
lessons	total hours	theory classes	problem classes	computer classes	tutorial	s evaluation	Total	Work in group	Personal work	Total
Lessons 1 & 2	51	10	5	3	1.25	0.75	20	1	30	31
Lesson 3	48	10	4	1	1.5	0.5	17	1	30	31
Lessons 4 & 5	51	10	5	3	1.25	0.75	20	1	30	31
Total	150	30	14	7	4	2	57	3	90	93

modality		hours	%	Total	
Presential	Theory classes	30	20		
	Problems classes	14	9.33		
	Computer classes	7	4.66		
	Clinic practice			57	
	Tutorials	4	2.66		
	External practice				
	Evaluation	2	1.33		
Non presential	work in group	3	2	93	
	Personal work	90			
	Total	150			

## 7. Evaluation of the student's learning results

An exam involving all the contents developed in the course will be held in each round of exams

In May and July's exams, the mark obtained in this exam represents 70% of the final mark of the course. *In order to pass the course, it is necessary to get at least 4 (out of 10) in the exam.* Those pupils with less than 4 in the exam will be marked with at most 4 in the course.

30% of the final mark of the course will be distributed as follows: 5% corresponding to the evaluation of Other Activities (OA); 10% corresponding to the evaluation of the computer classes (PL); 15% corresponding to the evaluation (knowledge, attitude, ...) of the activities developed in the other classes (TG, PA). In case the center does not offer OA to all the students of the year, that 5% will increase the percentage relative to TG-PA activities.

For those pupils with *Alternative evaluation*, a complementary quiz with short-answer questions and/or multiple choice questions besides a computer exam using R will be held in order to evaluate those skills related with PL, PA and TG. The quiz and the computer exam will correspond with 30% of the final mark.

In January's exams the mark of the exam will represent 100% of the final mark of the course.

In order to pass the course it will be necessary to get at least a final mark of 5 (out of 10).

### 8. Resources, bibliography and complementary documentation

Several documents related with the course will be available at Campus Virtual.

Reference books on Statistics can be consulted at the different libraries of this University. For example:

George C. Canavos "Applied probability and statistical methods" Little, Brown and Company (1984).

Scheaffer, Mendenhall, Wackerly "Mathematical statistics with applications", Brooks-Cole (2008).

Other books which will be of interest for the course (although there is not an English version of them) are:

García Pérez, Alfonso "Estadística básica con R", Colección Grado, UNED (2010)

Sesé Sánchez, Luis M. "Cálculo Numérico y Estadística Aplicada", Colección Grado, UNED (2011)