COURSE DATA

DATA SUBJECT

Code: 34192
Name: Informatics for Chemistry
Cycle: Undergraduate Studies
ECTS Credits: 6
Academic year: 2025-26

STUDY (S)

Degree	Center	Acad. year	Period
1110 - Degree in Chemistry	Facultat de Química	1	First quarter

SUBJECT-MATTER

Degree	Subject-matter	Character
1110 - Degree in Chemistry	Informática	BASIC

COORDINATION

CALBO ROIG JOAQUIN

SUMMARY

This subject aims to familiarize students with the computer tools useful in the learning and practice of the degree in chemistry and the acquisition of a critical attitude towards the results obtained.

The subject has an eminently practical and applied approach. The contents are adapted both to the needs of the student of the degree in chemistry when addressing other subjects, as well as other professional activities: office automation, applications of scientific utility and use of the Internet and its basic tools of communication and access to information.

The basic lines of the subject are aimed at knowledge of the contents and utilities of certain applications and in the performance of exercises that use the different tools of each application. Concretely:

- Basic tools for access to the user environment and e-learning of the University of Valencia.
- Learning of various applications, including:

1) A spreadsheet for data processing, graphical representations, statistical adjustment of data to functions, and basic numerical calculation. The Microsoft Excel program is used.

2) An algebraic manipulator capable of performing symbolic calculation, as well as numerical calculation. Mathematica program is used.

3) A molecular representation and modelling program. Depending on availability, ChemBioOffice/ ChemOffice, MarvinSketch or ChemSketch programs are used.

Learning the basic fundamentals of the Python language.

PREVIOUS KNOWLEDGE

RELATIONSHIP TO OTHER SUBJECTS OF THE SAME DEGREE

There are no specified enrollment restrictions with other subjects of the curriculum.

OTHER REQUIREMENTS

Operation of the keyboard and mouse.
Sound Management of the windows GUI system.
Run programs in multiprocessing environments and acknowledge the characteristic menu of a given program.
Basics of web browsing and search engines.
Sound handling of files.
Sound knowledge of the practical aspects of developing: arithmetic, symbolic algebra.

COMPETENCES / LEARNING OUTCOMES

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Act autonomously in learning, making well-founded decisions in various contexts, forming judgements based on experimentation and analysis, and applying knowledge to new situations.

Collaborate effectively in work teams, assume responsibilities and leadership roles, and contribute to collective improvement and development.

Communicate effectively both orally and in writing, adapting to the context and audience.

Demonstrate ability to communicate information, ideas, problems and solutions to both specialist and non-specialist audiences and using information technology, as appropriate.

Demonstrate ability to work in teams both in interdisciplinary teams and in an international context.

Demonstrate a commitment to ethics, equality values and social responsibility as a citizen and as a professional.

Demonstrate critical and self-critical thinking, considering professional ethics, moral values and social implications of the different activities carried out throughout the degree.

Demonstrate leadership and management skills, entrepreneurship, initiative, creativity, organization,

planning, control, leadership, decision making and negotiation.

Evaluate, interpret and synthesise chemical data and information.

Express ideas correctly, both orally and in writing, in any of the official languages of the Valencian Community.

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.

Learn autonomously.

Relate theory and experimentation.

Relate theory to experimentation.

Solve problems effectively.

Solve problems effectively.

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 be able to communicate information, ideas, problems and solutions to both expert and lay audiences.

Students must have acquired knowledge and understanding in a specific field of study, on the basis of general secondary education and at a level that includes mainly knowledge drawn from advanced textbooks, but also some cutting-edge knowledge in their field of study.

Students must have developed the learning skills needed to undertake further study with a high degree of autonomy.

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.

Understand and analyse, from the perspective of the degree programme, social inequalities based on sex and gender; integrate gender-sensitive approaches into problem-solving and solution design.

DESCRIPTION OF CONTENTS

Presentation of the course. UV user environment: Mail, Virtual Disk, Virtual Services, Virtual Classroom...

1. UV user environment.

The Bibliographic Information Service of the UV. Scientific databases: ChemNetBase, Web of Knowledge.

2. Worksheet 1. Expressions, formulas and functions

General Spreadsheet Concept: The Cell as a Computing Variable. Cell formats. Absolute and relative directions: Formulas and functions. Programming simple problems in the spreadsheet: solving equations with "Goal Seek" and basic use of Solver

3. Worksheet 2. Graphical presentation of data

Series generation. Data representation. Plotting of functions of known expression. Applications to problem solving.

4. Worksheet 3. Adjustment of data

Settings. Linear regression. Interpolation and extrapolation. Applications to problem solving.

5. Molecular representations

Conventions for chemical representation. Building and handling of 2D and 3D molecular structures. Fast obtention of stationary conformations. Property calculation

6. Algebraic manipulator 1. Variables, operators and lists

Introduction to the use of MA. Fundamental concepts of MA syntax. Substitution rules. Numerical results. Lists. Vectors and matrices as lists. List generation. Problem-solving applications.

7. Algebraic manipulator 2. Functions and equations

Predefined functions and programmer-defined functions. Solving equations and systems of equations. Derivation and integration of functions. Problem-solving applications

8. Algebraic manipulator 3. Graphical representations

Graphical representations in the MA. Graphical representation of lists of points. 2D and 3D graphic representations. Parametric representations. Problem-solving and data fitting applications

9. Introduction to the Python language

Jupyter notebooks. Basic data types. Lists and tuples. Flow control. Functions. Modules and packages. Using packages: math, numpy, scypy, matplotlib...

WORKLOAD

PRESENCIAL ACTIVITIES

Activity	Hours
Tutorials	12,00
Computer classroom practice	48,00
Total hours	**60,00**

NON PRESENCIAL ACTIVITIES

Activity	Hours
Attendance at other activities	0,00
Individual or group project	10,00
Independent study and work	50,00
Preparation of lessons	20,00
Preparation for assessment activities	10,00
Resolution of case studies	0,00
Total hours	**90,00**

TEACHING METHODOLOGY

The nature of the course implies intensive and almost exclusively use of "ICT" ("information and communication technologies"), in particular computer based tools. All the technically available issues in the classroom computers will be used in a practical way.

Through a website the students have information and materials that are common to all groups, as a complement of the virtual learning platform provided by the UVEG ("aula virtual") which is more group specif.

Since the work plan (section III) includes predominantly "directly supervised computer classroom practices" and, to a lesser extent, "seminars, activities related to acquisition of transversal skills, tests and exams", the development of the directly supervised part of the course is structured around the following points:

- Computer hands-on sessions supervised by a teacher.
- Seminars where students present their homework done and exposed by means of computational tools.
- Hands-on workshops where the students use the classroom computer resources to provide results aimed to complete a cooperative project.
- Evaluation sessions.

The students will be provided with exercise collections of chemical, physical and mathematical content to be solved with the applications they are introduced to. Teachers use "pilot" exercises to introduce each application, its procedures, commands, tools, and menus; then, the students can practice with proposed exercises under direct supervision. Additional students homework includes solving the collections of exercises and loading them up into mandatory terms. Additional exercises may be proposed that require using several applications and data exporting.

EVALUATION

For both the first and second calls, the evaluation criteria are as indicated in the following table:

Written, oral and/or experimental exams in laboratory and computer science subjects	55%
Evaluation of computer classroom sessions: attitude, skills, reports, memories and oral communication.	45%

Any student must obtain at least 4.0 out of 10 in each of the contributions to the overall rating. Otherwise, the grade of the subject will be fail. To pass the subject it is required to obtain an overall grade of 5.0 out of 10.

Final warning

Copying or plagiarism of any assignment that is part of the evaluation will make it impossible to pass the course, and the student will be subject to the appropriate disciplinary procedures.

Please note that, according to Article 13 d) of the University Student Statute (RD 1791/2010, December 30), "*it is the duty of a student to refrain from using or cooperating in fraudulent procedures in evaluation tests, in the work performed or in official University documents*".

REFERENCES

- BILLO, E.J. EXCEL for Chemists, A Comprehensive Guide, 2nd. Ed., Wiley-VCH, New York, 2001. ISBN 9780470381236

- PLANELLES, J., SERRANO, R. Informática aplicada a la química. Publicaciones de la Universitat Jaume I. Colección Universitas. Castellón, 2002. ISBN 9788480213875

- Help on line of the Spreadsheet, Molecular Modelizer, Computer Algebra System (CAS) and other software used in the course.

- Tutoriales de WXMaxima: http://andrejv.github.io/wxmaxima/tutorials/10minute_es.zip https://vimeo.com/channels/maximajaj http://maxima.sourceforge.net/docs/manual/es/maxima.html