COURSE DATA

DATA SUBJECT

Code: 34192
Name: Informatics for Chemistry
Cycle: Undergraduate Studies
ECTS Credits: 6
Academic year: 2026-27

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

It is not an essential requirement, although it is recommended to have basic knowledge of:

- Keyboard and mouse operation.
- File and window management in the Windows operating system.
- Running programs in multitasking environments and recognising a program's menu.
- Web browsing and the use of search engines.
- Practical mathematical aspects of development: arithmetic and symbolic algebra.

COMPETENCES / LEARNING OUTCOMES

1108 -

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 leadership and management skills, entrepreneurship, initiative, creativity, organization, planning, control, leadership, decision making and negotiation.

Evaluate, interpret and synthesise chemical data and information.

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.

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.

1110 - Degree in Chemistry

Act autonomously in learning, making informed decisions in different contexts, forming judgements based on experimentation and analysis, and transferring knowledge to new situations.

At the end of the course, the student will be able to relate theory and experimentation.

At the end of the course, the student will be able to solve problems effectively.

Collaborate effectively in teams, assuming responsibilities and leadership roles and contributing to collective improvement and development.

Communicate effectively, both orally and in writing, adapting to the characteristics of the situation and the audience.

Demonstrate critical and self-critical reasoning within the field of study, considering aspects such as professional ethics, moral values and the social implications of the different activities undertaken.

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

Understand and recognise, from within the discipline, inequalities based on sex and gender in society; integrate different needs and preferences related to sex and gender into problem-solving and solution design.

DESCRIPTION OF CONTENTS

1. UV User Environment.
Presentation of the course. UV user environment: mail, virtual disk, Virtual Secretary and Virtual Classroom. Bibliographic information service of the UV. Scientific databases: ChemNetBase and Web of Knowledge. Inserting formulas with Word and citing bibliography correctly. Installation of the subject software and use of UV Desktop.
2. Spreadsheet 1: Expressions, formulas, functions.
General spreadsheet concept: the cell as a computing variable. Cell formats. Absolute and relative references. Formulas and functions. Programming simple problems in the spreadsheet: solving equations with the Solver tool.
3. Spreadsheet 2: Graphical presentation of data.

Series generation. Data representation. Representation (X,Y) of functions of known expression. Application to problem solving.

4. Spreadsheet 3: Data adjustment.

Adjustments. Linear regression. Interpolation and extrapolation. Application to problem solving.

5. Molecular representation.

Chemical representations. Construction and handling of 2D and 3D molecular structures. Presentation of available chemical information. Rapid obtaining of stationary conformations. Calculation of structural and electronic properties.

6. Algebraic manipulator 1: Variables, operators and lists.

Introduction to the use of the algebraic manipulator. Fundamental concepts of syntax. Substitution rules. Numerical results. Lists. Vectors and arrays as lists. List generation. Application to problem solving.

7. Algebraic manipulator 2: Functions and equations.

Predefined functions and programmer-defined functions. Solving equations and systems of equations. Derivation and integration of functions. Application to problem solving and optimization exercises.

8. Algebraic manipulator 3: Graphical representations.

Graphical representations of functions. Graphical representation of point lists. 3D graphic representations. Parametric representations. Application to problem solving and data adjustment.

9. Introduction to the Python language.

Jupyter Notebooks. Basic data types. Lists and tuples. Flow control: conditionals and loops. Functions, objects and attributes. Modules and packages: math, numpy, scipy, matplotlib. Use of libraries for chemistry.

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	20,00
Independent study and work	40,00
Preparation of lessons	10,00
Preparation for assessment activities	20,00
Resolution of case studies	0,00
Total hours	**90,00**

TEACHING METHODOLOGY

The nature of the subject implies the intensive and almost exclusive use of "ICT" (new "information and communication technologies"), in particular computer tools. All those aspects that are technically available on the computers provided to students will be addressed in a practical way. Through a website, students have access to the information and materials necessary for the development of the subject, which can serve as a complement to the virtual classroom service offered by the UV as a monitoring panel, information on the development of the course, compulsory and optional activities, seminars, links and conferences of interest, etc.

Since the work plan predominantly includes "practical computer classroom classes" and, to a lesser extent, "seminars, assignments and activities related to the acquisition of transversal skills, tests and exams", the development of the face-to-face part of the subject is structured around:

- Explanation sessions and computer practices supervised by one or more teachers.
- Seminars where students: i) present a work that makes use of computer resources, or ii) carry out a project using computer resources, the result of which is necessary to complete a common project.

Students will be provided with collections of exercises of chemical, physical and mathematical content to be solved with the computer tools explained. The teacher will use "prototype exercises" to introduce the theoretical and practical concepts of each computer application in terms of techniques, commands, procedures and menus.
The sessions are completed with the completion of exercises in which the indicated techniques are applied and in which students, individually, are dedicated to solving practical problems posed by the teachers. During these practical sessions, students have the presence of one or more teachers who are in charge of answering their questions, so that the sessions can be considered supervised practices.
The additional non-face-to-face work may include the completion of the proposed collections of exercises or other activities designed by the teacher, which will include work for mandatory submission within specific deadlines.
Since the subject consists of several parts in which different types of computer applications are addressed, sessions will be dedicated to working on combined exercises that jointly use the techniques learned for problem solving. Logically, these problems will be more complex, as they will require the use of several applications and the transfer of information between them.

EVALUATION

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

Assessable Activity	Weighting	Nature of the Activity
a) Written and/or oral exams	60%	**RETAKEABLE.** The final exam can be retaken globally by taking an equivalent test in the second official call of the subject.
b) Continuous evaluation of the sessions in the computer room: attitude, skills, reports, memories and oral communication	40%	**NOT RETAKEABLE.** Due to their close link with face-to-face monitoring, continuous assessment and the daily work carried out in the computer room, these activities cannot be retaken in the second call.

Evaluation conditions:

- Any student must obtain at least a grade of 4.0 out of 10 in each of the two contributions (a and b) in order to calculate the overall grade. If this minimum is not reached in any of the parts, the final grade of the subject will be Fail. In case of not attending the exam (contribution a), the final

grade of the subject will be "Not Presented", regardless of the grade obtained in the continuous evaluation (contribution b).
- To pass the subject, it is necessary to obtain a final overall grade equal to or greater than 5.0 out of 10.

Final Warning
Copying or evident plagiarism in any task that is part of the evaluation will make it impossible to pass the subject and will result in the application of the corresponding disciplinary procedures.
It should be noted that, in accordance with article 13 d) of the University Student Statute (RD 1791/2010, of 30 December), *"it is the duty of a student to refrain from using or cooperating in fraudulent procedures in assessment tests, in the work carried out or in official documents of the University"*.

REFERENCES

Básica

- PLANELLES, J., SERRANO, R. *Computer Science Applied to Chemistry*. Publications of the Universitat Jaume I. Universitas Collection. Castellón, 2002. ISBN 9788480213875.
- BILLO, E. J. *Excel for Chemists: A Comprehensive Guide*. 3rd Edition. Wiley-VCH, New York, 2011. ISBN 978-0470381236.
- MICROSOFT CORPORATION. *Microsoft Excel Documentation and Support: Formulas, Functions, and Charts* [online]. Redmond, Washington: Microsoft, 2026. Available in: https://support.microsoft.com/excel.
- WOLFRAM, Stephen. *The Mathematica Book*. 5th ed. Champaign, Illinois: Wolfram Media, 2004. ISBN 978-1579550226.
- WOLFRAM RESEARCH. *Mathematica Documentation and Tutorial Center* [online]. Wolfram Research, Inc., 2026. Available in: https://reference.wolfram.com/.
- PYTHON SOFTWARE FOUNDATION / JUPYTER TEAM. *Updated official Python and Jupyter Notebook documentation and tutorials* [online]. 2026. Available in: https://docs.python.org/es/3/ and https://jupyter.org/documentation.
- MCKINNEY, W. *Python for Data Analysis: Data Wrangling with pandas, NumPy, and Jupyter*. 3rd Edition. O'Reilly Media, 2022. ISBN 978-1098104030.

Complementaria

- MAXIMA DEVELOPMENT TEAM. *Maxima Handbook* [online]. Official version in Spanish, 2026. Available in: http://maxima.sourceforge.net/docs/manual/es/maxima.html.
- PINE, D. J. *Introduction to Python for Science and Engineering*. CRC Press, 2024. ISBN 978-1032650333.