COURSE DATA

Data Subject	
Code	34192
Name	Informatics for chemistry
Cycle	Grade
ECTS Credits	6.0
Academic year	2017 - 2018

Study (s)

Degree	Center	Acad. year	Period
1108 - Degree in Chemistry	Faculty of Chemistry	1	First term

Subject-matter

Degree	Subject-matter	Character
1108 - Degree in Chemistry	4 - Information technology	Basic Training

Coordination

Name	Department
SANCHEZ MARIN, JOSE	999 - OTROS

SUMMARY

This course aims to familiarise students with the use of computer tools that are helpful in learning and practising towards the Degree in Chemistry and to provide them with a critical attitude towards the results obtained.

The course has a practical and applied approach. The contents are adapted both to the needs of the students of the Degree in Chemistry when addressing other subjects and to other professional activities: office automation, applications for scientific purposes and use of the Internet and of its basic tools for communication and access to information.

The subject is mainly designed to teach the contents and uses of certain software applications and to carry out exercises that use the different application-specific tools. Specifically:

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

1) A spreadsheet for data processing, graphical representation, statistical data adjustment to functions and basic numerical calculation.

2) An algebraic manipulator able to perform symbolic computation, plus numerical calculation.

3) A software for molecular modelling and plotting.

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

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

Other requirements

There are no enrolment restrictions on other subjects in the curriculum.

Ability to operate the keyboard and the mouse.

Ability to use the window system.

Ability to run programs in multiprocessing environments and to recognise the menu of a given program.

Basics of web browsing and search engines.

Ability to manage files.

Basic knowledge of the practical aspects of arithmetic, symbolic algebra, etc.

COMPETENCES (RD 1393/2007) // LEARNING OUTCOMES (RD 822/2021)

1108 - Degree in Chemistry

- Demonstrate leadership and management skills, entrepreneurship, initiative, creativity, organization, planning, control, leadership, decision making and negotiation.
- Solve problems effectively.
- Demonstrate ability to work in teams both in interdisciplinary teams and in an international context.
- Demonstrate ability to communicate information, ideas, problems and solutions to both specialist and non-specialist audiences and using information technology, as appropriate.
- Demonstrate a commitment to ethics, equality values and social responsibility as a citizen and as a professional.
- Learn autonomously.
- Evaluate, interpret and synthesise chemical data and information.
- Relate theory and experimentation.
- 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 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 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.
- Students must be able to communicate information, ideas, problems and solutions to both expert and lay audiences.
- Students must have developed the learning skills needed to undertake further study with a high degree of autonomy.
- 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.

LEARNING OUTCOMES (RD 1393/2007) // NO CONTENT (RD 822/2021)

The following learning outcomes have been defined for the subject Chemical Informatics taught in the Degree in Chemistry:

1. Capacity for managing information. (CG6, CG7, CE16, CT3)
2. Capacity for using information and communication technology (ICT) correctly. (CG6, CG7, CE16, CT3)
3. Capacity for using the ICT environment of electronic learning supported by the Universitat de València. (CG7, CT3)
4. Capacity for organisation and planning. (CG3, CE22)
5. Capacity for solving chemical problems using the ICT environment. (CG4, CG7, CT3)
6. Capacities for autonomous learning, simulated construction and 2D and 3D visualisation of organic and inorganic molecules. (CG7, CG8, CT3)
7. Capacity for teamwork. (CG5)

Minimum learning outcomes: subject to assessment and mandatory for achieving a **pass mark**:

At the end of the course, the student must **necessarily** be able to:

- Create a folder with a given name on the drive and directory indicated.
- Use the University of Valencia user environment to:
  - Send an e-mail with attachments through the University mail server
  - Search for information of interest selectively in a scientific database (accessible to UV users)
  - Use the functionalities of spreadsheets to:
    - Write formulas without basic syntax errors
    - Use numbers in scientific format (n.nn x 10n)

        - Propagate formulas (copy and paste operatively)
        - Draw basic scientific plots based on small data sets
        - Fix a graph's axis scaling, limits and format
        - Plot multiple data series in one chart
        - Fit data to a straight line and obtain the equation of the fitted line
        - Use the tool "Goal Seek" to solve single-variable equations numerically
    - Know the basic syntax of the algebraic manipulator for variables, operators, expressions, functions and lists and use its functionalities to:
        - Plot a single-variable function
        - Plot a list of points
        - Solve a single-variable equation symbolically
        - Solve a single-variable equation numerically
        - Solve a system of several-variable linear equations symbolically
        - Calculate explicit derivatives of single-variable functions
        - Calculate indefinite integrals of single-variable functions
        - Calculate definite integrals of single-variable functions
    - Use the functionalities of the 2D molecular modeller to:
        - Build simple organic and inorganic molecules
        - Replace functional groups and change atoms in a controlled manner
    - Use the functionalities of the 3D molecular modeller to:
        - Build simple organic and inorganic molecules
        - Replace functional groups and change atoms in a controlled manner
        - Measure distances and bond angles in 3D molecular representations
        - Obtain simple molecular structures that are chemically reasonable

Additional learning outcomes: subject to assessment and compulsory for obtaining **a mark higher than a pass**.

At the end of the course, in order to obtain a mark higher than a pass, in addition to having the skills required in the previous subsection ("minimum learning outcomes"), students must be able to:

- Use the functions of the operating system and computer network to:
    - Accurately find locations in the directory tree, disks and servers in the computer being used
    - Know the most common uses of the keyboard and mouse (editing text fields, writing non-alphanumeric characters, main keyboard functions and services, character sets, etc.)
    - Recognise applications, run them and have them ready to start working, where appropriate, in a new document
    - Create and manage documents from active applications
    - Perform copies, duplicates, renaming and back-ups of both documents and directories
    - Find information relevant to the degree subject areas on the Internet
    - Find information of interest in scientific network-accessible databases
    - Organise and plan information in accordance with instructions received
    - Export and import data between applications
    - Prepare an organised scientific document using combined computing resources
    - Use the functionalities of spreadsheets to:
        - Recognise the most common error conditions when using expressions

- Program simple algebraic mathematical expressions
- Program transcendental or simple functional mathematical expressions
- Generate numerical series in a controlled manner
- Perform basic operations on matrices and determinants
- Build crosstabs with the results obtained from data supplied, using relative and absolute cell addresses
- Perform and control XY plots from data tables
- Plot different sets of data with very different ranges on a single graph
- Fit data to straight lines with error estimates in the slope and intercept
- Fit data to various types of curves and obtain the corresponding equation
- Graphically interpolate a value from a fitted equation
- Numerically interpolate a value from a fitted equation
- Graphically extrapolate a value from a fitted equation
- Numerically extrapolate a value from a fitted equation

- Use the functionalities of the algebraic manipulator to:
  - Make an effective use of basic performance standards
  - Make an effective use of basic syntax rules
  - Find useful information in the program’s help section
  - Recognise error and warning messages
  - Manipulate basic algebraic and transcendental expressions symbolically
  - Perform operations using isolated data and using data lists
  - Replace an expression within another
  - Generate lists of values using indexes in a programmed manner
  - Use basic control structures (conditional "if" and "for" loops or equivalent)
  - Solve equations and systems of equations symbolically
  - Derive and integrate functions
  - Perform basic operations on vectors and matrices
  - Perform graphical plots of functions in a controlled manner
  - Plot two single-variable functions on the same graph
- Use the functionalities of the 2D and 3D molecular modeller (MM2D and MM3D) to:
  - Plot and recognise the 3D structure of organic molecules with common functional groups
  - Plot and recognise the 3D structure of common inorganic molecules
  - Recognise and measure dihedral bond angles in 3D molecular representations
  - Get chemically reasonable structures from assumed structures and optimise molecular geometries
  - Critically analyse the results of molecular optimisations
  - Optimise 3D molecular structures with theoretical models of molecular mechanics (MM) and quantum mechanics (QM)
  - Plot of several 3D molecules in the same document
  - Calculate molecular properties with MM2D and MM3D
  - Plot molecular surfaces with MM3D
  - Use molecular surfaces as a graphic support to display molecular properties
  - Plot 2D molecules, reactions, processes, etc. using the conventions for chemical representation
  - Recognise the terminology, nomenclature and basic structural properties of molecules

The learning outcomes that follow correspond to transferable skills that are progressively acquired throughout the curriculum. They are listed here because this subject can significantly contribute to achieving them:

- Improve the ability to work collaboratively in small teams.
- Understand the names and expressions that form the basic scientific or technical vocabulary in English related with applications and procedures studied in the course. (Even if the basic course materials are in the official languages of the CV, much of the relevant chemical information that can be obtained from the Internet, the commands in the algebraic manipulation software and in the molecular modeller (2D and 3D), as well as the "help" section of these programs are in English, which allow students to get familiar with an important part of the basic English vocabulary related to the contents taught.)
- Write and make presentations in the native language correctly.
- Improve the ability to choose from among many options. It is common for applications to offer several options to solve problems without that substantially altering the content or nature of the solution. Students must choose and justify their choices. This provides excellent training in making decisions with immediate effects.

DESCRIPTION OF CONTENTS

1. UV user environment. Electronic resources

Presentation of the course. Running applications: editing math expressions. Internet and LAN at the UV. User environment: Mail. Virtual Disk. Virtual services. UV e-learning environment: UV virtual classroom. The UV bibliographical information service. Scientific databases: searches in databases and management of search results.

2. Worksheet 1. Expressions, formulas and functions

General concept of worksheet: the cell as a computer variable. Cell formats. Absolute and relative cells. Formulas and functions. Matrices and vectors. Programming simple problems on the worksheet.

3. Worksheet 2. Graphical presentation of data

Representation of data. Generation of series. Graphical representations with parametric dependencies. Representation (X, Y) of functions of a known expression. Applications to problem solving.

4. Worksheet 3. Adjustment of data

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

5. Worksheet 4. Numerical solution of equations

Search for values that meet conditions. Search target. Solver. Applications to problem solving.

6. Algebraic manipulator 1. Variables, operators, expressions

Introduction to the use of the AM. Basic concepts of syntax of the AM. Symbolic algebraic manipulations. Substitution rules. Numerical results. Applications to problem solving.

7. Algebraic manipulator 2. Lists, matrices, vectors

Lists. Operations between lists. Vectors and matrices as lists. List generation. Lists of pairs of numbers (x,y). Graphical representation of lists of points. Applications to problem solving.

8. Algebraic manipulator 3. Functions and equations

Predefined functions and functions defined by the programmer. Solving equations and systems of equations. Derivation and integration of functions. Control structures (conditions, loops). Applications to problem solving.

9. Algebraic manipulator 4. Graphical representations

Graphical representations in the AM. 2D and 3D graphical representations. Parametric representations. Applications to problem solving.

10. Molecular representation 1. 2D molecular representations

2D chemical representation conventions. Construction and management of 2D molecular structures. Calculation of properties.

11. Molecular representation 2. 3D molecular representation

Construction and management of 3D molecular structures. Fast obtainment of stationary configurations. Calculation of properties of molecular structures.

WORKLOAD

ACTIVITY	Hours	% To be attended
Computer classroom practice	48,00	100
Tutorials	12,00	100
Development of group work	10,00	0
Study and independent work	50,00	0
Preparation of evaluation activities	10,00	0
Preparation of practical classes and problem	20,00	0
TOTAL	**150,00**	

TEACHING METHODOLOGY

The nature of the course implies intensive and almost exclusive use of ICT (information and communication technologies), in particular, computer-based tools. All the applications to be studied and available from the computers provided will be dealt with from a practical perspective.

The subject's website provides the students with the information and materials that are common to all groups, as a supplement to the virtual learning platform provided by the UVEG ("aula virtual"), which is more group-specific.

Since the work plan (section III) includes predominantly "practical lessons in the computer room" and, to a lesser extent, "seminars, activities related to the acquisition of transferable skills, tests and exams", face-to-face teaching will be structured around:

- Computer practical sessions supervised by an instructor
- Seminars in which students must present a piece of work prepared and presented using computer tools
- Hands-on workshops in which students must use computer resources to obtain the results needed to complete a cooperative project
- Evaluation sessions

Students will be provided with exercise booklets on chemistry, physics and mathematics to be solved with the applications explained in class. Lecturers 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 homework includes solving exercise booklets and submitting them within mandatory terms. Additional exercises requiring the use of several applications and data exports may be proposed.

EVALUATION

In all cases, **the minimum learning outcomes** (see section "LEARNING OUTCOMES") must have been **SUCCESSFULLY** achieved to pass the course.

First examination sitting: the final mark of the course is calculated from two marks:

a) That from continuous assessment

b) That from the final exam

As regards continuous assessment, throughout the semester students will be presented with a set of tasks, both individual and collective, whose main function is to obtain ongoing information on their progress regarding the learning outcomes outlined in this guide, and thus be able to advise them more efficiently. These tasks can be divided into three sections:

a) Work done during classroom sessions

b) Exercises carried out autonomously and submitted by students throughout the course

c) Minor team projects

The weighting of each of these sections towards the course final mark is as follows:

- Work carried out in practical classes and exercises submitted throughout the year: 30%
- Teamwork: 15%

Thus, the sum of these elements (i. e., those corresponding to continuous assessment) accounts for 45% of the final mark. The average mark for this set of activities must be of at least 4.0 out of 10.

The remaining 55% of the mark will be based on a final exam consisting of an individual practical exam with a series of exercises testing each of the three parts of the syllabus:

Part 1: Introduction, user environment and molecular representation (unit 1 and 10-11).

Part 2: Spreadsheet (units 2-5)

Part 3: Algebraic manipulator (units 6-9)

The weighting of each part towards the course final mark is as follows:

- Part 1: 10%
- Part 2: 25%
- Part 3: 20%

A minimum mark of 4.0 out of 10 must necessarily be achieved in each of these three parts. Otherwise, the subject will be marked as a fail. A pass mark requires an overall mark of 5.0 out of 10.

For the **second examination sitting,** one final exam will be held with the same characteristics and conditions as for the first sitting. The marks for continuous assessment will be carried forward, as well as the percentages to be applied. However, if a student wishes to improve his or her grade for the section of exercises carried out autonomously, he/she can do it by completing new exercises.

REFERENCES

Basic

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