COURSE DATA

Data Subject

Code	34192
Name	Informatics for chemistry
Cycle	Grade
ECTS Credits	6.0
Academic year	2018 - 2019

Study (s)

Degree	Center	Acad. year	Period
1110 - Degree in Chemistry	Faculty of Chemistry	1	First term

Subject-matter

Degree	Subject-matter	Character
1110 - Degree in Chemistry	4 - Informática	Basic Training

Coordination

Name	Department
SANCHEZ DE MERAS, ALFREDO	315 - Physical Chemistry

SUMMARY

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

The course has a practical and applied approach. The contents are oriented to the needs of both the student's degree in chemistry in addressing other subjects, and also to other professional activities: offimatics, applications of scientific utility and management of the Internet and its basic tools of communication and access to information.

The course basic lines are directed to the knowledge of the contents of certain utilities and applications and exercises that use different tools of each application. Specifically:

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

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

2)   An algebraic manipulator able to perform symbolic computation, plus numerical. Programs Maxima/wxMaxima are used.

3)   A program of molecular modeling and plotting. The suite of programa ChemBioOffice/ChemOffice, which includes among other the ChemBio3D and ChemBioDraw programs.

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.

OUTCOMES

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

The following results of learning are allocated to the subject "Informatics Applications in Chemistry" of the BSc "Degree in Chemistry":

1. Effective capacity of management of the information.
2. Capacity of correct use of the ICT, i.e. "information and communication technologies".
3. Effective use of the ICT environment for electronic education supported by the Universitat de València.
4. Capacity of organization and planning.
5. Capacity for solving chemical problems using the ICT environment.
6. Autonomous learning capacities for simulated construction and 2D and 3D visualization of organic and inorganic molecules.
7. Capacity to team work.

Minimum learning outcomes: are assessable and mandatory for obtain **the passing grade**:

At the end of the course, the student, in an **indispensable way**, must be able to:

- Create a folder on the drive and directory and the name indicated.

- Use the user environment the University of Valencia to:
  - Send an e-mail with attachments through the mail server of the University
  - Search selectively information of interest in a scientific database (accessible to UV users)
  - Use the functionality of the spreadsheet to:
    - Write formulas without basic syntax errors
    - Use numbers in scientific format (n.nn x 10n)
    - Propagate formulas (copy and paste operatively)
    - Perform basic scientific plots, from small data sets in the right way for it
    - Handle axe scale, limits and format of a graph
    - 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 numerically solve single-variable equations
  - Know the basic syntax of the algebraic manipulator for use variables, operators, expressions, functions, and lists and use their capabilities to:
    - Plot a single variable function
    - Plot a list of points
    - Symbolically solve a single-variable equation
    - Numerically solve a single- variable equation
    - Symbolically solve a system of several variable linear equations
    - Calculate explicit derivatives of single variable functions
    - Calculate indefinite integrals of single variable functions
    - Calculate definite integrals of single variable functions
  - Use functionalities of the 2D Molecular Modeler to:
    - Build simple organic and inorganic molecules
    - Replace functional groups and change atoms in a controlled way
  - Use molecular functionalities 3D Modeler:
    - Build simple organic and inorganic molecules
    - Replace functional groups and change atoms in a controlled way
    - Measure distances and bond angles on 3D molecular representations
    - Obtain simple molecular structures that be chemically reasonable

Additional learning outcomes: are assessable and required for obtaining **grades higher than passing grade**.

In addition to the skills required in the preceding subparagraph ("minimal learning outcomes"), at the end of the course, the student receiving a grade higher than the passing grade, must be able to:

- Use the functions of the operating system and computer network to:
  - Accurately situate in the directory tree, disks, and servers from the computer being used
  - Know the extended use of the keyboard and mouse (text field editing, write non-alphanumeric characters, main keyboard functions and services, character sets, etc.)
  - Recognize applications, open them to execute them and leave them in a position to start working, where appropriate, into a new document
  - Create and manage documents from active applications
  - Perform in a controlled manner copies, duplicates, rename and back up of both documents

and directories
- Find information relevant to the Degree subjects in the Web in a controlled way
- Find information of interest in a controlled way in scientific data bases accessible by network
- Organize and plan information in accordance with instructions received
- Export and import data between applications
- Develop an organized scientific document using combined computing resources
- Use the functionality of the spreadsheet to:
    - Recognize the most common error conditions using expressions
    - Program simple algebraic mathematical expressions
    - Program transcendent mathematical expressions or simple functional
    - Generate numerical series in a controlled way
    - 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 the 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 of the slope and intercept
    - Fit data to various types of curves obtaining 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 functions of algebraic manipulator to:
    - Make effective use of basic performance standards
    - Make effective use of the basic rules of syntax
    - Find information in a useful way from the program help
    - Acknowledge error and warning messages
    - Symbolically manipulate basic algebraic and transcendental expressions
    - Perform operations using isolated data and using data lists
    - Replace an expression in another
    - Generate lists of values in a programmed way using indexes
    - Use basic control structures (conditional "if" and "for" loops or equivalent)
    - Symbolically solve equations and systems of equations
    - Derive and integrate functions
    - Perform basic operations on vectors and matrices
    - Perform in a controlled way graphical plots of functions
    - Plot two single variable functions on the same graph
- Use the functions of 2D and 3D Molecular Modeler (MM2D and MM3D) to:
    - Plot and recognize the 3D structure of organic molecules with common functional groups
    - Plot and recognize the 3D structure of common inorganic molecules
    - Recognize and measure dihedral bond angles in 3D molecular representations
    - Get chemically reasonable structures from assumed structures and optimize molecular geometries
    - Critically analyze the results of molecular optimizations
    - Optimize 3D molecular structures with theoretical models of molecular mechanics (MM) and quantum mechanics (MQ)
    - 3D Plot of several molecules in the same document
    - Calculate molecular properties with MM2D and MM3D

- Plot molecular surfaces with MM3D
- Use molecular surfaces as graphic support to display molecular properties
- 2D Plot of molecules, reactions, processes, etc. using the conventions of chemical representation
- Recognize the terminology, nomenclature and basic structural properties of molecules

Learning outcomes that follow correspond to transferable skills progressively acquired throughout the curriculum. They are listed here because this subject can contribute relevantly to their achievement:

- 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 seen in the course (Although the basic course documentation is given in the official languages of the CV, much of the relevant chemical information can be obtained from the Web, the commands of the algebraic manipulation program and the molecular modeler (2D and 3D), and the "help" of these programs are in English, which allows students to familiarize themselves 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 among many options. It is common for applications to resolve problems choosing among several options without that substantially alters the content or nature of the solution. Students must choose and justify their choices. This is excellent training in decision making 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 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.

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EVALUATION

In any case, **the minimum learning outcomes** (see section LEARNING OUTCOMES) have to be **COMPLETELY** credited to pass the course.

First call: the course grade is calculated from two grades:

a)   That from the continuous assessment

b)   That from the final exam

As regards the continuous evaluation, a set of tasks, both individual and collective, will be developed throughout the semester, whose main function is to obtain information on a continuous basis on the progress of each student regarding the learning outcomes outlined in this guide, and thus be able to guide him/her more efficiently. These tasks can be divided into three sections:

a)   Work done during class sessions

b)   Exercises worked autonomously and delivered by students throughout the course

c)   Small team projects

The weight of each of these sections on the final grade for the course is as follows:

- Work done in practical classes and exercises delivered throughout the year: 30%
- Teamwork: 15%

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

The other 55% of the grade will be a final exam consisting in an individual practical test that will include a series of exercises for each of the three parts of the syllabus:

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

Part 2: Spreadsheet (items 2-5)

Part 3: Algebraic Manipulator (items 6-9)

The weight of each part in the final grade for the course is as follows:

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

To be considered the exam grade must be at least 4.0 out of 10 in each of these three parts. Otherwise, the grade for the course will be fail. To pass the course it is required to obtain an overall rating of 5.0 out of 10.

For the **second call,** one final exam will be held with the same characteristics and conditions that at first call. The grades of the sections of continuous assessment will be kept, as well as the percentages to be applied. However, if a student wishes to improve the grade corresponding to section of exercises performed autonomously, he/she can do it by performing new exercises.

REFERENCES

Basic

- 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