COURSE DESCRIPTION

COURSE DETAILS

Title (of the course): **QUÍMICA COMPUTACIONAL APLICADA**
Code: 100477
Degree/Master: **GRADO DE QUÍMICA** Year: 4
Name of the module to which it belongs: APLICADO
Field: QUÍMICA (OPTATIVA 3)
Character: OPTATIVA Duration: SECOND TERM
ECTS Credits: 3.0 Classroom hours: 30
Face-to-face classroom percentage: 40.0% Study hours: 45
Online platform: http://www3.uco.es/amoodle

LECTURER INFORMATION

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PREREQUISITES AND RECOMMENDATIONS

Prerequisites established in the study plan

The student will be able to matriculate in optional subjects once he has passed the 60 basic training credits and at least 30 other obligatory credits

Recommendations

It is convenient to have good knowledge on General Mathematics and Quantum Chemistry.
It is recommended that the student has at least the B1 level of English

INTENDED LEARNING OUTCOMES

CB3	written and oral communication in the native language
CB5	The capacity for data management and to generate information / understanding
CB10	Ability to study independently for continued professional development.
CE6	Principles of quantum mechanics and its place in the description of the structure and properties of atoms and molecules.
CE21	The ability to show knowledge and understanding of the essential facts, concepts, principles, and theories relating to chemistry
CE22	The ability to apply knowledge to solve qualitative and quantitative problems according to previously developed models
CE26	To gain skills in managing and processing chemical data and information.
CE31	interpretation of data from previous observations and measurements in the laboratory in terms of

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their significance and the theories that support them

CU2 To understand and improve basic IT skills

OBJECTIVES

To get knowledge about the main principles of Computational Chemistry and the different calculation methods and its applications in the prediction of the physico-chemical properties of the molecules plus the design of new compounds with predefined properties.

CONTENT

1. Theory contents

1. Theoretical content

Lesson 1. Principles of Computational Chemistry. General aspects. Molecular models and visualization of molecules. Coordinate systems. Potential Energy Surfaces (PES). Dihedral Angle: conformations and configurations. Molecular mechanics (MM). Quantum mechanical force fields.

Lesson 2. Quantum Mechanics. Schrödinger equation. Molecular Hamiltonian. Born-Oppenheimer approximation. "Ab Initio" methods. Hartree-Fock method or self-consistent field method. Density Functional Theory (DFT). Comparison between the different methods. Hybrid methods.

Lesson 3. Simulation approaches. Optimization of the geaometry. Molecular Dynamics (MD). Monte Carlo Simulation and Langevin Dynamics.

Lesson 4. Applications. Definition of relationship between the molecular structure and the physico-chemical properties. Quantitative correlation between the structure and the activity (QSAR). Designing of compounds directed by QSAR.

2. Practical contents

2. Practical contents

Calculation with molecular mechanics. Semi-empirical calculations. Ab Initio calculations. Optimization of the molecular geometry. Molecular dynamics. Quantitative correlation between structure and activity. Determination of

QSAR parameters.

METHODOLOGY

General clarifications on the methodology (optional)

Seminars will take place at the computers classroom. Attendance to lectures and seminars is mandatory

Methodological adaptations for part-time students and students with disabilities and special educational needs

Part-time students will be interviewed in each individual case. The modifications in the methodology will be designed to better match each situation.

Face-to-face activities

Activity	Large group	Medium group	Total
Assessment activities	3	-	3
Lectures	14	-	14

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Activity	Large group	Medium group	Total
Seminar	-	13	13
Total hours:	***17***	***13***	***30***

Off-site activities

Activity	Total
Exercises	10
Self-study	35
Total hours	***45***

WORK MATERIALS FOR STUDENTS

Coursebook
Dossier
Exercises and activities

EVALUATION

Intended learnig	Case study/clinical case discussion/scientific work discussion	Problem solving	Real and/or simulated tasks
CB10	X	X	X
CB3		X	X
CB5	X	X	X
CE21	X	X	
CE22	X		X
CE26	X	X	
CE31	X	X	
CE6	X	X	X
CU2	X	X	X
Total (100%)	***60%***	***20%***	***20%***
Minimum grade	***4***	***4***	***4***

(*)Minimum grade necessary to pass the course

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Method of assessment of attendance:

Attendance to the lecture is mandatory

General clarifications on instruments for evaluation:

Software will be provided by the person in charge

Clarifications on the methodology for part-time students and students with disabilities and special educational needs:

The final practical work represents 60% of the final grade. During the seminars the students will have to solve different practical problems, which represents 20% of the grade, they must also consider certain tasks, which represents another 20% of the final grade.

Part-time students will be interviewed in each individual case. The modifications in the methodology will be designed to better match each situation.

Qualifying criteria for obtaining honors:

Average qualification equal to or greater than 9. The MH number will depend on the students numbers, in accordance with the UCO regulations

BIBLIOGRAPHY

1. Basic Bibliography

Computational Chemistry. E. G. Lewars. Ed: Springer. 2011, 2ª ed.
Computational Medical Chemistry for Drug Discovery. P. Bultink (Ed.) Ed: Marcel Dekker. 2004
Theoretical and Computational Chemsitry. Juan Andrés y Juan Beltran. Editorial: Universitat Jaume I. 2000
Physical Chemistry. Atkins y de Paula. Ed. Panamericana, 2008. 8ª Edición
Physical Chemistry. Thomas Engel y Philip Reid. Ed. Pearson Addison Wesley. 2006.
Physical Chemistry. J. Bertrán, J. Núñez, Ed. Ariel Ciencia, 2002

2. Further reading

None

COORDINATION CRITERIA

Tasks deadlines
Tasks performance

SCHEDULE

Period	Assessment activities	Lectures	Seminar
1# Week	0.0	2.0	0.0
2# Week	0.0	2.0	0.0
3# Week	0.0	2.0	2.0

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Period	Assessment activities	Lectures	Seminar
4# Week	0.0	2.0	2.0
5# Week	0.0	2.0	3.0
6# Week	0.0	2.0	3.0
7# Week	0.0	2.0	3.0
8# Week	3.0	0.0	0.0
Total hours:	***3.0***	***14.0***	***13.0***

The methodological strategies and the evaluation system contemplated in this Course Description will be adapted according to the needs presented by students with disabilities and special educational needs in the cases that are required.