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 Classroom hours: 30
Face-to-face classroom percentage: 40% Study hours: 45
Online platform: http://www3.uco.es/amoodle

LECTURER INFORMATION

Name: CAMACHO DELGADO, LUIS (Coordinator)
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Name: MIGUEL ROJAS, GUSTAVO DE
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PREREQUISITES AND RECOMMENDATIONS

Prerequisites established in the study plan

Prerequisites established in the study plan.
The student will be able tomatriculate 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 their significance and the theories that support them

COURSE DESCRIPTION

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*
Seminar	-	13	*13*
Total hours:	***17***	***13***	***30***

Off-site activities

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

COURSE DESCRIPTION

WORK MATERIALS FOR STUDENTS

Dossier
Exercises and activities
Coursebook

EVALUATION

Intended learnig outcomes	Tools		
	Objective tests	Problem solving	Real and/or simulated tasks
CB10		x	x
CB3	x	x	x
CB5		x	x
CE21	x	x	
CE22	x		x
CE26		x	
CE31	x	x	
CE6	x	x	x
CU2		x	x
Total (100%)	**45%**	**45%**	**10%**
Minimum grade.(*)	**3**	**3**	**2**

(*) Minimum grade necessary to pass the course

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:
Final exam represents 45% of the marks and the resolution of practical problems another 45%. The students are asked to analyze potential applications shown in the literature with a written report. This issue represents a 10% of the marks.
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: *Nota media igual o superior a 9. El número de MH dependerá del número de alumnos matriculados, de acuerdo con la normativa de la UCO*

BIBLIOGRAPHY

1. Basic Bibliography:

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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	Activity		
	Assessment activities	Lectures	Seminar
1# Week	0	2	0
2# Week	0	2	0
3# Week	0	2	2
4# Week	0	2	2
5# Week	0	2	3
6# Week	0	2	3
7# Week	0	2	3
8# Week	3	0	0
Total hours:	***3***	***14***	***13***

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.