



IDENTIFYING DATA

(*)Tese de Máster

Subject	(*)Tese de Máster			
Code	V11M030V01201			
Study programme	(*)Máster Universitario en Química Teórica e Modelización Computacional. R.D. 1393/2007			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	30	Mandatory	2nd	2nd
Teaching language	English			
Department				
Coordinator	Nieto Faza, Olalla			
Lecturers	Nieto Faza, Olalla Silva López, Carlos			
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Web				
General description	(*)Introduction to research through a simple research project			

Competencies

Code	
A2	(*)Adquirir formación en los métodos de modelización
A3	(*)Aplicar los métodos teóricos y de modelización a sistemas químicos en general
A4	(*)Aplicar los métodos teóricos y de modelización a sistemas bioquímicos
A5	(*)Aplicar los métodos teóricos al estudio de la reactividad y la catálisis
A6	(*)Aplicar los métodos teóricos y de modelización a la Química Atmosférica y a la Astroquímica
A7	(*)Aplicar los métodos teóricos y de modelización a la Nanociencia
A8	(*)Aplicar los métodos teóricos y de modelización al diseño de materiales
B1	(*)Mejorar la comunicación oral y escrita en Inglés u otros idiomas europeos
B7	(*)Ser capaz de obtener y manejar bibliografía científico técnica

Learning aims

Expected results from this subject	Typology	Training and Learning Results
(*)To learn how to tackle chemical problems by designing a suitable computational strategy	Know How	A2 A3 A4 A5 A6 A1 A2
(*)To compile all the pertinent bibliographic references and to select the most relevant information.	Know How	B1
(*)To learn how to dimension the required computations according to the existing hardware and software resources.	Know How	A3 A4 A5 A6 A1 A2

(*)To carry out the necessary computations, discuss critically the results and re-design the computational strategy if needed.	Know How	A3 A4 A5 A6 A1 A2
(*)To write a detailed report on the methods and results and defend it in public in front of a tribunal.	Know How	B1

Contents

Topic

(*)Setup and framing of the problem	(*)(*)
(*)Design of a a research plan	(*)(*)
Theoretical analysis and Computation	(*)(*)
Data analysis and report writing.	(*)(*)

Planning

	Class hours	Hours outside the classroom	Total hours
(*)Proyectos	28	700	728
(*)Trabajos e proyectos	2	20	22

*The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.

Methodologies

	Description
(*)Proyectos	(*)A simple research project. Three results are presented in a detailed written report and in a public talk in front of a tribunal.

Personalized attention

Methodologies	Description
Proyectos	

Assessment

	Description	Qualification
(*)Proyectos	(*)Assessment of the design and execution of the research project by the tutor(s)	85
(*)Trabajos e proyectos	(*)Assessment of the report and talk given by the student following the tribunal's recommendation.	15

Other comments on the Evaluation

Sources of information

R.A. Day and B. Gastel, **How to write a scientific paper**, 6th,
W.C. Booth, G.G. Colomb, J.M. Williams, **The Craft of Research**, 3rd,
scopus.com,
A.M. Coghill, L. R. Garson, **The ACS Style Guide: Effective Communication of Scientific Information**, 3rd,

Recommendations