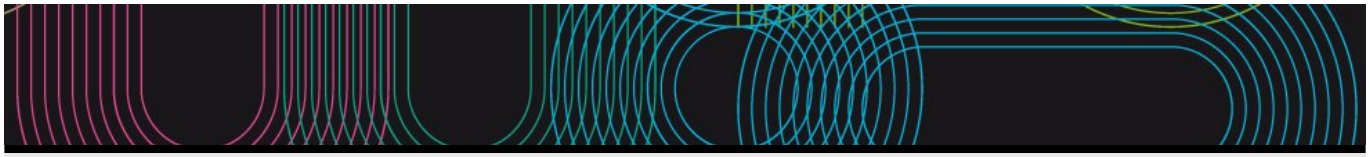

IDENTIFYING DATA				
(*)Ferramentas informáticas e de comunicación en química				
Subject	(*)Ferramentas informáticas e de comunicación en química			
Code	V11G200V01401			
Study programme	(*)Grao en Química			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	6	Mandatory	2nd	2nd
Teaching language	English			
Department				
Coordinator	Estevez Valcarcel, Carlos Manuel			
Lecturers	Estevez Valcarcel, Carlos Manuel Vaz Araújo, Belén			
E-mail	cestevez@uvigo.es			
Web				
General description	The course aims to familiarize students with the use of chemical information sources (scientifical and technical in general) with emphasis on its use through the Internet, as well as with the use of all types of software tools for statistical calculations and chemical modeling . Attention is also paid to the acquisition of important communication skills (writing scientific and technical documents, academic, web design, etc).			

Competencies	
Code	
A20	(*)Avaliar, interpretar e sintetizar datos e información química
A22	(*)Procesar datos e realizar cálculo computacional relativo a información e datos químicos
A23	(*)Presentar material e argumentos científicos de xeito oral e escrita a unha audiencia especializada
A24	(*)Recoñecer e analizar novos problemas e propor estratexias para solucionalos
A29	(*)Demostrar habilidades para os cálculos numéricos e a interpretación dos datos experimentais, con especial énfase na precisión e a exactitude
B1	(*)Comunicarse de forma oral e escrita en polo menos unha das linguas oficiais da Universidade
B2	(*)Comunicarse a nivel básico en inglés no ámbito da Química
B3	(*)Aprender de forma autónoma
B4	(*)Procurar e administrar información procedente de distintas fontes
B5	(*)Utilizar as tecnoloxías da información e das comunicacións e manexar ferramentas informáticas básicas
B6	(*)Manexar as matemáticas, incluíndo aspectos tales como análise de erros, estimacións de ordes de magnitude, uso correcto de unidades e modos de presentación de datos
B7	(*)Aplicar os coñecementos teóricos á práctica
B9	(*)Traballar de forma autónoma
B10	(*) Traballar nun contexto tanto nacional como internacional
B14	(*) Analizar e sintetizar información e obter conclusións
B15	(*)Avaliar de modo crítico e construtivo o entorno e a si mesmo

Learning aims		
Expected results from this subject	Training and Learning Results	
To know the different sources of scientific and technical information	A20	B2 B4 B5 B9 B14

To understand the basics of running a Science library and know how to perform an advanced use of its services		B2 B4 B5 B9 B14
To classify scientific journals based on their theme or objective	A20	B2 B5 B9 B10 B15
To distinguish the different types of contributions to scientific journals (full text articles, brief articles, preliminary communications, etc).		B1 B2 B3 B4 B5 B9 B10
To know the basic characteristics of other sources: technical reports, conference proceedings, patents, dissertations, government publications, standards, videos, dictionaries, encyclopedias, directories, databases and "handbooks".	A20	B2 B5 B10
To know the basic characteristics of other sources: technical reports, conference proceedings, patents, dissertations, government publications, standards, videos, dictionaries, encyclopedias, directories, databases and "handbooks".	A20	B2 B5 B10
To know the structure and function of an abstracting or indexing service	A20	B2 B5 B10
To know the basic characteristics of other sources: technical reports, conference proceedings, patents, dissertations, government publications, standards, videos, dictionaries, encyclopaedias, directories, databases and "handbooks".	A20 A23	B2 B3 B4 B5 B9 B14
To know the basic characteristics of other sources: technical reports, conference proceedings, patents, dissertations, government publications, standards, videos, dictionaries, encyclopaedias, directories, databases and "handbooks".	A20 A23	B2 B3 B4 B5 B9 B14
To know the structure and function of an abstracting or indexing service, in particular the I.S.I. Web of knowledge or the Chemical Abstract Service	A20 A23	B2 B3 B4 B5 B9 B14
To know the basics of the internet's architecture (IP addresses, protocol hierarchies, etc.) and to develop expertise in the use of the essential services of the Internet: remote connections ("telnet" type), file transfer ("ftp", type), web browsers, etc.		B3 B5 B9
To know how to search for different types of online resources: educational, technical or scientific.	A23	B2 B3 B4 B5 B9 B14
To know alternative ways to disseminate the results, for example, the principles of web page design applied to those of technical or scientific interest	A20 A23	B2 B3 B4 B5 B9 B14
To know which items are required in the identification of a scientific paper or patent to be included in an indexing service	A20	B2 B3 B4 B5 B9 B14

Knowing how to use controlled vocabulary	A20 A23	B2 B3 B4 B5 B9 B14
To know how to plan and perform a literature search in bibliographic databases using SciFinder (CAS), WOK (ISI) or other indexing services,	A20 A23 A24	B2 B3 B4 B5 B9 B14
To know how use the web sites of scientific journals	A20	B2 B3 B4 B5 B9 B14
To know how to find and use some databases of chemical interest (molecular and crystal structure, chemical thermodynamics, kinetics, spectroscopy, etc).	A20 A22	B2 B3 B4 B5 B9 B14
To be aware of the different options for managing bibliographic references	A20 A23	B2 B3 B4 B5 B9 B14
To know how to use at least one of the most common reference management software programs to perform the most typical tasks (import / export references, modifying, adding or sorting them).	A20 A23	B2 B3 B4 B5 B9 B14
Knowing the basic principles of the drafting of scientific papers, technical reports, dissertations or master's thesis and, if possible, gaining some expertise in the use of computer templates	A23	B2 B3 B5 B9
To be aware of the present capabilities of the Molecular Modelling software and their relation to the Theoretical Methods of Physical Chemistry.	A22	B2 B3 B4 B5 B9 B14
To know how to use the most straightforward sections and utilities of M.M. software to solve simple chemical problems; the same with chemical processing software.		B5 B6 B7 B9
To know how to use statistical program packages to perform data fitting, graphical and other kinds of statistical analysis	A29	B5 B6 B7 B9 B14

Contents

Topic	
The scietific literature: general aspects.	Structure and classification of the literature. General rules of a literature search. Function, organization and use of a scientific library.

Information Sources	Books. Journals. Technical reports. Conference Proceedings. Patents. Thesis. Government Publications. Standards. Videos. Dictionaries. Directories Encyclopedias Databases
Using Internet	Basic Internet services. Remote connection and file transfer utilities. Search engines. Electronic lists and subscription services. Other services. Structure, function and design of web pages.
Indexing and abstracting services	Identification of a scientific paper. The ISI Web of Knowledge (WOK). The Chemical Abstract Service (CAS) and the Scifinder. Other abstracting services. Handbooks.
Bibliographic Managers	Classification of bibliographic references: general principles. Use of popular software packages: Refworks and Endnote as examples.
Preparation of a scientific, technical or academic document	Parts of a scientific document. References, tables and figures : general principles. Use of computer templates. General aspects of the scientific style and the use of English. How to write: CVs, progress reports, grant requests and other academic documents.
Using Statistical Sofware	2 and 3D graphics. Statistical Analysis. Data fitting.
Chemical and Process Modelling and Simulation	Introduction: what can and should be modelled. Modelling electronic structure Modelling chemical dynamics Modelling Spectroscopy Modelling Chemical Processes

Planning			
	Class hours	Hours outside the classroom	Total hours
Master Session	13	26	39
Practice in computer rooms	26	52	78

Troubleshooting and / or exercises	2	18	20
Others	3	4	7
Long answer tests and development	1.5	4.5	6

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

Methodologies

	Description
Master Session	The theoretical aspects of the subject are presented
Practice in computer rooms	Computer lab exercises: literature searches, use of bibliographic managers, use of statistical packages, report writing.
Troubleshooting and / or exercises	Report or article writing in English language. Simple exercises with modelling software
Others	Issues raised by the students are discussed and clarified

Personalized attention

Methodologies	Description
Practice in computer rooms	The student is helped by providing adequate guidelines. Since all lectures are given in the computer room, the student will be helped mostly there in a practical and effective way.
Others	The student is helped by providing adequate guidelines. Since all lectures are given in the computer room, the student will be helped mostly there in a practical and effective way.
Troubleshooting and / or exercises	The student is helped by providing adequate guidelines. Since all lectures are given in the computer room, the student will be helped mostly there in a practical and effective way.

Assessment

	Description	Qualification
Practice in computer rooms	Typically, literature searches	40
Troubleshooting and / or exercises	Tipically, database searches and use of utilities of modelling software.	20
Long answer tests and development	Written exam consisting of short questions.	40

Other comments on the Evaluation

Attendance at practical lectures (seminars) is compulsory. The student will be given a rating (0-10) as long as he/she has attended 3 or more seminar sessions, has delivered at least two reports on the exercises or practices proposed by the teacher or has done a written exam.

If the student fails in the first call he/she will be asked to improve some of the exercises or perform new ones provided by the teacher. In addition he/she will have to undergo a more thorough exam, which will weight 50% of the final grade.

Sources of information

Douville, J.A., **The literature of chemistry**, 1st,

Kaplan, S.M., **The English-Spanish Spanish-English dictionary of chemistry**, 1st,

Maizell, R.E., **How to find chemical information: a guide for practising chemists, educators and students**, 3d,

Day, R.A.; Gastel, B., **How to write and publish a scientific paper**, 6th,

Hirst, D.M., **A Computational approach to chemistry**, 1st,

Cramer, C.J., **Essentials of Computational Chemistry: Theories and Models**, 2nd,

References 1,2 and 4, are considered "basic". A list "topic dependent" references (including other web resources and software) will be handed to the student in due course.

Recommendations

Subjects that are recommended to be taken simultaneously

(*)Química física II/V11G200V01403

Subjects that it is recommended to have taken before

(*)Física III/V11G200V01301
(*)Química física I/V11G200V01303