

60455 - Bibliographic resources and databases

Información del Plan Docente

Academic Year	2016/17
Academic center	100 - Facultad de Ciencias
Degree	543 - Master's in Molecular Chemistry and Homogeneous Catalysis
ECTS	2.0
Course	1
Period	First semester
Subject Type	Optional
Module	---

1. Basic info

1.1. Recommendations to take this course

Class attendance and resolution of the exercises that teachers propose for each database are mandatory.

1.2. Activities and key dates for the course

The information about schedules, calendars and exams is available at the websites of the Sciences Faculty, <https://ciencias.unizar.es/calendario-y-horarios> , and the Master, <http://masterqmch.unizar.es> .

Controls and supervised individual or iteam-based practical work related to different bibliographic resources will be made throughout the course. The presentation of practical works will be done according to the schedule to be announced well in advance.

2. Initiation

2.1. Learning outcomes that define the subject

The student must identify how to access and manage different types of library resources available.

The student must recognize how to plan a literature search on specific research topics, and to select the databases of adequate scientific data.

The student should discern how to analyze and classify the information obtained, and to distinguish the most useful in each case.

The student must practice reference management software in order to organize bibliographic cites.

2.2. Introduction

Chemical search information is a set of operations that aim to make available to the student/researcher adequate information to answer permanent or occasional questions work-related. In this course, the students acquire basic skills in handling information that will be of great use to your research and your future professional practice.

The purpose of the search and the subject on which we have to locate information determine the type of information sources to be consulted (statistics, books, monographs, journal articles, dissertations ...) and therefore the resources that allow to access them. The development of new technologies and ease of web publishing, coupled with the wealth of information available, require to access resources that guarantee, through a previous selection processes prior, the

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recovery of reliable quality information, such as catalogues or databases.

3.Context and competences

3.1.Goals

The aim of the course is that students develop research skills in both general and specific bibliographic resources, and they acquire the necessary abilities to develop research skills in an autonomous way, one of the basic proposals put forward by the European Higher Education Area.

3.2.Context and meaning of the subject in the degree

The course is part of the Structural Characterization Module. This is a cross optional course of 2 ECTS taught in the first term which intend to give students the fundamental tools to carry out chemical researches, regardless of the particular area that are going to specialize later. It is essential to know how to access to available scientific information in a reliable manner and how to manage it.

3.3.Competences

To be able to recognize and to determine what information is needed in a given context.

Capacity to locate potential sources of information in their discipline, both general and specialized (search engines, databases, specialized information resources) and to use the most appropriate.

To choose tools and design appropriate information search strategies according to the needs and to access available sources.

To understand and to select the information obtained. To organize and present a clear, accurate and legible report including citing sources and background documents employees.

To use and to understand the importance, for both future own activity and coworkers, of reference management software in order to organize bibliographic references.

To evaluate critically the effectiveness, efficiency and quality of both the search process and the information obtained. To optimize information searches.

3.4.Importance of learning outcomes

Learning outcomes obtained in this course are key in order to have an overview of a specific problem. Essential skills for current students and professionals are developed. In this context, it is a contemporary subject that intends to fulfill the current demand of exigency, competitiveness and ability to communicate in an international environment.

4.Evaluation

The continuous assessment of this course is based on the following activities, weighted as indicated:

1. Formative evaluation by themes: based on self-assessment exercises that measure the gradual acquisition of theoretical knowledge, as well as exercises and practical activities (50%)
2. Final evaluation of global exercises that include all databases to be realized at the end of the classes (50%)

The students that have not passed the subject or wish to improve their score have the option to carry out a global test either in the first or the second call. This test will consist on the presentation of the information required in different global exercises that entail the management of databases used throughout in a critical way.

The number of official examination calls per registration and their use will be subjected to the statements of the

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Regulation of Permanence in Master Studies and [Regulation of the Learning Assessment](#) . The latest document will also regulate the general design and scoring criteria of the assessment activities, as well as the exam schedules and timetable for the post-examination review.

5. Activities and resources

5.1. General methodological presentation

The classroom training activities will consist of interactive lectures that allow students to know the possibilities offered by the available library resources. In addition, the supervised resolution of a set of exercises, individually or in small groups, will be carried out in the classroom and, more general, self-assessment on homework.

The course requires online access to several databases, so the classes are held in the computer room and, whenever possible, with an individual access to each database by the student. The aim is that the students can follow teacher's explanations interactively from their own computer.

Personal study is facilitated with teaching materials accessible in a web environment.

5.2. Learning activities

Interactive lectures (0.8 ECTS).
Problem-solving sessions (0.4 ECTS).
Computer practices (0.8 ECTS).
Small groups or customized tutoring.

5.3. Program

1. Introduction to Computational Chemistry.
2. Introduction to computational environments and programs of use in chemistry.
3. The concept of potential energy surface.
4. Empirical methods: Molecular mechanics, fundamentals, applications and limits.
5. Quantum chemistry methods: WFT y DFT.
6. Analysis of output: Study of wavefunction. Molecular properties.
7. Solvation and solvent effects.
8. Applications to structural analysis, molecular reactivity and reaction mechanisms.
- 9 . Use of computational chemistry programs.

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5.4.Planning and scheduling

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The students will be provided with different scholar material either at reprography or through the University's web tool: <https://moodle2.unizar.es/add>.

5.5.Bibliography and recommended resources

SciFinder Training Materials. Available in: <http://www.cas.org/training/scifinder>

ScienceDirect Training Tutorials. Available in: <http://trainingdesk.elsevier.com/products/ScienceDirect>

Beilstein and Gmelin Databases. Further information at: <http://www.columbia.edu/itc/chemistry/chem-tutorial/beilstein.html>

Cambridge Crystallographic Data Centre (CCDC). General information and user guide: <https://www.ccdc.cam.ac.uk/pages/Home.aspx> , <https://www.ccdc.cam.ac.uk/Lists/DocumentationList/conquest116.pdf>

Inorganic Crystal Structure Database (ICSD). General information and user guide: http://www.fiz-karlsruhe.de/icsd_home.html , http://www.fiz-karlsruhe.de/fileadmin/be_user/ICSD/PDF/sci_man_ICSD_v1.pdf

Cómo Interpretar Referencias Bibliográficas. Available in: <http://biblioteca.unizar.es/buscar/referencias.php>

Gestores Bibliográficos. <http://biblioteca.unizar.es/buscar/gestores.php> .

Help Guides: Refworks, <http://biblioteca.unizar.es/buscar/gestores/refworks.php> ; Mendeley, http://www.americalatina.elsevier.com/sul/es/mendeley/3288_Mendeley_User_Guide_ES.pdf

Guía rápida de uso del catálogo de la Biblioteca de la Universidad de Zaragoza. http://biblioteca.unizar.es/documentos/guia_catalogo.pdf

Motores de búsqueda de información científica y académica. L. Codina. "Hipertext.Net", Nº 5, 2007. <http://www.upf.edu/hipertextnet/numero-5/accesibilidad.html>

Cómo elaborar, un trabajo académico. Material de Autoformación biblioteca Universidad Carlos III de Madrid. http://portal.uc3m.es/portal/page/portal/biblioteca/aprende_usar/autoformacion , <http://uc3m.libguides.com/TFM/> .