

60455 - Bibliographic resources and databases

Información del Plan Docente

Academic Year	2017/18
Faculty / School	100 - Facultad de Ciencias
Degree	543 - Master's in Molecular Chemistry and Homogeneous Catalysis
ECTS	2.0
Year	1
Semester	First semester
Subject Type	Optional
Module	---

1.General information

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

1.2.Recommendations to take this course

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

1.3.Context and importance of this course 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.

1.4.Activities and key dates

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.Learning goals

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2.1. Learning goals

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. Importance of learning goals

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.

3. Aims of the course and competences

3.1. Aims of the course

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. 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.

4. Assessment (1st and 2nd call)

4.1. Assessment tasks (description of tasks, marking system and assessment criteria)

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.

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The number of official examination calls per registration and their use will be subjected to the statements of the *Regulation of Permanence in Master Studies* and the *Regulation of the Learning Assessment* (<http://www.unizar.es/ice/images/stories/calidad/Reglamento%20Evaluacion.pdf>). 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. Methodology, learning tasks, syllabus and resources

5.1. Methodological overview

The methodology followed for this course will consist of interactive lectures that allow students to know the possibilities offered by the available library's resources. In addition, the supervised solving of a set of exercises, individually or in small groups, will be carried out in the classroom as well as 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 the teacher's explanations interactively from their own computer.

Classroom materials will be available via Moodle. These include a repository of the lecture notes used in class, the course syllabus, as well as other course-specific learning materials, for the students' personal study.

5.2. Learning tasks

The course includes the following learning tasks:

- Interactive lectures (0.8 ECTS).
- Problem-solving sessions (0.4 ECTS).
- Computer practice sessions (0.8 ECTS).
- Small group or individualized tutorials.

5.3. Syllabus

The course will address the following topics:

Topic 1. Introduction to Computational Chemistry.

Topic 2. Introduction to computational environments and programs of use in chemistry.

Topic 3. The concept of potential energy surface.

Topic 4. Empirical methods: Molecular mechanics, fundamentals, applications and limits.

Topic 5. Quantum chemistry methods: WFT y DFT.

Topic 6. Analysis of outputs: Study of wavefunction. Molecular properties.

Topic 7. Solvation and solvent effects.

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Topic 8. Applications to structural analysis, molecular reactivity and reaction mechanisms.

Topic 9. Use of computational chemistry programs.

5.4. Course planning and calendar

Further information concerning the timetable, classroom, assessment dates and other details regarding this course, will be provided on the first day of class or please refer to the Faculty of Science <https://ciencias.unizar.es/calendario-y-horarios>, and the Master's, <http://masterqmch.unizar.es>.

Students will be provided with different teaching material either at reprography or through the University's virtual platform <https://moodle2.unizar.es/add>.

5.5. Bibliography and recommended resources

URLs LIST:

Data Base Reaxys. <https://www.elsevier.com/solutions/reaxys>

Chemistry Data Bases access from Library of the University of Zaragoza. http://roble.unizar.es/search*spi~S11/d?SEARCH=Quimica

Cambridge Crystallographic Data Centre (CCDC). General information and user guide. <http://www.ccdc.cam.ac.uk/pages/Home.aspx>

How to understand Bibliographic References. <http://biblioteca.unizar.es/ayuda-y-formacion/referencias>

Elsevier ScienceDirect Learn & Support. <https://www.elsevier.com/solutions/sciencedirect/support>

Bibliographic References Managers. <http://biblioteca.unizar.es/node/606>

Quick guide to the use the catalog of the Library of the University of Zaragoza. http://biblioteca.unizar.es/sites/biblioteca.unizar.es/files/documentos/guia_catalogo.pdf

Inorganic Crystal Structure Database (ICSD). General information and user guide. <http://www.fiz-karlsruhe.de/icsd.html>

Lluís Codina. Search engines for scientific and academic information online. "Hipertext.net", núm. 5, 2007. <http://www.hipertext.net>

<http://www.upf.edu/hipertextnet/numero-5/motores-busqueda.html>

Scifinder Training Materials. <http://www.cas.org/training/scifinder>

University Carlos III. Library guide to support UC3M students in their Master's Degree Work.

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<http://uc3m.libguides.com/TFM/>