# COURSE DATA

## DATA SUBJECT

**Code:** 44709
**Name:** Computational organic chemistry
**Cycle:** Master's Degree
**ECTS Credits:** 4
**Academic year:** 2026-27

## STUDY (S)

| Degree | Center | Acad. year | Period |
| --- | --- | --- | --- |
| 2226 - Master's degree in Organic Chemistry | Facultat de Química | 1 | Annual |

## SUBJECT-MATTER

| Degree | Subject-matter | Character |
| --- | --- | --- |
| 2226 - Master's degree in Organic Chemistry | Computational organic chemistry | COMPULSORY |

## COORDINATION

ESCORIHUELA FUENTES JORGE

# SUMMARY

The subject Computational Chemistry deals with the study of different computational techniques as useful tools in the study of chemical properties and mechanistic studies with high interest in the rational drug design.

# PREVIOUS KNOWLEDGE

## RELATIONSHIP TO OTHER SUBJECTS OF THE SAME DEGREE

There are no specified enrollment restrictions with other subjects of the curriculum.

## OTHER REQUIREMENTS

The subject Computational Chemistry requires a solid background in Organic Chemistry and Biochemistry

# COMPETENCES / LEARNING OUTCOMES

Ampliar los conceptos básicos en los que se apoyan las diferentes técnicas computacionales, especialmente aquellas empleadas en Química Orgánica como herramientas útiles en estudios de propiedades químicas y estudios mecanísticos.

Be able to access to information tools in other areas of knowledge and use them properly.

Competencias de gestión tales como la capacidad para la planificación y gestión de tiempo y recursos, así como para dirigir y tomar decisiones.

Conocer las bases químicas para el diseño racional de fármacos mediante la utilización de técnicas computacionales y de modelado molecular.

Poseer habilidades sociales, un buen nivel de comunicación oral y escrita, así como capacidad para trabajar en equipo y con personas de diferentes procedencias.

Saber participar en debates y discusiones, dirigirlos y coordinarlos y ser capaces de resumirlos y extraer de ellos las conclusiones más relevantes y aceptadas por la mayoría.

Ser capaces de valorar la necesidad de completar su formación científica, en lenguas, en informática, asistiendo a conferencias o cursos y/o realizando actividades complementarias, autoevaluando la aportación que la realización de estas actividades supone para su formación integral.

Students should apply acquired knowledge to solve problems in unfamiliar contexts within their field of study, including multidisciplinary scenarios.

Students should be able to integrate knowledge and address the complexity of making informed judgments based on incomplete or limited information, including reflections on the social and ethical responsibilities associated with the application of their knowledge and judgments.

Students should communicate conclusions and underlying knowledge clearly and unambiguously to both specialized and non-specialized audiences.

Students should demonstrate self-directed learning skills for continued academic growth.

Students should possess and understand foundational knowledge that enables original thinking and research in the field.

Use different presentation formats (oral, written, slide presentations, boards, etc.) to communicate knowledge, proposals and positions.

## DESCRIPTION OF CONTENTS

### 1. Computational Organic Chemistry. Introduction

Introduction. Concepts. Relationship with other areas. Pharmaceutical Industry applications.

Computational biological chemistry. Drug Discovery and design.

## 2. Quantum Chemistry

Quantum chemistry. Methods in quantum mechanics. Ab initio methods. Semi-empiric methods. Density functional theory (DFT) methods. Exploration of potential energy surfaces: energy minima and transition states. Reaction mechanisms. Electronic properties. Thermodynamic properties. Solvation models.

## 3. Molecular mechanics

Molecular mechanics. Forces fields. Bonding terms. No bonding terms. Force fields parametrization. Energy optimization. Conformational analysis. Molecular dynamics. Treatment of the solvent effect. Trayectory analysis. Hybrid methods QM/MM

## 4. Computational chemistry in drug design.

Computational chemistry in drug design. Molecular recognition. Ligand-receptor interactions. Structure-activity relationship. Drug-like properties of the products. Generation of molecules. Molecular description. Drug design based on the structure of data bases, macromolecule-ligand interactions, protein-ligand and protein-protein docking, virtual screening. Drug design based on the ligand: QSAR-2D, QSAR.3D, pharmacophores. Macromolecules modeling. Structure prediction. Combination of experimental data: NMR and X-Ray crystalography

## 5. Practice

PRACTICE PROGRAM (informatics classroom): molecular modeling and determination of some properties of organic compounds and drugs. Studies of organic reaction mechanisms. Visualization and handling of ligand-receptor complexes. Protein-ligand and protein-protein Docking. Identification of relevant interactions in molecular recognition processes. Use of bibliographic data bases of 3D structures. Use of informatics resources for the calculation of drug-like properties of organic compounds

# WORKLOAD

## PRESENCIAL ACTIVITIES

| Activity | Hours |
|---|---|
| Theory | 20,00 |
| Seminar | 20,00 |
| **Total hours** | **40,00** |

## NON PRESENCIAL ACTIVITIES

| Activity | Hours |
|---|---|
| Attendance at other activities | 0,00 |
| Individual or group project | 10,00 |
| Independent study and work | 40,00 |
| Preparation of lessons | 0,00 |
| Preparation for assessment activities | 10,00 |
| Resolution of case studies | 0,00 |
| **Total hours** | **60,00** |

# TEACHING METHODOLOGY

The subject is formulated in a manner that the student is the principal actor of its own learning. From the beginning of the course, students will have the whole didactic material necessary and the teaching will be structured in the following manner:

• Master classes (in person): In these classes the basic concepts of the subject will be introduced. Theoretical themes will be imparted, developing the contents of the program with the aid of Power Point presentations. Additionally, chemoinformatic resources and web pages will be also employed.

Active participation of the students will be encouraged by means of question proposal related to the application of previously acquired concepts. Furthermore, the establishment of discussions will be also promoted.

• Seminars (in person).- Seminars will be imparted with the aim to get a closer interaction between the teacher and the students. In those seminars, we intend that the students apply some of the acquired knowledge by means of the use of some computational tools: Gaussian. GaussView, DS Visualizar, RasMol, Molekel, AutoDock, Glide, Amber, etc. This activity will be dedicated to the resolution of problems and questions with an active participation of the students.

• Written assignment.-

In those assignments, the student will show the knowledge of the imparted concepts and the use of computational techniques explained during the course

# EVALUATION

The assessment of the subject will be carried out through a combination of written tests, individual assignments, and oral presentations, with the aim of evaluating both the theoretical knowledge and practical skills of the students. The assessment criteria and weightings will be as follows:

**Multiple-choice exam (60%)**
A written exam in the form of a questionnaire will be administered, including multiple-choice questions. The purpose of this exam is to assess the students understanding of the theoretical content covered throughout the course.

**Submission of a Report (20%)**
Students will be required to write and submit a report in which they apply the knowledge acquired, developing a critical analysis or a practical proposal related to the subject matter.

**Oral presentation of published Work (20%)**
Students must select a published academic paper or article related to the subject and deliver an oral presentation on it. The presentation will be evaluated based on synthesis ability, clarity of exposition, subject mastery, and the ability to answer questions.

To pass the subject, students must obtain a minimum score of 4 out of 10 in each of the three components and a weighted average of at least 5 out of 10.

## REFERENCES


- Frank Jensen, Introduction to Computational Chemistry, 3rd Edition, John Wiley & Sons, Inc., 2016.
- Christopher J. Cramer, Essentials of Computational Chemistry: Theories and Models, 2nd Edition, John Wiley & Sons, Inc., 2004
- David C. Young. Computational Drug Design. A Guide for Computational and Medicinal Chemists, John Wiley & Sons, Inc., 2009.
- Andrew R. Leach, Molecular Modelling, Principles and Applications, 2nd Edition, Pearson, Prentice, Hall, 2001.
- Guy H. Grant, W. Graham Richards, Computational Chemistry. Oxford University Press, 1996.
- Steven M. Bachrach. Computational Organic Chemistry. Wiley-Blackwell. 2007.

- J. Naidoo, John Brady, Martin J. Field, Jiali Gao, and Michael Hann. Modelling Molecular Structure and Reactivity in Biological Systems. Royal Society of Chemistry Cambridge. 2006.
- Errol G. Lewars. Computational Chemistry: Introduction to the Theory and Applications of

Molecular and Quantum Mechanics. Springer. 2nd ed. 2011.
- S. L. Schreiber, T. M. Kapoor, G. Wess. Chemical Biology: From Small Molecules to Systems Biology and Drug Design. Wiley. 2007.
- Raimund Mannhold (Editor) (2008). Molecular Drug Properties: Measurement and Prediction. Wiley/VCH, Weinheim, Germany
- David Young. Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems. WileyBlackwell. 2009.
- Gaussian Website: http://www.gaussian.com/
- AutoDock Website: http://autodock.scripps.edu/
- The World Association of Theoretical and Computational Chemists, WATOC. http://www.ch.ic.ac.uk/watoc/.index.html
- Amber Molecular Dynamics package Website: www.ambermd.org
- Zdock Website: http://zdock.umassmed.edu/
- Protein Data Bank: (http://www.rcsb.org)
- Cambridge Structural Database System: http://www.ccdc.cam.ac.uk/prods/csd/csd.html
- Drug Bank: http://www.drugbank.ca