COURSE DATA

Data Subject	
Code	44709
Name	Computational organic chemistry
Cycle	Master's degree
ECTS Credits	4.0
Academic year	2022 - 2023

Study (s)

Degree	Center	Acad. year	Period
2226 - M.D. in Organic Chemistry	Faculty of Chemistry	1	Annual

Subject-matter

Degree	Subject-matter	Character
2226 - M.D. in Organic Chemistry	5 - Computational organic chemistry	Obligatory

Coordination

Name	Department
DEL POZO LOSADA, CARLOS	325 - Organic Chemistry

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

OUTCOMES

2226 - M.D. in Organic Chemistry

- 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.
- Be able to access to information tools in other areas of knowledge and use them properly.
- 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.
- Poseer habilidades sociales, un buen nivel de comunicación oral y escrita, así como capacidad para trabajar en equipo y con personas de diferentes procedencias.
- Competencias de gestión tales como la capacidad para la planificación y gestión de tiempo y recursos, así como para dirigir y tomar decisiones.
- 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.
- 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.
- Conocer las bases químicas para el diseño racional de fármacos mediante la utilización de técnicas computacionales y de modelado molecular.

LEARNING OUTCOMES

- Knowledge of the basic concepts where the different computational techniques are sustained, specially those used in Organic Chemistry and Chemical Biology related with the Pharmaceutical Industry, as useful tools in the study of chemical properties and mechanistic studies.

. Knowledge of the chemical bases for the rational drug design and for the understanding of molecular recognition processes of biological interest through the use of computational techniques and molecular modeling.

- Design, selection and/or development products and chemical processes efficiently (ODS 7) that minimize their impact in the environment (ODS 14 and 15), taking advantage of the alternative row materials and generating the minor amount of residues possible (ODS 11)

- Knowledge of some techniques uses in the study of molecular recognition of biological processes with relevance for drug design

- Ability of the students to combine NMR data with the ones obtained through computational chemistry techniques and molecular modeling for the understanding, at atomic level, of the structural requirements of ligand-receptor molecular recognition with biomedical interest and therefore, make progress in drug design and understanding of biological processes.

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. DFT. Exploration of potential energy sufaces: energy minima and transition states. Electronic properties. Thermodinamic properties

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

ACTIVITY	Hours	% To be attended
Theory classes	20,00	100
Seminars	20,00	100
TOTAL	**40,00**	

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

There will be a continuous evaluation based on the following and interaction with the students throughout the on-site classes (25%). Furthermore, written assignments will weight 25%, questionnaires and informs have to be done for the students as personal work (50% weight). Final evaluation of the students will be a summary of all of those activities and work.

REFERENCES

Basic

- Andrew R. Leach, Molecular Modelling, Principles and Applications, 2nd Edition, Pearson, Prentice Hall, 2001.
- Grant, G.H.; Richards, W.G.; Computational Chemistry. Oxford University Press, 1996.
- David C. Young. Computational Drug Design. A Guide for Computational and Medicinal Chemists. John Wiley & Sons, Inc., Hoboken, NJ. 2009.
- Steven M. Bachrach. Computational Organic Chemistry. Wiley-Blackwell. 2007.

Additional

- 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