Universitat Autònoma de Barcelona

2022/2023

Advanced Chemistry

Code: 42429
ECTS Credits: 9

Degree	Type	Year	Semester
4313385 Industrial Chemistry and Introduction to Chemical Research	OT	0	1

Contact

Name: Montserrat Lopez Mesas

Email: montserrat.lopez.mesas@uab.cat

Use of Languages

Principal working language: english (eng)

Teachers

Joan Carles Bayón Rueda

Marta Figueredo Galimany

Agustí Lledos Falco

José Peral Perez

Joan Pau Bayon Rueda

Maria Jose de Montserrat Esplandiu Egido

José Vidal Gancedo

Roger Bofill Arasa

Maria del Mar Puyol Bosch

Gregori Ujaque Perez

Gonzalo Guirado Lopez

Míriam Pérez Trujillo

Ona Illa Soler

Manel Alcala Bernardez

Maria Jesús Sánchez Martín

Prerequisites

The student must hold a Bachelor's degree in Sciences or Biosciences, preferred Chemistry, Material Science, Nano-science, Biotechnology or Environmental Sciences

- Intermediate english level

Objectives and Contextualisation

Advanced essential chemistry topics are studied for carrying out interdisciplinary chemical research.

Competences

- Correctly apply new information capture and organisation technologies to solve problems in professional activity.
- Define specialised concepts, principles, theories and facts in the different areas of Chemistry.
- Evaluate responsibility in the management of information and knowledge in the field of Industrial Chemistry and Chemical Research.
- Identify information in the scientific literature using the appropriate channels and integrating said information to approach and contextualise a research issue.
- Innovate in chemical synthesis and analysis methods related with different areas of Chemistry.
- Possess and understand knowledge that provides a basis or opportunity for originality in the development and/or application of ideas, often in a research context
- Propose alternatives for the solving of complex chemical problems in different chemical specialities.
- Student should possess an ability to learn that enables them to continue studying in a manner which is largely self-supervised or independent
- Students should know how to apply the knowledge acquired and the capacity to solve problems in new or little-known areas within broader (or multidisciplinary) contexts realted to thier area of study
- Students should know how to communicate their conclusions, knowledge and final reasoning that they hold in front of specialist and non-specialist audiences clearly and unambiguously
- Use scientific terminology in the English language to defend experimental results in the context of the chemistry profession.

Learning Outcomes

1. Correctly apply new information capture and organisation technologies to solve problems in professional activity.
2. Elucidate the structure of complex chemical compounds on the basis of the appropriate chemical analysis and structural determination techniques.
3. Evaluate responsibility in the management of information and knowledge in the field of Industrial Chemistry and Chemical Research.
4. Identify information in the scientific literature using the appropriate channels and integrating said information to approach and contextualise a research issue.
5. Implement strategies for chemical analysis for the study of specific systems.
6. Interfaces characterize and describe the chemical reactions on the surface
7. Possess and understand knowledge that provides a basis or opportunity for originality in the development and/or application of ideas, often in a research context
8. Recognize properties of conventional solvents, ionic liquids and supercritical fluids.
9. Recognize special catalytic processes applied to the synthesis.
10. Student should possess an ability to learn that enables them to continue studying in a manner which is largely self-supervised or independent
11. Students should know how to apply the knowledge acquired and the capacity to solve problems in new or little-known areas within broader (or multidisciplinary) contexts realted to thier area of study
12. Students should know how to communicate their conclusions, knowledge and final reasoning that they hold in front of specialist and non-specialist audiences clearly and unambiguously
13. Use numeric methods in the study of chemical reactions.
14. Use scientific terminology in the English language to defend experimental results in the context of the chemistry profession.
15. Using different microscopy and spectroscopy techniques to the study of materials and biomolecules

Content

- Chemical speciation, non destructive analysis, miniaturization

- Chemometrics

- Surface chemistry (heterogeneous catalysis, self-assembled monolayers)

- Conventional and non-conventional solvents

- Applications of computational techniques in chemistry.

- Structure determination in chemistry (NMR, EPR, Microscopy)

- Synthesis and catalysis (Basic principles and strategies in the design of organic synthesis, Stereoselective synthesis, Homogeneous catalysis, Non-aromatic and aromatic carbo- and heterocycles, Total synthesis)

Methodology

Design and train of oral presentations

Theorical and excersise lectures

Collaborative activities and seminars

Annotation: Within the schedule set by the centre or degree programme, 15 minutes of one class will be reserved for students to evaluate their lecturers and their courses or modules through questionnaires.

Activities

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Collaborative activities and seminars	56	2.24	1, 2, 4, 11, 12, 10, 7, 13, 14, 3
Type: Supervised			
Design and train of oral presentations	6	0.24	1, 2, 4, 11, 12, 10, 7, 13, 14, 3
Type: Autonomous			
Theoretical and exercise lectures	137	5.48	1, 2, 4, 11, 12, 10, 7, 13, 14, 3

Assessment

- Every professor decides the number and typology of evaluation activities: oral presentations, written exams, delivery of discussed articles, small tests...

- The final mark of the module will be the sum of the mark of every professor multiplied by the percentage of his classes in the total teaching of the module. It should be higher than 5.0 to pass.

- The marks of the written exams of the individual matters must be above 3.5 in order to average with other marks of the professor and/or the module.

- There will be a period in January to repeat written exams with marks under 5.0. In the case of exams under 3.5 will be mandatory to the student, in case of exams between 3.5 and 5.0 would be optional to the student.

- In the case that a student will not arrive to a 3.5 mark after the retaking exam in January, the coordinator of the module could decide to average this mark with the rest of the module. However, this option can only be considered for two written exams in the whole master.

- The marks of other evaluations activities (i. e. oral presentations) will average with the rest of the marks of the professor/module independently of the value. There will not be option of repeating these other evaluation activities.

- When the student does not reach a minimum of two thirds of the total activitites of the module, the mark will be considered "not avaluated".

VERY IMPORTANT: Partial or total plagiarising will immediately result in a FAIL (0) for the plagiarised exercise (first-year students) or the WHOLE subject (second-, third- and fourth-year students). PLAGIARISING consists of copying text from unacknowledged sources -whether this is part of a sentence or a whole text - with the intention of passing it off as the student's own production. It includes cutting and pasting from internet sources, presented unmodified in the student's own text. Plagiarising is a SERIOUS OFFENCE. Students must respect authors' intellectual property, always identifying the sources they may use; they must also be responsible for the originality and authenticity of their own texts.

In the event of a student committing any irregularity that may lead to a significant variation in the grade awarded to an assessment activity, the student will be given a zero for this activity, regardless of any disciplinary process that may take place. In the event of several irregularities in assessment activities of the same subject, the student will be given a zero as the final grade for this subject.

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Exams, oral presentations and reports	100	26	1.04	1, 5, 6, 2, 4, 11, 12, 10, 9, 8, 7, 15, 13, 14, 3

Bibliography

- S. Warren, *Organic Synthesis: The Disconnection Approach*,John Wiley & Sons, 1982
- E.J. Corey, X.-M. Cheng: *The Logic of Chemical Synthesis*, Wiley - Interscience, 1989
- Paul Wyatt, S. Warren: *Organic Synthesis: Strategy and Control*, John Wiley & Sons, 2007
- J. Clayden, N. Greeves, S. Warren: *Organic Chemistry*, Chap. 30, Oxford University Press, 2nd Edition, 2012
- Nicolaou, K. C.; Sorensen, E. J. *Classics in Total Synthesis. Targets, Strategies, Methods*, VCH, Weinheim, 1996
- Nicolaou, K. C.; Snyder, S. A. *Classics in Total Synthesis II. More Targets, Strategies, Methods*, 2003
- Wiley & VCH. Weinheim, 2003
- Any general book of Organic Chemistry to consult reactions
- J.A. Weil, J.R. Bolton, E. Wertz. "Electron Spin Resonance, Elementary Theory and Practical Applications". 2ª Ed., John Wiley & Sons, New York, 1994.
- N.M. Atherton. "Electron Spin Resonance, Theory and Applications". John Wiley, 1994.
- Introduction to Surface Chemistry and Catalysis, 2nd Edition, G.A. Somorjai, Y. Li, Wiley, 2010, ISBN: 978-0-470-50823-7
- G. Ramis y M.C. García. Quimiometría, Síntesis, España (2001).
- C.Mongay, Quimiometría,U. Valencia, 2005
- J.C. Miller and J.N. Miller. Statistics and chemometrics for analytical chemistry 4rd ed., Prentice Hall, Essex, England (2000). Versión traducida (2002).
- D.L. Massart, B.G.M. Vandegiste, L.M.C. Buydens, S.Dejong, P.J. Lewi and J. Smeyers- Verbeke. Handbook on Chemometrics and Qualimetrics, Elsevier, Amsterdam (1997).
- Introduction to Computational Chemistry, F. Jensen, Wiley 2002
- Essentials of Computational Models, Theories and Models, Wiley, 2004

Software

ChemDraw Professional 17.0

https://chemaxon.com/products/marvin

https://www.acdlabs.com/resources/freeware/chemsketch/index.php

Gaussian

COPASI

TopSpin 4.0 - NMR software for academia