Universidad Zaragoza

Academic Year/course: 2021/22

60450 - Synthetic strategies in advanced organic chemistry

Syllabus Information

Academic Year: 2021/22
Subject: 60450 - Estrategias en síntesis orgánica avanzada
Faculty / School: 100 - Facultad de Ciencias
Degree: 543 - Master's in Molecular Chemistry and Homogeneous Catalysis
ECTS: 6.0
Year: 1
Semester: First semester
Subject Type: Compulsory
Module:

1. General information

1.1. Aims of the course

This subject constitutes one of the fundamental pillars of the Master in *Molecular Chemistry and Homogeneous Catalysis*, since it provides the knowledge to address the synthesis of organic molecules from simply precursors, a field of growing interest in chemical research. The student should be able to propose an experimental procedure to synthesize a new or existing molecule using tools of Organic Chemistry, Organometallic Chemistry and Catalysis.

These approaches and objectives agree with the following Sustainable Development Goals (SDGs) of the United Nations Agenda 2030 (https://www.un.org/sustainabledevelopment/es/), in such a way that the acquisition of the learning results of this subject provides training and competence to contribute to a certain extent to its achievement. Goal 3: Health and well-being, Goal 7: Affordable and clean energy and Goal 13: Climate Action.

1.2. Context and importance of this course in the degree

The subject S*ynthetic strategies in advanced organic chemistry* is included in the mandatory module *Molecular Chemistry and Catalysis* and is lectured in the first quarter with a teaching load of 6 ECTS: 3 ECTS theoretical and 3 ECTS problem-solving.

Research aimed to the preparation of organic molecules with specific properties is a field of great interest, both academically and in the industry: pharmaceutical products, cosmetic, photovoltaic materials, polymers, food industry, etc.

1.3. Recommendations to take this course

The knowledge of the basic concepts of Organic Chemistry (structure and reactivity of the mail functional groups and chemical bond theory) is recommended.

Continuous work and class attendance, especially the resolution of the proposed problems, facilitates the success in this course.

2. Learning goals

2.1. Competences

a) To identify the different available tools for the preparation of organic molecules

b) To integrate the acquired knowledge in Organic Chemistry, Organometallic Chemistry and Catalysis and apply them to solving problems related to the organic synthesis.

c) To design reasonable synthetic routes for the preparation of organic molecules starting from common or easily prepared products. Student should be able to predict the stereochemistry of a reaction as well as to select the right reagent basing on structural and mechanistic criteria.

d) To assimilate and evaluate critically research findings in Molecular Chemistry and Catalysis.

e) To develop experimental protocols of advanced organic synthesis.

f) To know the use of update scientific bibliography and database in order to apply them in a specific synthetic problem.

2.2. Learning goals

To overcome the subject:

a) The student must know the principles of retrosynthesis and, how to apply them to the synthesis of an organic molecule from readily accessible starting products.

b) The student must know the usual synthetic methods to build the carbon skeleton in organic molecules (linear chains, rings, formation of carbon-carbon bonds) and the interconversion of the most important functional groups.

c) The student should make use of basic organic synthetic chemistry tools, taking into account the compatibility and incompatibility between the present functional groups.

d) The student must know the mechanism of the organic reactions and its relationship with issues such as: chemoselectivity, regioselectivity and stereoselectivity.

e) The student should be able to solve practical problems and general issues of synthetic organic chemistry.

f) The student must propose reasonable synthetic procedures for a relative complex organic compound, taking into account the stereochemistry of each step.

g) The student should be able to conduct a critical analysis of the different synthetic alternatives for the same compound and to defend the final proposal synthesis.

h) The student should be able to conduct a critical analysis of the synthesis described in the scientific literature for a product of interest.

i) The student should be able to obtain information from literature sources and base data, and include that information in reports or presentations.

The student should be able to elaborate experimental procedures for a given organic molecule.

2.3. Importance of learning goals

One of the most important challenges for a chemist is the synthesis of organic molecules (known or unknown). Learning outcomes of this subject are very important because they will allow the student to propose a reasonable synthesis of a molecule in the laboratory, taking into account its structural features. They also will allow them to assess its effectiveness and the study of possible alternatives. The student will have to combine the acquired knowledge in both Degree and Master subjects, developing their ability as a researcher.

3. Assessment (1st and 2nd call)

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

The student must demonstrate that he/she has achieved the intended learning outcomes through the following assessment activities: continuous assessment and/or a global exam

1.- Continuous assessment

Throughout the semester there will be two partial examinations, P1 and P2, to solve several organic synthesis problems and/or related questions. The first partial (P1) will take place in November and the second one (P2) after the Christmas holidays, before the official exam period.

Likewise, progressive learning will be evaluated by solving problems, tasks through the Moodle platform, discussion in the classes of problems or specific proposals raised throughout the course, which will allow obtaining a grade of problems (Pr)

The final grade will be obtained by applying the following formula:

Continuous grade = 0,3 x P1 + 0,5 x P2 + 0,2 x Pr

To pass, it will be necessary to achieve a minimum qualification of 5 (out of 10). Given the nature of the course, the partial tests do not eliminate matter.

2.- Global exam

Students who do not use the continuous assessment system, who do not pass the course through this procedure or who want to improve their grade, will have the right to take a global exam to be held during the global exams period. This exam will consist in the resolution of several organic synthesis problems and/or related questions.

To pass, it will be necessary to achieve a minimum qualification of 5 (out of 10). The final grade will be the best between the continuous grade and the global exam.

For the realization of both the global and partial exams, the use of molecular models, notes of the subject or textbooks will be allowed.

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 (https://ciencias.unizar.es/normativas-asuntos-academicos).

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.

4. Methodology, learning tasks, syllabus and resources

4.1. Methodological overview

The methodology followed in this course is oriented towards achievement of the learning objectives. A wide range of teaching and learning tasks are implemented, such as:

1.- Interactive theory sessions (3 ECTS).

2.- Problem-solving sessions (3 ECTS).

4.2. Learning tasks

This is a 6 ECTS course organized as follows:

Interactive theory sessions (3 ECTS: 30 hours). The theory sessions are focused on acquisition of knowledge of advanced organic synthesis.

Training activity of seminars and problem-solving sessions (3 ECTS: 30 hours). With this activity students, individually or in small groups, will solve practical cases.

Theory and problem-solving sessions are prepared for face to face training.

Teaching and assessment activities will be carried out in the classroom with all students onsite unless, due to the health situation, the provisions issued by the competent authorities and the University of Zaragoza arrange to carry them out by telematics means or in a reduced rotating capacity.

4.3. Syllabus

The course will address the following topics:

Topic 1. *The bases of retrosynthetic analysis*.

The retrosynthetic analysis. Disconnections. The synthon concept. Electrophile synthons. Nucleophile synthons. Synthetic equivalents. Type of transformations. Financial considerations in the retrosynthetic analysis. Starting products.

Topic 2. *Formation of simple Carbon-Carbon bonds*.

Carbanions of type d^1. Carbanions of type d^2: synthesis from enolates. Alkylation. Alkylation of compounds with active methylenes. Alkylation of 1,3-dicarbonyl compounds. Aldolic condensation. Michael type additions. Carbanions of type d: syntheses from organometallic compounds: organolithium and organomagnesium compounds. Organocuprates. Substitutions, additions and conjugate additions. Coupling reactions catalysed by palladium. Reactions with p-allyl palladium complexes.

Topic 3. *Formation of multiple carbon-carbon bonds*.

Alkene syntheses. Elimination reactions. Condensation of carbonyl compounds with ylide and other carbanions. Syntheses mediated by metallic carbenes, metathesis reactions. Alkyne syntheses. Elimination reactions. Condensation reactions.

Topic 4. *Formation of cyclic compounds*.

Cyclopropanes: Carbene additions. Cyclopentanes. Cyclohexanes and cyclohexenes: cycloadditions [4+2]. Robinson annelation. Syntheses mediated by metallic carbenes, Ring closing metathesis (RCM).

Topic 5. *Protecting groups in organic synthesis*.

Protection of hydroxyl groups: formation of ethers, esters, diols. Protection of carboxylic acids: esters. Protection of amine groups: amide, carbamate and substituted amines. Protection of carbonyl groups: acetal, thioacetal and enol derivatives.

Topic 6. *Oxidations and reductions*.

Alcohol oxidations. Oxidations with Cr (VI), Oxidations with RuO4. Oxidations with DMSO. Dess-Martin oxidation. Alkene oxidations. Dihydroxylation of alkenes. Epoxydation of alkenes. Oxidative cleavage of alkenes and glycols. Baeyer-Villiger oxidation. Other oxidations.

Catalytic hydrogenation. Hydrogenations in absence of hydrogen. Reductions with metallic hydrides of group 13 (B, Al). Reductions with active metals. Deoxygenation of carbonyl compounds. Other reductions.

4.4. 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 website, https://ciencias.unizar.es/calendario-y-horarios and the Master's http://masterqmch.unizar.es.

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

The subject *Synthetic strategies in advanced organic chemistry* will be lectured in the first semester, like the other three compulsory subjects of the Master and the optional subjects *Fundamental methodologies in synthesis* and *Bibliographic resources and databases*.

Throughout the course two partial examinations will be made, in order to learn more deeply some issues. Every partial examination corresponds roughly a third of the complete syllabus. The completion dates will be communicated well in advance.