VNIVERSITAT DE VALÈNCIA

Course Guide
34223 Fine Organic Chemistry

COURSE DATA

Data Subject	
Code	34223
Name	Fine Organic Chemistry
Cycle	Grade
ECTS Credits	6.0
Academic year	2020 - 2021

Study (s)

Degree	Center	Acad. year	Period
1110 - Chemistry Degree	Faculty of Chemistry	4	First term

Subject-matter

Degree	Subject-matter	Character
1110 - Chemistry Degree	17 - Organic Chemistry Applied	Optional

Coordination

Name	Department
BLAY LLINARES, GONZALO	325 - Organic Chemistry

SUMMARY

Organic chemistry is the branch of chemistry, which studies the structure and reactivity of carbon compounds, generally known as organic molecules. Most of the key compounds for life such as lipids, carbohydrates, amino acids, proteins and nucleic acids are among these molecules. Other daily life substances such as fuels, glues, paints or textile fibers are also organic molecules. Those displaying pharmacologic activity, being the base of drugs form an important group of organic compounds. Pesticides, fertilizers and herbicides have change agriculture and preservatives have contributed modifying our feeding habits. Having said that, not every organic molecules are beneficial; many of them are harmful either for health or for the environment and, for this reason, new compounds showing better properties to those presenting problems are seek.

The knowledge of the structure and reactivity of organic compounds is aimed to the development of new ways for the synthesis of compounds maintaining all the beneficial characteristics while minimizing the undesired side effects.

The elective subject Fine Organic Chemistry is regarded as a continuation and extension of the knowledge acquired in the subjects Organic Chemistry I, II and III. The objectives aimed to be achieved by the students after studying this subject are summarized in the following points:

- Perceive the structural changes produced in molecules after the individual application of each reaction studied during previous subjects.
- Perceive the structural changes produced in molecules after the sequential application of two or more of the reactions studied in previous subjects.
- Combine sequences of synthetic organic reactions aimed to a defined structural modification.
- Analyze organic syntheses from the final compounds by inverse sequence (retrosynthetic analysis).
- Perceive the existing relationships among the diverse functional groups in an objective molecule as a key element of retrosynthetic analysis.
- Perceive the stereochemical aspects of the objective molecule as a key element of retrosynthetic analysis.
- Identify aspects related to selectivity in organic synthesis.
- Design synthesis of high added value organic compounds from given available starting materials in several reaction containing sequences.
- Perceive the additional practical aspects, which must be taken into account by the chemist in the industry when designing a large-scale synthesis of high added value compounds.
- Regarding the later point, take into consideration the “green chemistry” principles.

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

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

Other requirements

This knowledge should enable the student to:
Represent in a clear and appropriate form the structure of compounds and their bonds, distinguishing between empirical formula, molecular formula and Developer formula.
Identify the different functional groups in organic molecules.
Name and formulate simple organic compounds: hydrocarbons (alkanes, alkenes, alkynes and aromatics), halogen derivatives, oxygenated compounds (alcohols, ethers, aldehydes, ketones, acids and esters) and nitrogenated ones (a

OUTCOMES

1108 - Grado de Química

- Develop capacity for analysis, synthesis and critical thinking.
- Show inductive and deductive reasoning ability.
- Demonstrate leadership and management skills, entrepreneurship, initiative, creativity, organization, planning, control, leadership, decision making and negotiation.
- Solve problems effectively.
- Demonstrate ability to work in teams both in interdisciplinary teams and in an international context.
- Demonstrate a commitment to ethics, equality values and social responsibility as a citizen and as a professional.

- Ability to recognise chemical elements and their compounds: preparation, structure, reactivity, properties and applications.
- Recognise and analyse new problems and plan strategies to solve them.
- Recognise and evaluate chemical processes in daily life.
- Develop sustainable and environmentally friendly methods.
- Students must be able to apply their knowledge to their work or vocation in a professional manner and have acquired the competences required for the preparation and defence of arguments and for problem solving in their field of study.
- Students must have the ability to gather and interpret relevant data (usually in their field of study) to make judgements that take relevant social, scientific or ethical issues into consideration.
- Students must be able to communicate information, ideas, problems and solutions to both expert and lay audiences.
- Students must have developed the learning skills needed to undertake further study with a high degree of autonomy.
- Express oneself correctly, both orally and in writing, in any of the official languages of the Valencian Community.
- Have basic skills in the use of information and communication technology and properly manage the information obtained.

LEARNING OUTCOMES

The previous section includes the competences contained in the document VERIFICA. This subject addresses part of the learning results of the matter Applied Organic Chemistry that allow to acquire specific knowledge of chemistry, cognitive skills and general skills recommended by the EUROPEAN CHEMISTRY THEMATIC NETWORK (ECTN) for the Chemistry Eurobachelor® Label. The following table lists the learning outcomes acquired in the subject Fine Organic Chemistry related to the competences of the degree in Chemistry.

SPECIFIC KNOWLEDGE OF CHEMISTRY	
The learning process should allow the degree graduates to demonstrate:	
	Competences of the subject Fine Organic Chemistry that contemplate the learning outcomes EUROBACHELOR®
Major aspects of chemical terminology, nomenclature, conventions and units.	Demonstrate knowledge of the main aspects of chemical terminology, nomenclature, conventions and units..(CE1)
The major types of chemical reaction and the main characteristics associated with them.	Demonstrate knowledge of the main types of chemical reaction and their main characteristics.(CE4)
The properties of aliphatic, aromatic, heterocyclic and organometallic compounds.	Demonstrate knowledge of the main types of chemical reaction and their main characteristics.(CE4) Ability to recognise chemical elements and their compounds: preparation, structure, reactivity, properties and applications..(CE7). Demonstrate knowledge of the principles, procedures and techniques for the determination, separation, identification and characterisation of chemical compounds.(CE8). Show knowledge of the structure and reactivity of the main classes of biomolecules and the chemistry of the main biological processes..(CE12).
Major synthetic pathways in organic chemistry, involving functional group interconversions and carbon carbon and carbonheteroatom bond formation	Demonstrate knowledge of the main types of chemical reaction and their main characteristics.(CE4) Ability to recognise chemical elements and their compounds: preparation, structure, reactivity, properties and applications..(CE7). Demonstrate knowledge of the principles, procedures and techniques for the determination, separation, identification and characterisation of chemical compounds.(CE8). Show knowledge of the structure and reactivity of the main classes of biomolecules and the chemistry of the main biological processes..(CE12).

COMPETENCES AND COGNITIVE SKILLS	
The learning process should allow the degree graduates to demonstrate:	
	Competences of the subject Fine Organic Chemistry that contemplate the learning outcomes EUROBACHELOR®
Ability to demonstrate knowledge and understanding of the facts, concepts, principles and fundamental theories related to the topics mentioned above.	Demonstrate knowledge and understanding of essential facts, concepts, principles and theories related to the areas of chemistry..(CE13).
Ability to apply this knowledge and understanding to the solution of common qualitative and quantitative problems.	Solve qualitative and quantitative problems following previously developed models..(CE14). Recognise and analyse new problems and plan strategies to solve them..(CE15). Understand the qualitative and quantitative aspects of chemical problems..(CE24).
Competences to present and argue scientific issues orally and in writing to a specialized audience.	Relate chemistry with other disciplines.(CE26). Prepare reports, surveys and industrial and environmental projects in the field of chemistry..(CE27). Demonstrate ability to communicate information, ideas, problems and solutions to both specialist and non-specialist audiences and using information technology, as appropriate. (CG6). Students must be able to communicate information, ideas, problems and solutions to both expert and lay audiences..(CB4).

GENERAL COMPETENCES	
The learning process should allow the degree graduates to demonstrate:	
	Competences of the subject Fine Organic Chemistry that contemplate the learning outcomes EUROBACHELOR®
Ability to apply practical knowledge to solve problems related to qualitative and quantitative information.	Solve problems effectively..(CG4). Solve qualitative and quantitative problems following previously developed models..(CE14). Relate theory and experimentation..(CE22). Recognise and evaluate chemical processes in daily life..(CE23). Understand the qualitative and quantitative aspects of chemical problems..(CE24).
Competences in information management, in relation to primary and secondary sources, including information retrieval through on-line searches.	Demonstrate ability to communicate information, ideas, problems and solutions to both specialist and non-specialist audiences and using information technology, as appropriate..(CG6). Have basic skills in the use of information and communication technology and properly manage the information obtained.(CT2).
Skills related to information technology such as word processing, spreadsheet, recording and storage of data, internet use related to the subjects.	Demonstrate ability to communicate information, ideas, problems and solutions to both specialist and non-specialist audiences and using information technology, as appropriate..(CG6). Have basic skills in the use of information and communication technology and properly manage the information obtained.(CT2).

Competences in oral and written communication, in one of the main European languages, in addition to the language of the country of origin.	Demonstrate ability to work in teams both in interdisciplinary teams and in an international context..(CG5). Demonstrate a commitment to ethics, equality values and social responsibility as a citizen and as a professional. (CG7). Express oneself correctly, both orally and in writing, in any of the official languages of the Valencian Community. (CT1). Students must be able to communicate information, ideas, problems and solutions to both expert and lay audiences..(CB4). Have basic skills in the use of information and communication technology and properly manage the information obtained.(CT2).
Study skills necessary for professional development. These will include the ability to work autonomously.	Demonstrate leadership and management skills, entrepreneurship, initiative, creativity, organization, planning, control, leadership, decision making and negotiation..(CG3). Demonstrate ability to work in teams both in interdisciplinary teams and in an international context..(CG5). Learn autonomously.(CG8). Demonstrate the ability to adapt to new situations..(CG9). Students must have developed the learning skills needed to undertake further study with a high degree of autonomy.(CB5).

DESCRIPTION OF CONTENTS

1. Chemoselectivity and protecting groups

Chemoselectivity. Definition and applications. Reactivity towards nucleophiles. Reducing agents. Hydride transfer. Catalytic hydrogenation. Hydrogenolysis. Dissolving metal reductions. Selectivity in oxidation reactions. Chemoselectivity in the reactions of dianions. Kinetic chemoselectivity. Use of protecting groups: importance and choice. Classification. Peptide synthesis.

2. Functional groups interconversion.Retrosynthetic analysis

Fundamental strategies in retrosynthetic analysis. Synthons. Functional groups interconversion based strategies. Carbon-heteroatom bond disconnections: 1,2-diX and 1,3-diX disconnections. Synthesis of simple bond functions (alcohols, amines, etc).

3. Disconnection of functional groups.

Disconnection of functional groups based strategies. Disconnections of C-C bonds. Disconnections of aromatic systems. 1,1 C-C disconnections: the use of organometallic reagents. Disconnection of carbon-carbon multiple bonds. 1,3 and 1,5 disconnections of two groups. Natural reactivity and the concept of Umpolung. 1,2 and 1,4 disconnections of two groups.

4. Diastereoselectivity

Diastereoselectivity: definitions. Stereoselective reactions. Prochirality. Enantiotopic vs diastereotopic. Crams rule vs FelkinAhn model. The effect of electronegative atoms. Chelation, rate, and stereoselectivity. Stereoselective reactions of acyclic alkenes. The Houk model. Stereoselective epoxidation. Stereoselective enolate alkylation. Diastereoselectivity in aldol reactions. Single enantiomers from diastereoselective reactions.

5. Asymmetric Synthesis

Nature is asymmetric. The chiral pool. Resolution can be used to separate enantiomers. Chiral auxiliaries. Alkylation of enolates. Enantiomeric excess. Chiral reagents. Asymmetric catalysis: catalytic asymmetric hydrogenation of alkenes. Auxiliary-controlled vs Asymmetric catalysis. Asymmetric epoxidation: examples. Asymmetric dihydroxylation. Asymmetric formation of C-C bonds. Asymmetric conjugate addition. Organocatalysis: examples. Asymmetric aldol reactions. Enzymes as catalyst

6. Industrial scale synthesis. Processes scale up

Practical considerations of large scale processes. Choice of routes and reagents. Choice of solvents. Optimization. Purification of final products. Example of the synthesis of high added value compounds: pesticides, pharmaceuticals, colorings, etc.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	51,00	100
Tutorials	9,00	100
Study and independent work	90,00	0
TOTAL	**150,00**	

TEACHING METHODOLOGY

The subject is outlined so that the student is the protagonist of its own learning and is structured as follows:

- Teaching material. - The students will have at their disposal the teaching material from the beginning of the year.
- Theoretical and problem classes.- They will be dedicated to exposing students to the most fundamental aspects of the subject. These classes are supplemented by personal study time. Some classes will be devoted to demonstrative problem solving by the teacher interacting with students
- Tutorials.- They will be distributed uniformly throughout the course, the duration of each of these sessions being 1 hour. Ther, the teacher will evaluate the overall learning process of the students. The tutorials will be mainly devoted to the active resolution of problems by the students. Students must previously have worked on the problems that will be solved and will present them in class for discussion and correction. In the tutoring sessions, controls can be programmed that will consist of solving problems individually, with the support of study material, which will be collected and evaluated by the teacher. Problems or other online activities may also be raised to be worked autonomously by the student. Likewise, the tutorials will serve to solve all the doubts that may have arisen throughout the classes and will guide the students on the most useful working methods for solving the problems that may arise.
- Organic Chemistry Seminars. - They will consist of the exposition and discussion by a couple or group of students of an article in a scientific journal related to organic synthesis.

EVALUATION

The professor will carry out the evaluation of learning in a continuous manner. The different items which will be evaluated are the following:

1.Direct evaluation by the professor (1 point): several aspects hill be taken into consideration in this evaluation, among which is worth noting:

- Attendance and reasoned and clear participation in the posed discussions.
- Progress in the use of the characteristic language of organic chemistry.
- Solution of problems and posing of doubts.
- Critical spirit.

2. Tutorials (as a whole 2 points): the mark of each student in this item will take into consideration:

- Assistance and exposition of problems and exercises.
- Problem solving and autonomous learning activities assigned
- Control exercises

• Seminars.

3.Exams (7 points): will take place on the date shown by the Faculty and will be common to every group of the subject. It will consist of theoretic-practical questions related to the matter taught during the teaching period. The global pass of the subject implies having obtained a minimum scoring of 3 points out of the 7 total.

In the evaluation of the second call, the qualification got in the continuous evaluation (item 1- **"**Direct evaluation by the professor" and item 2- "Tutorials") from the first call Hill be kept and the part corresponding to the item 3 -"Exams"- will be evaluated again.

The student could be evaluated only with a written exam on the contents of the subject treated during lectures, tutorials and seminars, so that the teacher can evaluate whether the student has acquired the skills and knowledge related to the subject. This test will be 100% of the overall grade and the student must obtain a score of 5 over 10.

In this case the student must resign from the continuous evaluation and choose this type of assessment presenting a written application at the registry of the secretary of the department.

REFERENCES

Basic

- COREY, E. J.; CHENG, X. M. The Logic of Chemical Synthesis, John Wiley and Sons, 1998.
- CLAYDEN, J.; GREEVES, N.; WARREN, S.; WOTHERS, P. Organic Chemistry, Oxford: Oxford University Press, 2001, Caps. 30-34.
- WYATT P., WARREN, S. Workbook for Organic Synthesis. Strategy and Control, John Wiley and Sons, 2008.
- CARDA, M.; MARCO, J. A.; MURGA, J.; FALOMIR, E. Análisis retrosintético y síntesis orgánica. Resolución de ejemplos prácticos, Castellón: Publicacions de la Universitat Jaume I, 2010.
- CABRI, W.; DI FABIO, R.; From Bench to Market. The Evolution of Chemical Synthesis, Oxford: Oxford University Press, 2000.
- ANDERSON, N. G. Practical Process Research and Development, 2 Ed., Elsevier, 2012.
- ChemBioOffice Ultra, PerkinElmer (CambridgeSoft) Amplia selección de aplicaciones y funcionalidades que permite a químicos y biólogos dibujar, formular, modelar y editar estructuras moleculares químicas y biológicas así como simular espectros de RMN de protón y carbono.

Additional

- LEE, S.; ROBINSON, G. Process Development. Fine Chemicals from Grams to Kilograms, Oxford: Oxford Science Publications, 1995.
- SAUNDERS, J. Top Drugs. Top Synthetic Routes, Oxford: Oxford Science Publications, 2000.

ADDENDUM COVID-19

This addendum will only be activated if the health situation requires so and with the prior agreement of the Governing Council

Contents

The contents initially collected in the teaching guide are maintained.

Volume of work and temporary planning of teaching

Regarding the workload:

The different activities described in the Teaching Guide are maintained with the intended dedication.

Regarding the temporary teaching planning:

The material for the follow-up of the classroom theory classes allows to continue with the temporary teaching planning both in days and hours, both if the teaching is classroom-based or not.

Teaching methodology

Theory classes and classroom tutoring will tend to the maximum possible face-to-face teaching, always respecting the health restrictions that limit the capacity of the classrooms to 50% of their usual occupation. Depending on the capacity of the classroom and the number of students enrolled, some of the students may need to follow the classes synchronously in an auxiliary classroom. If this situation arises, students will attend the main classroom or auxiliary classroom for weekly rotary shifts (preferably in alphabetical order). However, the rotation system will be fixed once the actual enrollment data is known, guaranteeing, in any case, that the percentage of face-to-face teaching of all students enrolled in the subject is the same.

If there is a closure of the facilities for health reasons that totally or partially affects the classes of the course, they will be replaced by non-face-to-face sessions following the established schedules and using the tools of the virtual classroom.

Evaluation

The evaluation system described in the Teaching Guide of the subject in which the different evaluable activities have been specified as well as their contribution to the final grade of the subject is maintained.

If there is a closure of the facilities for health reasons affecting the development of any face-to-face evaluable activity of the subject, it will be replaced by a test of a similar nature that will be carried out in virtual mode using the computer tools licensed by the University of Valencia. The contribution of each evaluable activity to the final grade of the subject will remain unchanged, as set out in this guide.

Bibliography

The bibliography recommended in the Teaching Guide is kept as it is accessible.