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	2018 - 2019

Study (s)

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

Subject-matter

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

Coordination

Name	Department
FUSTERO LARDIES, SANTOS	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 - Degree in Chemistry

- 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

1 Apply the knowledge of basic organic chemistry to design and prepare selectively organic compounds with high added value.
2 To know the interest and the incidence of natural products and fine chemical products obtained in the various areas of daily life.
3 Learn to assess the importance of stereochemical aspects of the products studied both in their synthesis and their practical application.
4 Learn to acquire, use and transmit bibliographic information related to organic compounds.
5 Acquire an overview of the organic chemical industry
6 Know the main organic compounds of industrial interest
7 Understand how organic compounds are prepared from their primary sources

8 To assess the problems associated with scaling and sustainability of the reactions of preparation of compounds with high added value
9 Perceiving sustainable chemistry as a viable way to develop chemistry in our days
10 Know how to organize and plan tasks
11 Teaming up with a serious and professional behavior and gender perspective

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.
- Theoretic classes. - Will be aimed to show the students the most fundamental aspects of the matter. These classes are complemented by personal study time.
- Problems classes. - In these classes the specific application of the knowledge acquired by the students in the theoretic classes will be carried out. The students will have to, previously, have worked on the problems to be solved. The solution of those problems will be carried out, in certain cases, by the professor and in other occasions by the students, Esther in groups or individually.
- Tutorials. - Will consist of sessions uniformly spread along the year, lasting each session 1 hour. During them, the professor will evaluate the global learning process of the students, which may be previously organized in working teams. In tutored sessions the homework entrusted by the professor to the mentioned work teams may be collected. Equally, tutorials will serve to solve every doubt that may have arisen along the classes and will guide the students about the most useful working methods for solving the problems they may encounter.

Organic Chemistry Seminars. - Seminars will be carried out along the semester, in the dates that will be gathered in the year calendar. Those seminars will be devoted to a more profound discussion of selected examples of organic synthesis, which level requires a more detailed study. After the discussion of each topic, some related practical problems would be solved.

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.
- Attendance.
- Contents and written submission of homework entrusted by the professor to each work team. The qualification will be a global mark for the working team and Hill count equally for each of its members.

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

In order to get a qualification in this item, a minimum attendance to 4 seminars and 6 tutorials will be mandatory.

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- "Organic Chemistry Seminars and 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.

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.