

**COURSE DATA****Data Subject**

<b>Code</b>	36453
<b>Name</b>	Química Orgánica I
<b>Cycle</b>	Grade
<b>ECTS Credits</b>	6.0
<b>Academic year</b>	2018 - 2019

**Study (s)**

<b>Degree</b>	<b>Center</b>	<b>Acad. Period year</b>
1110 - Degree in Chemistry	Faculty of Chemistry	2 First term

**Subject-matter**

<b>Degree</b>	<b>Subject-matter</b>	<b>Character</b>
1110 - Degree in Chemistry	9 - Organic Chemistry	Obligatory

**Coordination**

<b>Name</b>	<b>Department</b>
ASENSIO AGUILAR, GREGORIO	325 - Organic Chemistry

**SUMMARY**

Organic chemistry is the branch of chemistry that studies the structure and reactivity of carbon compounds, generally known as organic molecules. Among these molecules are most of the essential compounds for life, such as lipids, carbohydrates, amino acids, proteins and nucleic acids. Organic substances are also many substances with which we come into direct contact, such as fuels, glues, paints or textile fibers. A large group of organic compounds are those that have pharmacological activity and that are the basis of medicines. Pesticides, fertilizers and herbicides have changed agriculture and preservatives have helped to modify our eating habits. However, not all organic compounds are beneficial; there are many of them that are harmful to health or to the environment and therefore, it is necessary to continue preparing compounds with better properties to replace those that present problems.

The knowledge of the structure and reactivity of organic compounds has the purpose of opening paths for the preparation of compounds that maintain all their beneficial characteristics, minimizing undesirable side effects.



The study of Organic Chemistry is based on the general knowledge acquired in the subjects of Chemistry I and Chemistry II of the first year. As, the systematic study of functional groups characteristic of organic compounds will be carried out from this knowledge, it is highly recommended to have passed the above-mentioned subjects before approaching the study of Organic Chemistry I. This subject together with Organic Chemistry II and III constitute the theoretical foundations of the compulsory Organic Chemistry Module of the Degree in Chemistry and should be treated as a whole to show the complete perspective of the area of knowledge.

The objectives that are intended to achieve in this subject can be summarized in the following points:

- To set the student's knowledge about the structure and bond in organic compounds. Study the different types of representation of organic molecules.
- To apply the general rules of nomenclature for organic compounds.
- To study the stereochemistry of organic compounds and the appropriate nomenclature rules.
- To identify the different functional groups present in organic molecules.
- To study the reactivity of the different functional groups that only contain carbon-carbon bonds
- To study the methods for obtaining these functional groups.
- To study the mechanisms of the most important reactions in which these functional groups are involved.
- To design synthesis of organic compounds from certain starting products and involving more than one reaction step.

## 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 study of Organic Chemistry I is based on the knowledge acquired in General Chemistry I and General Chemistry II.

## COMPETENCES (RD 1393/2007) // LEARNING OUTCOMES (RD 822/2021)

### 1110 - 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 communicate information, ideas, problems and solutions to both specialist and non-specialist audiences and using information technology, as appropriate.
- Demonstrate a commitment to ethics, equality values and social responsibility as a citizen and as a professional.
- Learn autonomously.
- Demonstrate the ability to adapt to new situations.
- Acquire a permanent sensitivity to quality, the environment, sustainable development and the prevention of occupational hazards.
- Demonstrate knowledge of the main aspects of chemical terminology, nomenclature, conventions and units.
- Interpret the variation of the characteristic properties of chemical elements according to the periodic table.
- Demonstrate knowledge of the main types of chemical reaction and their main characteristics.
- Demonstrate knowledge of the principles of thermodynamics and kinetics and their applications in chemistry.
- Ability to recognise chemical elements and their compounds: preparation, structure, reactivity, properties and applications.
- Demonstrate knowledge and understanding of essential facts, concepts, principles and theories related to the areas of chemistry.
- Solve qualitative and quantitative problems following previously developed models.
- Recognise and analyse new problems and plan strategies to solve them.
- Evaluate, interpret and synthesise chemical data and information.
- Recognise and evaluate chemical processes in daily life.
- Develop sustainable and environmentally friendly methods.
- Relate chemistry with other disciplines.
- 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 (RD 1393/2007) // NO CONTENT (RD 822/2021)**

- To demonstrate knowledge of the main aspects of terminology and organic nomenclature.
- To understand the structural properties and reactivity of compounds and functional organic groups by applying them to the solution of synthetic and structural problems.
- To elucidate the structure of simple organic compounds using spectroscopic techniques.
- To explain in a comprehensible way phenomena and processes related to Organic Chemistry.
- To acquire and use bibliographic and technical information related to organic compounds.
- To write and expose in the native language with correction.
- To effectively perform the tasks assigned as a member of a team with a gender perspective.
- To demonstrate knowledge of sustainable methodologies in organic chemistry.
- To demonstrate critical reasoning
- To demonstrate autonomous learning
- To solve problems with rigor.

## **DESCRIPTION OF CONTENTS**

### **1. Polar Covalent Bonds; Acids and Bases**

1.1 Polar Covalent Bonds: Electronegativity. 1.2 Polar Covalent Bonds: Dipole Moments. 1.3 Formal Charges. 1.4 Resonance. 1.5 Rules for Resonance Forms. 1.6 Drawing Resonance Forms. 1.7 Acids and Bases: The BrønstedLowry Definition. 1.8 Acid and Base Strength. 1.9 Predicting AcidBase Reactions from pKa Values. 1.10 Organic Acids and Organic Bases. 1.11 Acids and Bases: The Lewis Definition. 1.12 Noncovalent Interactions Between Molecules.



**2. Organic Compounds: Alkanes, Cycloalkanes and their Stereochemistry**

2.1 Functional Groups. 2.2 Alkanes and Alkane Isomers. 2.3 Alkyl Groups. 2.4 Naming Alkanes. 2.5 Physical and chemical properties of alkanes. 2.6 Conformations of Ethane. 2.7 Conformations of Other Alkanes. 2.8 Naming Cycloalkanes. 2.9 CisTrans Isomerism in Cycloalkanes. 2.10 Stability of Cycloalkanes: Ring Strain. 2.11 Conformations of Cycloalkanes. 2.12 Conformations of Cyclohexane. 2.13 Axial and Equatorial Bonds in Cyclohexane. 2.14 Conformations of Monosubstituted. 2.15 Cyclohexanes Conformations of Disubstituted Cyclohexanes. 2.16. Conformations of Polycyclic Molecules.

**3. Stereochemistry at Tetrahedral Centers**

3.1 Enantiomers and the Tetrahedral Carbon. 3.2 The Reason for Handedness in Molecules: Chirality. 3.3 Optical Activity. 3.4 Pasteurs Discovery of Enantiomers. 3.5 Sequence Rules for Specifying Configuration. 3.6 Diastereomers. 3.7 Meso Compounds. 3.8 Racemic Mixtures and the Resolution of Enantiomers. 3.9 A Review of Isomerism. 3.10 Chirality at Nitrogen, Phosphorus, and Sulfur.

**4. An Overview of Organic reactions**

4.1 Kinds of Organic Reactions. 4.2 How Organic Reactions Occur: Mechanisms. 4.3 Radical Reactions: alkane halogenation. 4.4 Polar Reactions. 4.5 An Example of a Polar Reaction: Addition of HBr to Ethylene. 4.6 Using Curved Arrows in Polar Reaction Mechanisms. 4.7 Describing a Reaction: Equilibria, Rates, and Energy Changes. 4.8 Describing a Reaction: Bond Dissociation Energies. 4.9 Describing a Reaction: Energy Diagrams and Transition States. 4.10 Describing a Reaction: Intermediates. 4.11 A Comparison Between Biological Reactions and Laboratory Reactions.

**5. Alkenes: Structure, Reactivity, Reactions and Synthesis**

5.1 Industrial Preparation and Use of Alkenes. 5.2 Calculating Degree of Unsaturation. 5.3 Naming Alkenes. 5.4 CisTrans Isomerism in Alkenes. 5.5 Alkene Stereochemistry and the E,Z Designation. 5.6 Stability of Alkenes. 5.7 Electrophilic Addition Reactions of Alkenes. 5.8 Orientation of Electrophilic Additions: Markovnikovs Rule. 5.9 Carbocation Structure and Stability. 5.10 The Hammond Postulate. 5.11 Evidence for the Mechanism of Electrophilic Additions: Carbocation Rearrangements. 5.12 Preparing Alkenes. 5.13 Halogenation of Alkenes: Addition of X<sub>2</sub>. 5.14 Halohydrins from Alkenes: Addition of HOX. 5.15 Hydration of Alkenes: Addition of H<sub>2</sub>O by Oxymercuration. 5.16 Hydration of Alkenes: Addition of H<sub>2</sub>O by Hydroboration. 5.17 Reduction of Alkenes: Hydrogenation. 5.18 Oxidation of Alkenes: Epoxidation and Hydroxylation. 5.19 Oxidation of Alkenes: Cleavage to Carbonyl Compounds. 5.20. 5.20 Radical Additions to Alkenes: Chain-Growth Polymers. 5.21 Reaction Stereochemistry: Addition of H<sub>2</sub>O to an Achiral Alkene.



## **6. Alkynes: An Introduction to Organic Synthesis**

6.1 Naming Alkynes. 6.2 Preparation of Alkynes: Elimination Reactions of Dihalides. 6.3 Reactions of Alkynes: Addition of HX and X<sub>2</sub>. 6.4 Hydration of Alkynes. 6.5 Reduction of Alkynes. 6.6 Oxidative Cleavage of Alkynes. 6.7 Alkyne Acidity: Formation of Acetylide Anions. 6.8 Alkylation of Acetylide Anions.

## **7. Alkyl Halides. Reactions of Alkyl Halides**

7.1 Names and Properties of Alkyl Halides. 7.2 Preparing Alkyl Halides. 7.3 Reactions of Alkyl Halides: Grignard Reagents. 7.4 Organometallic Coupling Reactions. 7.5 Oxidation and Reduction in Organic Chemistry. 7.6 The Discovery of Nucleophilic Substitution Reactions. 7.7 The S<sub>N</sub>2 Reaction. Characteristics of the S<sub>N</sub>2 Reaction. 7.8 The S<sub>N</sub>1 Reaction. 7.9 Characteristics of the S<sub>N</sub>1 Reaction.. 7.10 Elimination Reactions: Zaitsevs Rule. 7.11 The E2 Reaction and the Deuterium Isotope Effect. 7.12 The E2 Reaction and Cyclohexane Conformation. 7.13 The E1 and E1cB Reactions. 7.14 Biological Elimination Reactions. 7.15 A Summary of Reactivity: S<sub>N</sub>1, S<sub>N</sub>2, E1, E1cB, and E2.

## **8. Structure Determination: Mass Spectrometry and Infrared Spectroscopy**

8.1 Mass Spectrometry of Small Molecules: Magnetic-Sector Instruments. 8.2 Interpreting Mass Spectra. 8.3 Mass Spectrometry of Some Common Functional Groups. 8.4 Spectroscopy and the Electromagnetic Spectrum. 8.5 Infrared Spectroscopy. 8.6 Interpreting Infrared Spectra. 8.7 Infrared Spectra of Some Common Functional Groups

## **9. Structure Determination: Nuclear Magnetic Resonance spectroscopy**

9.1 Nuclear Magnetic Resonance Spectroscopy. 9.2 The Nature of NMR Absorptions. 9.3 Chemical Shifts. 9.4 <sup>13</sup>C NMR Spectroscopy: Signal Averaging and FTNMR. 9.5 Characteristics of <sup>13</sup>C NMR Spectroscopy. 9.6 Uses of <sup>13</sup>C NMR Spectroscopy. 9.7 <sup>1</sup>H NMR Spectroscopy and Proton Equivalence. 9.8 Chemical Shifts in <sup>1</sup>H NMR Spectroscopy. 9.9 Integration of <sup>1</sup>H NMR Absorptions: Proton Counting. 9.10 SpinSpin Splitting in <sup>1</sup>H NMR Spectra. 9.11 Uses of <sup>1</sup>H NMR Spectroscopy..



## WORKLOAD

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

## TEACHING METHODOLOGY

The subject is designed so that the student is the protagonist of his/her own learning. The subject structure is:

- Theory classes and questions.- Theory lessons will introduce the students to the most fundamental aspects of the subject. The question sessions will be dedicated to the application of the specific knowledge that students have acquired in theory classes. Students must have previously worked on the questions to be solved. The answers will be discussed in class by both the teacher and the students. The classes should be complemented by personal study time.
- Tutoring.- In them the overall learning process of the students will be evaluated. In the tutorial sessions the professor could entrust written reports to the students. Furthermore, the tutorials will serve to solve any doubts that may have arisen during the classes and guide students on the most convenient work methods.
- Seminars-Talks: The Seminars-Talks will deal with complementary aspects of their formation in Organic Chemistry and will be dedicated to the presentation by a specialist of a relevant topic in current Chemistry. For this task, students will attend the event and answer a questionnaire prepared by the teacher.

## EVALUATION

For learning assessment, the teacher can use two modalities. The student must opt for one of them and communicate his choice to the secretary of the department according to the written form available. The student must communicate the preferred modality during the first month of the semester. On behalf of the teacher's programming, the student will be evaluated with the B modality if there is no communication within this first month period.

The minimum global qualification to pass the subject in any modality will be 5 points out of 10.



## FIRST CALL

### Modality A

Continuous evaluation through the course. In this case, the following sections will be considered:

**1. Direct evaluation by the teacher (5%):** this evaluation will take into account different aspects, among which include:

Assistance and reasoned and clear participation in the discussions and questions in the class

Progress in the use of the language specific to organic chemistry

Troubleshooting and raising doubts

Critical spirit

**2. Tutorials and Seminars (globally 15%):** In this section the following aspects will be considered:

Assistance

Content and written presentation of the exercises proposed by the teacher (if applicable).

Rational and clear participation in the discussions.

**3. Exams (80%):** will be held on the date indicated by the Faculty and will be common to all groups of the subject. It will consist of theoretical and practical questions related to the subject explained during the teaching period. The global passing of the subject will necessarily entail having obtained a minimum score of 5 out of 10 points on the exam.

### Modality B

Evaluation with only a written exam on the contents of the subject dealt with in theory classes and tutorials, so that the teacher can thus assess whether the student has acquired the skills and knowledge related to the subject. This exam will be 100% of the overall score.

The exam will be held on the date indicated by the Faculty and will be common to all groups of the subject. In this modality, the teacher may take into account the participation of students in theory classes and tutorials for the final grade.

## SECOND CALL

In the second call evaluation for students who have chosen modality A, the grade obtained by the student in the first call for sections 1 and 2 will be maintained but, section 3 will be re-evaluated.





## REFERENCES

### Basic

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- QUIÑOÁ CABANA, E.; RIGUERA VEGA, R. Nomenclatura y representación de los compuestos orgánicos, McGraw-Hill/Interamericana, 2013. Disponible en formato papel y electrónico en la biblioteca.
- ChemBioOffice Ultra, Perkin Elmer (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

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