

COURSE SYLLABUS 2018-19

Basic information on the course			
Course:	Organic Synthesis		
Course code:	5093217	Plan:	Chemistry degree (2009)
Academic Year:	2018/2019	Undergraduate/Graduate:	Undergraduate
Degree Year:	3rd	Type:	Obligatory
Duration:	1 semester		
TIME DISTRIBUTION ACCORDING TO REGULATIONS			
Credits:	9 ECTS		
Total time:	225h (90h in class + 135h of autonomous work)		
USE OF LEARNING PLATFORM:		Teaching support	

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OTHER IMPORTANT INFORMATION

Content justification

Organic Synthesis is one of the most powerful tool available to our civilization for the preparation of new products. The ability to make drugs, pesticides, flavorings, preservatives, plastics, insulation, textiles, paints, dyes, etc. is the result of the design and subsequent implementation by synthetic organic chemists of a series of techniques based on adequate organic chemistry reactions. This course provides an overview of the current issues and solutions, ranging from the initial rational approach to the ultimate preparation and structural design. The main objectives are:

- The understanding of the basic principles of the retrosynthetic analysis.
- The knowledge of the general methods of protection of functional groups.
- The knowledge of the main strategies of asymmetric synthesis.
- Expanding the knowledge on reactivity in organic chemistry.

These objectives can be achieved by the study of the tools for synthesis and retrosynthesis and also by solving exercises in synthesis, starting with simple cases which will progressively increase in complexity.

Courses related in Study Plan

The course "Organic Synthesis", a part of the "Organic Chemistry" matter of the Fundamental Module of the Degree in Chemistry is a compulsory 9 ECTS course, 3 of which correspond to "Experimental laboratory in Organic Chemistry". The pillars of this course are the Organic Chemistry I and Organic Chemistry II also included within that matter of Organic Chemistry of the Fundamental Module and taught in the second year of the Degree. On the other hand, the Organic Synthesis is the logical basis for further courses of this matter: Enhancement of Organic Chemistry, 6 ECTS, taught in the second semester of the third year and Experimentation in Organic Chemistry, 6 ECTS, taught in the fourth year. Furthermore, a feature of modern Organic Chemistry is its interaction with other traditional areas of chemistry and other disciplines (medicine, biochemistry, materials science, etc.). Therefore, there is a close relationship between this course and other branches of chemistry as well as Biochemistry, Biological Chemistry and Materials Science. Finally, the synthesis of organic compounds at industrial level links with the matter of Chemical Engineering included in the Basic module of the Degree.

Pre-required knowledge

To address properly this subject is essential to have achieved a positive assessment of the competencies acquired in the courses "Organic Chemistry I" and "Organic Chemistry II".

All the recommended bibliography or reading is mostly in English.

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COMPETENCES

General competences

Key competences University of Almeria

- Knowledge of a second language.
- Ability of criticism and self-criticism.
- Ability to learn how to work independently.
- Ability for management and planning.

Specific competences

- **C11.** Properties of aliphatic, aromatic, heterocyclic and organometallic compounds.
- **C13.** The main synthetic routes in organic chemistry, including the interconversion functional groups and the formation of carbon-carbon and carbon-heteroatom bonds.
- **Q3.** Competency to assess, explain and summarize data and chemical information.
- **Q6.** Skill in handling and processing computer data and chemical information
- **P3.** Ability for observation, monitoring and measurement of properties, events or chemical changes, and the systematic and reliable recording of documentation.
- **P4.** Ability to handle standard chemical instrumentation, like that used for structural elucidations and chemical separations.
- **P5.** Interpretation of data from observations and measurements in the laboratory in terms of its significance and the scientific theories.

LEARNING OUTCOMES

Each student who has passed the subject of Organic Synthesis will be able, at the level of the third year in the Degree in Chemistry, to perform the following tasks:

- To plan the preparation of reports and the study time and to self-organize in a chemical laboratory to carry out the relevant experience within a reasonable time and in an efficient way.
- To conduct a comprehensive reading of scientific texts in a foreign language.
- To interpret data derived from observation and establish links with appropriate theories. Accurately identify both the fundamental and the superfluous elements in a written report or an oral presentation, either from mate students or its own.
- To organize the work and time, to meet deadlines; to prepare classes; to organize the study time. To have autonomous access to relevant information sources. To search and summarize basic bibliographical sources related to chemistry.
- To predict some fundamental properties of aliphatic, aromatic and organometallic compounds. To be able to reason the reactivity of aliphatic, aromatic and organometallic compounds. To know and justify the inorganic properties of organometallic compounds.
- To analyze what reagents would be able to react with an organic molecule on the basis of its constitution and the way they would react. To propose transformations of functional groups according to their reactivity. To propose simple synthesis of organic compounds by sequences of functional group transformations.

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- To correlate the reactivity of multifunctional molecules with that of the functional groups within them. To evaluate, interpret and summarize chemical data obtained in an experimental laboratory in chemistry. To evaluate, interpret and summarize data and information obtained from different sources on chemical aspects.
- To handle chemical databases. To select information for the resolution of specific chemical problems. To prepare reports based on the results of the treatment of chemical information with the appropriate software.
- To develop protocols for the recording of data, which will guarantee the reproducibility of an experiment, conducted in the laboratory. To correlate the observed changes in the course of an experiment with the obtained results. To be able to carry out observation, monitoring and measurement of properties or chemical and / or physical changes in a certain material or reaction.
- To interpret the data obtained at the different stages of the experiments. To explain any differences between the results experimentally obtained and those expected. To prepare reports of the results with scientific rigor and conciseness.

In short, at a more specific level, the student will be able to:

- Design its own synthesis, properly planning all the phases involved in the synthetic design.
- Perform synthesis in the laboratory using conventional techniques for chemical separation, purification and structural elucidation of compounds.
- Analyze and evaluate the results obtained when performing synthesis in the laboratory, and to propose, if necessary, the appropriate improvements.

CONTENTS

THEORETICAL CONTENTS:

MODULE I: SYNTHETIC DESIGN TOOLBOX

Chapter 1. Synthetic Design

- Methodology of the retrosynthetic analysis.
- Types of transformations.
- General Strategy of the retrosynthetic analysis.
- Types of synthesis.
- Inversion of the polarity of the carbonyl group (umpolung).
- Domino reactions.

Chapter 2. Stereochemical considerations of the synthetic design

- Chiral molecules with one stereogenic center.
- Chirality without stereogenic carbon.
- Chiral molecules with two or more stereogenic centers.
- Separation of enantiomers.
- Stereochemistry of the C=C and C=N double bonds.
- Stereoisomerism in cyclic structures.
- Prochirality, homotopic, enantiotopic and diastereotopic groups and faces.
- Stereochemical classification of the reactions.
- Strain and molecular mechanics.
- Conformation of acyclic molecules.

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- Conformation of cyclic molecules.
- Anomeric effect.

Chapter 3. Protecting groups in organic synthesis

- Concept and characteristics of protecting groups.
- Protection of the hydroxyl group.
- Protection of the carbonyl group.
- Protection of diols.
- Protection of carboxylic acids.
- Protection of the amino group.
- Protection of multiple bonds.

MODULE II: FUNCTIONAL GROUP MANIPULATION TOOLBOX

Chapter 4. Oxidation

- Oxidation of alcohols.
- Allylic oxidation of alkenes.
- Oxidation of ketones and aldehydes.

Chapter 5. Reduction

- Catalytic hydrogenation.
- Reduction by dissolving metals.
- Group III hydride-transfer reagents.
- Reductions with soluble metals.
- Reductive deoxygenation of carbonyl compounds.

Chapter 6. Reactivity of π -carbon-carbon bonds

- Oxymercuration-reduction.
- Hydroboration.
- Epoxidation and azidination.
- Dihydroxylation.
- Degradation of C=C double bonds.
- Palladium-catalysed oxidation of alkenes.

MODULE III: C-C BOND FORMATION TOOLBOX

Chapter 7. Formation of carbon-carbon bonds via enolates

- Generation of carbanions by deprotonation.
- Regioselectivity and stereoselectivity in the formation of enolates.
- Alkylation of enolates.
- Generation and alkylation of dianions.
- Influence of the solvent in the alkylation of enolates.
- Oxygen versus carbon alkylation.
- Alkylation of carbon nucleophiles by conjugate addition.
- Aldol addition and related reactions.
- Nitrogen analogs of enols and enolates.
- Addition reactions to imines and iminium ions.
- Acylation of carbanions.

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Chapter 8. Formation of carbon-carbon bonds via organometallic reagents

- Preparation and properties of organomagnesium and organolithium reagents.
- Reactivity of organomagnesium and organolithium reagents.
- Organozincates.
- Copper organometallic intermediates.
- Reactions with palladium organometallic intermediates.
- Alkene metathesis.

Chapter 9. Pericyclic reactions

- The Diels-Alder cycloaddition reaction.
- 1,3-Dipolar cycloaddition reactions.
- [3,3]-Sigmatropic rearrangements.
- [3,2]-Sigmatropic rearrangements.

Chapter 10. Formation of carbon-carbon π -bonds

- β -elimination reactions.
- Pyrolytic *syn*-eliminations.
- Synthesis of alkenes from hydrazones.
- Stereodefined synthesis of alkenes from alkynes.
- The Wittig and related reactions.
- Alkene metathesis.

PRACTICAL CONTENTS:

MODULE IV. LABORATORY EXPERIMENTAL TECHNIQUES

Organic synthetic reactions

- Setting the reaction: use of the scale and volumetric measurement devices.
- Stoichiometric calculations.
- Monitoring the reaction. Thin layer chromatography.
- Work-up of the reaction. Calculations on the crude weight.

Isolation and purification of the product of an organic synthetic reaction

- Liquid liquid extraction.
- Gravity filtration.
- Filtration under reduced pressure.
- Crystallization.
- Distillation.
- Evaporation of solvent in the rotatory evaporator.

Interpretation of the results of a reaction

- Calculation of the yield of the reaction.
- Reaction product characterization: spectroscopy, melting point, boiling point.

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COMPETENCY ASSESSMENT

Criteria and assessment tools

This course has two alternative evaluation systems: a continuous evaluation system or a single examination system.

CONTINUOUS EVALUATION SYSTEM

The student must carry out the activities proposed by the lecturer, actively participating in them. The activities to be evaluated are listed below along with the weighting used for the rating:

The course is taught in the classroom (part A) and in the laboratory (part B).

To pass the course, a minimum grade of 5 out of 10 in each of the two sections, A and B is required. The final grade will be the result of the following weighting: Part A 80% and Part B 20%

Part A. Blocks I to III. Organic Synthesis toolbox.

This part deals with the general competencies "Ability to learn how to work independently", as well as specific competencies **C11** "Properties of aliphatic, aromatic, heterocyclic and organometallic compounds" and **C13** "The main synthetic routes in organic chemistry, including the interconversion functional groups and the formation of carbon-carbon and carbon-heteroatom bonds". Their assessment is carried out considering:

- Regular checks: 80%
- Rational synthetic proposal of an organic molecule, elaboration of a written document and its oral presentation: 20%

Part B. Block IV. LABORATORY EXPERIMENTAL TECHNIQUES.

In addition to the student autonomous work, the activities of this section are developed in the laboratory, being mandatory the attendance to all sessions. In this part the general competencies "Knowledge of a second language", "Ability of criticism and self-criticism" and "Ability for management and planning" as well as the specific competencies **Q3** "Competency to assess, explain and summarize data and chemical information", **Q6** "Skill in handling and processing computer data and chemical information", **P3** "Ability for observation, monitoring and measurement of properties, events or chemical changes, and the systematic and reliable recording of documentation", **P4** "Ability to handle standard chemical instrumentation, like that used for structural elucidations and chemical separations" and **P5** "Interpretation of data from observations and measurements in the laboratory in terms of its significance and the scientific theories" Their assessment is carried out considering:

- Work in the laboratory: 20%
- Laboratory notebook and results report: 50%
- Questions to be solved in autonomous working hours: 30%

SINGLE EXAMINATION SYSTEM.

It will be applied in all ordinary and extraordinary calls for those students who do not benefit from continuous assessment. It will consist of a written exam on the date fixed by the Faculty of Experimental Sciences.

Follow-Up Mechanisms

Assessment instruments

- Progress report.
- Tests, exercises, problems.

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- Observations of the process.
- Final assessment of reports, works and projects.
- Final tests (whether written or oral).

Monitoring mechanisms:

- Attendance to tutorials.
- Attendance and participation in seminars.
- Access to the virtual platform.
- Participation in communication tools (e mails, discussion forums).
- Submitting classroom activities.
- Submitting of tutorial activities.
- Submitting of virtual platform activities.

COURSE MATERIALS

Recommended course materials

1. Zweifel, G.S.; Nantz, M.H.; Somfai, P. *Modern Organic Synthesis: An Introduction* 2nd Ed. John Wiley & Sons Inc. 2017.
2. Carruthers, W.; Coldham, I.; Carruthers, W. *Modern methods of organic synthesis*. 4th Ed. Cambridge University Press. 2004.
3. Hoffman, R. V. *Organic Chemistry: An Intermediate Text*. 2nd Ed. Wiley-Interscience. 2004.
4. Morris, D.G. *Stereochemistry*. Royal Society of Chemistry. 2001.
5. Sundberg, R.J.; Carey, F.A. *Advanced Organic Chemistry Part B*. 5th Ed. Springer. 2007.
6. Cranwell, B.; Harwood, L. M.; *Experimental Organic Chemistry*. 3rd Ed. John Wiley & Sons Inc. 2017.

Complementary

1. Li, J.J. *Name Reactions: A Collection of Detailed Mechanisms and Synthetic Applications*. 5th Ed. Springer, 2014
2. Kürti, L.; Czakó, B. *Strategic applications of Named Reactions in Organic Synthesis*. Elsevier. 2005.
3. Warren, S.; Wyatt, P. *Organic synthesis: the disconnection approach*. 2nd Ed. John Wiley & Sons Inc. 2008.
4. Wyatt, P. *Organic synthesis: strategy and control*. John Wiley & Sons Inc. 2007.
5. Hanson, J. R. *Organic synthetic methods*. Royal Society of Chemistry. 2002.
6. Smith, M.B. *Organic synthesis*. 4th Ed. Academic Press. 2016.
7. Sundberg, R.J.; Carey, F.A. *Advanced Organic Chemistry Part A: Structure and Mechanism*. 5th Ed. Springer. 2007.
8. Smith, M.B. *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*. 7th Ed. John Wiley & Sons Inc. 2013.

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9. Martínez Grau, M. Á. *Técnicas experimentales en síntesis orgánica*. Síntesis. 1998.

Couse materials available in UAL's library

WEBSITE

- *Virtual Textbook of Organic Chemistry*:
<http://www2.chemistry.msu.edu/faculty/reusch/VirtTxtJml/intro1.htm>
- *Organic Synthesis Search*
<https://www.organic-chemistry.org/synthesis/>

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