COURSE: ADVANCED ORGANIC SYNTHESIS

SUBJECT: Advanced Organic Synthesis
MODULE: Drug Research Module
PROGRAM: University Master's Degree in Pharmaceutical Chemistry

GENERAL CHARACTERISTICS *

<table>
<thead>
<tr>
<th>Type</th>
<th>☐ Basic training, ☑ Compulsory ☐ Optional</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>☐ Final Project Work, ☐ External Practices</td>
</tr>
</tbody>
</table>

Duration: Semester
Number of ECTS credits: 5
Language: Spanish, Catalán and English

DESCRIPTION

BRIEF DESCRIPTION AND JUSTIFICATION (The meaning of the course in relation to the program. Between 100 and 200 words.)

The introduction by E. J. Corey in 1967 of retrosynthetic analysis as a systematic methodology for the organic synthesis design definitely changed the way by which organic chemists propose synthetic itineraries for a given molecule. This course develops in nine chapters the aforementioned methodology including the disconnection of carbon-carbon bonds (needed for the disconnection of monofunctional and difunctional systems), the disconnection of carbon-heteroatom bonds (living a particular attention to the construction of heterocyclic systems) and the study of those methods used to modify functionality (transformation of functional groups and use of protecting groups). A special attention is given to the economic and environmental implications of Organic Synthesis and to the use of computer tools to help retrosynthetic analysis. Finally, the course covers the Asymmetric Synthesis methods, Combinatorial Chemistry methodology, and their implications in the synthesis of new drugs.

COMPETENCES (Of the course in relation with preassigned competences in this area.)

Basic competences

• CB6 - To possess and understand knowledge to provide a basis or opportunity to be original in developing and / or applying ideas, often within a research context.

• CB7 - Students can apply their acquired knowledge and capability to solve problems in new or unfamiliar environments within broader (or multidisciplinary) contexts related to their field of study.

• CB9 - Students are able to communicate their conclusions to specialist and non-specialist audiences in a clear and unambiguous manner.

• CB10 - Students possess the learning skills to enable them to continue studying in a manner that may be largely self-directed or autonomous.

Specific competences

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- E8 - Students will acquire the knowledge of retrosynthetic analysis, new reactions and synthetic methodologies to apply them in research of drugs.

- E9 - Ability to develop synthetic routes for multifunctional organic molecules through application of the method of the “retrosynthetic methodology”.

Transversal competences
- T1 - Ability to communicate in English and use English as a working Language.
- T3 - Ability to assess the impact of the use of chemistry in the sustainable development of society.

PREREQUISITES * (Modules, materials, subjects or skills necessary to follow the course. Subjects can be stated that should have been completed.)

The corresponding to access master studies. Students who had reached the master from undergraduate degrees or degree in chemistry will not require any additional training supplement. For other qualifications, must have completed additional training previously.

CONTENTS (Sections that make up the syllabus, to a second level of detail.)

Chapter 1: Introduction to organic synthesis
1.1 Historical background. 1.2. Organic synthesis: Science and art. 1.3. Retrosynthetic analysis. 1.4. Objectives of the Organic synthesis.

Chapter 2: Retrosynthetic analysis
2.1. Retrosynthetic analysis methodology. 2.2. Retrosynthetic transformations. 2.3. Retrosynthetic analysis strategies. 2.4. Monofunctional and difunctional systems. 2.5 Praxis of retrosynthetic analysis. 2.6. In silico retrosynthetic analysis.

Chapter 3: Strategies and tactics in organic synthesis
3.1. General criteria for the evaluation of a synthesis. 3.2. Convergent vs linear synthesis. 3.3. Yield and conversion. 3.4. Selectivity and specificity. 3.5. Environmental efficiency. 3.6 Bibliography in organic synthesis. 3.7. Generic starting materials. 3.8. Tactical approaches to the synthesis of compounds.

Chapter 4: Protecting groups in organic synthesis
4.1. Strategies in synthesis: protecting groups. 4.2. Alcohol protective groups. 4.3. Amine protecting groups. 4.4. Carbonyl protecting groups. 4.5. Carboxylic acid protecting groups. 4.6. Orthogonal protecting groups. 4.7 Summary of protective groups.

Chapter 5: Functional group transformation
5.1. Transformations of functional groups. 5.2 Transformations of \( Csp^3 \). 5.3. Transformations on \( Csp^2 \) and \( Csp \). 5.4. Transformations on aromatic nuclei. 5.5. Transformations of polar groups.

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Chapter 6: Construction of open chain compounds

6.1. Introduction: open chain compounds. 6.2 Synthons and their synthetic equivalents. 6.3 Disconnections in nonfunctional and monofunctional systems. 6.4. Difunctional systems disconnections.

Chapter 7: Construction of carbocyclic and heterocyclic compounds

7.1. Strategies for synthesis of carbocycles and heterocycles. 7.2 Disconnections of carbocycles. 3-membered rings. 7.3 Disconnections of carbocycles. 4-membered rings. 7.4 Disconnections of carbocycles. 5 and 6-membered rings. 7.5. Disconnections of polycycles. 7.6. Disconnection of heterocycles. 3-Membered rings. 7.7 Disconnections of heterocycles. 4-Membered rings. 7.8 Disconnections of heterocycles. 5 and 6-membered rings

Chapter 8: Asymmetric synthesis


Chapter 9: Advanced techniques and applications in synthesis


METHODOLOGY

TRAINING ACTIVITIES * (Complete the table relating activities, workload in ECTS credits and skills.)

<table>
<thead>
<tr>
<th>Training activities</th>
<th>Hours / ECTS</th>
<th>Competences</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sessions of exposition of concepts</td>
<td>1,15</td>
<td>E8, E9, T1, T3, CB6, CB7</td>
</tr>
<tr>
<td>Sessions solving exercises, problems and cases</td>
<td>0,15</td>
<td>E8, E9, T1, T3, CB7</td>
</tr>
<tr>
<td>Seminars</td>
<td>0,07</td>
<td>E8, E9, T1, T3, CB7, CB9</td>
</tr>
<tr>
<td>Presentations</td>
<td>0,1</td>
<td>E8, E9, T1, T3, CB9, T1</td>
</tr>
<tr>
<td>Activities of personal study by students</td>
<td>3,33</td>
<td>E8, E9, T1, T3, CB6, CB7, CB9, CB10</td>
</tr>
<tr>
<td>Evaluation activities (exams, monitoring controls ...)</td>
<td>0,15</td>
<td>E8, E9, T1, T3, CB9</td>
</tr>
<tr>
<td><strong>TOTAL</strong></td>
<td><strong>5</strong></td>
<td>E8, E9, T1, T3, CB9</td>
</tr>
</tbody>
</table>

TEACHING METHODOLOGY (Justifying the teaching methods used in relation to the competences and contents of the course. Between 100 and 200 words.)

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The course consists of about 40-45 hours of lectures. All the material used during the lectures will be delivered to the student. The presentation of the topics will be complemented by discussion and resolution of problems and case studies.

There will be a short examination of chapter 5. In addition, two synthetic exercises regarding chapters 6 and 7 will be proposed. The final exam consists of a set of synthetic problems (3-4 exercises).

Course activities:

- **Sessions of exposition of concepts**: Exposition of contents through presentation or explanation (possibly including demonstrations) by a professor.
- **Sessions solving exercises, problems and cases**: Solving exercises, approach / problem solving and presentation / discussion of cases by a professor with the active participation of students.
- **Seminars**: open discussion with the teacher in order to review, discuss and answer questions about materials and topics presented in the sessions of exposure sessions concepts and solving exercises, problems and cases.
- **Presentations**: Oral presentation to a teacher and possibly other students by a student. It can be a paper prepared by the student by searching the published literature or a summary of a practical or project undertaken by the student.
- **Activities of personal study by students**: Personal work required to acquire the skills of each subject and assimilate the knowledge presented in the sessions of exposure sessions concepts and solving exercises, problems and cases, using, when necessary, the consultation recommended material.
- **Evaluation activities (testing, monitoring controls ...)**: Oral and / or written examinations carried out during the course of a semester or after it.

### EVALUATION

#### ASSESSMENT SYSTEM *

(Complete the table relating evaluation methods, competences and weight in the qualification of the subject.)

<table>
<thead>
<tr>
<th>Evaluation Methods</th>
<th>%</th>
<th>Competences</th>
</tr>
</thead>
<tbody>
<tr>
<td>Final Exam</td>
<td>40%</td>
<td>E8, E9, T1, T3 / CB6, CB7</td>
</tr>
<tr>
<td>Follow-up exams</td>
<td>30%</td>
<td>E8, E9, T1, T3 / CB6, CB7</td>
</tr>
<tr>
<td>Project and presentation</td>
<td>25%</td>
<td>E8, E9, T1, T3 / CB9, CB10</td>
</tr>
<tr>
<td>Participation</td>
<td>5%</td>
<td>T1</td>
</tr>
</tbody>
</table>

#### LEARNING OUTCOMES

(Explanation of the embodiments that allow competences evaluation of student, relating them to the competences and evaluation methods.)

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**Objective 1:**
Students should demonstrate their skills to apply retrosynthetic analysis to the disconnection of monofunctional and difunctional systems.

**Objective 2:**
Students should demonstrate their ability to interpret the results.

**Objective 3:**
Students should demonstrate their knowledge of new reactions and synthetic methodologies, such as asymmetric synthesis methods, functional groups protection, etc., to deal / to resolve / to discuss theoretical or practical questions in the light of the principles of the Organic Synthesis.

**Objective 4:**
Students should demonstrate skills to develop synthetic itineraries for organic multifunctional molecules by using the methodology of the "backward step".

**Objective 5:**
Students should demonstrate knowledge about the economic and environmental implications in the synthetic processes, both in those proposed by the students themselves and in those discussed in the classroom.

**QUALIFICATION** (Explanation of the system used for the grade of the student.)

The grade of this course depends on the following items:

<table>
<thead>
<tr>
<th>Item</th>
<th>Percentage</th>
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<tbody>
<tr>
<td>Final Exam</td>
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</tr>
<tr>
<td>Follow-up exams</td>
<td>30%</td>
</tr>
<tr>
<td>Papers and presentations</td>
<td>25%</td>
</tr>
<tr>
<td>Participation</td>
<td>5%</td>
</tr>
</tbody>
</table>

The final grade (first examination) is calculated using the results of the final exam (EF), the average of the follow-up exams (AS), the grade of a presentation (chapter V) and a synthetic roadmap (T) and class participation (P):

$$\text{Grade} = 40\% \text{ EF} + 30\% \text{ AS} + 25\% \text{ T} + 5\% \text{ P}$$

The final grade (following examinations) in the following examinations is given by:

$$\text{Grade} = 90\% \text{ EF} + 10\% \text{ T} \text{ (synthetic roadmap grade)}$$

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ASSESSMENT OF THE COMPETENCES (Define calculation expressions for each competence and the relevant evaluation methods.)

<table>
<thead>
<tr>
<th>Competences</th>
<th>Evaluation Methods</th>
<th>Observations</th>
</tr>
</thead>
<tbody>
<tr>
<td>To possess and understand knowledge to provide a basis or opportunity to be original in developing and / or applying ideas, often within a research context (CB6).</td>
<td>Final Exam Follow-up</td>
<td>50% EF + 50% AS</td>
</tr>
<tr>
<td>Students can apply their acquired knowledge and capability to solve problems in new or unfamiliar environments within broader (or multidisciplinary) contexts related to their field of study (CB7).</td>
<td>Final Exam Follow-up</td>
<td>50% EFE + 50% AS</td>
</tr>
<tr>
<td>Students can communicate their conclusions, and the knowledge and rationale underpinning these, to specialist and non-specialist audiences in a clear and unambiguous manner (CB9).</td>
<td>Project and presentation</td>
<td>T</td>
</tr>
<tr>
<td>That students have the learning skills to enable them to continue studying in a manner that may be largely self-directed or autonomous (CB10)</td>
<td>Project and presentation</td>
<td>T</td>
</tr>
<tr>
<td>Ability to communicate effectively both orally and in writing with specialized partners and non-specialized public (T1)</td>
<td>Project and presentation Participation</td>
<td>95% T + 5% P</td>
</tr>
<tr>
<td>Ability to assess the impact of the use of chemistry in the sustainable development of society (T3)</td>
<td>Project and presentation Participation</td>
<td>95% T + 5% P</td>
</tr>
<tr>
<td>Students will acquire the knowledge of retrosynthetic analysis, new reactions and synthetic methodologies to apply them in research of drugs (E8)</td>
<td>Final Exam Follow-up</td>
<td>50% EFE + 50% AS</td>
</tr>
<tr>
<td>Ability to develop synthetic routes for multifunctional organic molecules through application of the method of the “retrosynthetic methodology” (E9)</td>
<td>Final Exam Follow-up</td>
<td>50% EFE + 50% AS</td>
</tr>
</tbody>
</table>

BIBLIOGRAPHY (Recommended and accessible to students.)

BASIC BIBLIOGRAPHY (*):

- Lecture Notes (available on the Blackboard platform, http://moodle.iqs.url.com)

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COMPLEMENTARY MATERIAL:


DOCUMENT HISTORY

PREVIOUS CHANGES (Indicate date and author / s, most recent first)
September 30th, 2014. Dr. David Sánchez García
September 5th, 2016. Dr. David Sánchez Garcia

LAST REVISION (Indicate date and author / s.)
October 18th, 2016. Dr. David Sánchez García

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