SUBJECT: CHEMICAL PROCESS

MATTER: Process Chemistry
MODULE: Drug Production
STUDIES: Master in Pharmaceutical Chemistry

GENERAL FEATURES *
Type: ☐ Basic Training ☑ Compulsory ☐ Elective
☐ Master's thesis work, ☐ Outside practical
Duration: Semester Semester / s: 2
Number of ECTS credits: 5
Language / s: English

DESCRIPTION

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

The mission of the process chemists is to find the ideal industrial synthesis for a NCE taking into account factors such as safety, environmental considerations and price. The aim of this course is to provide chemical language, knowledge and development principles of organic synthesis processes on an industrial scale, particularly within the environment of the pharmaceutical industry. Consequently, the course focuses on the production of drugs at a relatively small scale (tens to hundreds of kg) and not about the manufacture of organic compounds at the level of hundreds of tons. Special attention is devoted to the selection of reagents and solvents commonly used in industry.

POWERS (Of course put in relation to the powers preassigned in the field.)

• Knowledge and understanding that provide a basis or opportunity for originality in developing and / or applying ideas, often in a research context (CB6).
• That the students can apply their knowledge and their ability to solve problems in new or unfamiliar environments within broader (or multidisciplinary) contexts related to their field of study (CB7).
• Students can communicate their conclusions, and the knowledge and rationale underpinning these, to specialist and non-specialist audiences clearly and unambiguously (CB9).
• Students must possess the learning skills that enable them to continue studying in a way that will be largely self-directed or autonomous (CB10)
• Have knowledge of the development process on an industrial scale synthesis to be applied in the production of drugs (E13)
• Ability to select industrial synthetic routes taking into account economic, environmental and safety aspects (E14)
• Ability to communicate in English and use English as a working language (T1)
• Ability to assess the impact of the use of chemistry in sustainable development of society (T3)

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PREVIOUS REQUIREMENTS* (Modules, materials, subjects or knowledge necessary for the pursuit of the subject. Consist must have completed courses that can be made.)

The corresponding to access to master studies. Students who have accessed the master from undergraduate degrees or degree in chemistry will not require any additional further training. For other qualifications, they must first have completed additional training.

CONTENTS (As a ratio of the sections that constitute the agenda of the same, up to a second level detail.)

Chapter 1: Introduction
1.1. The pharmaceutical industry: Phases of drug development. 1.2. Industrial production of drugs: development. 1.3 Process Scale up: from gram to kilogram, role of the process chemist. 1.4. Scalability of basic laboratory operations.

Chapter 2: Selecting the synthetic route
2.1. Characteristics of an Industrial synthetic route. 2.2. Economic criteria: cost evaluation. 2.3. Safety criteria. 2.4 Environmental criteria. 2.5. Green Chemistry: waste disposal.

Chapter 3: Reagent selection
3.1. Characteristics of the reagents used in industry scale. 3.2. Industrial Classification of reagents ACCORDING to use: bases, oxidizers, reductants, catalysts, polymer-supported reagents, biocatalysts. 3.3. Starting materials: affordable sources of starting materials.

Chapter 4: Solvent selection
4.1. Characteristics of an ideal industrial solvent. 4.2. Solvents suitable for scaling. 4.3. Industrial Solvents used at scale. 4.4. Uses of solvents. 4.5. Water in Industrial reactions. 4.6. Azeotropic drying.

Chapter 5: The Industrial-scale reaction
5.1. The reactor and Its components. 5.2. Batch Processes and continuous. 5.3. Procedures for Establishing the reaction conditions. 5.4. Control of the reaction. 5.5. Optimization of the reaction. 5.6. Scaling reactions. 5.7. Industrial chiral synthesis. 5.8. Troubleshooting.

Chapter 6: Isolation Process

Chapter 7: Purification of products
7.1. Purification operations. 7.2. Chromatography. 7.3. Recrystallization. 7.4. Disagregation.

Chapter 8: Characteristics of the end product

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# METHODOLOGY

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

<table>
<thead>
<tr>
<th>Training activities</th>
<th>ECTS</th>
<th>competences</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sessions of exposition of concepts</td>
<td>1.15</td>
<td>E13, E14, T1, T3, CB6, CB7, CB10</td>
</tr>
<tr>
<td>Sessions solving exercises, problems and cases</td>
<td>0.15</td>
<td>E13, E14, T1, T3, CB6, CB7</td>
</tr>
<tr>
<td>Seminars</td>
<td>0.07</td>
<td>E13, E14, T1, T3, CB6, CB7, CB9, CB10</td>
</tr>
<tr>
<td>Presentations</td>
<td>0.1</td>
<td>E13, E14, T1, T3, CB6, CB7, CB9</td>
</tr>
<tr>
<td>Activities of personal study by students</td>
<td>3.33</td>
<td>E13, E14, T1, T3, CB7, CB9</td>
</tr>
<tr>
<td>Evaluation activities (testing, monitoring controls ...)</td>
<td>0.15</td>
<td>E13, E14, T1, T3, CB6, CB7</td>
</tr>
<tr>
<td><strong>TOTAL</strong></td>
<td><strong>5</strong></td>
<td></td>
</tr>
</tbody>
</table>

## EXPLANATION OF TEACHING METHODS (Justifying the teaching methods used in relation to the skills and course contents. Between 100 and 200 words.)

The course is taught through lectures (40-45 h) covering the various aspects of the program and which are the basis of an individual or group project in which students have to study the possible industrialization of a synthetic multi-step process from all points of view (reagents, solvents, economic criteria, safety criteria, environmental criteria, sustainability, etc). This study will be presented in the form of PowerPoint presentation in class.

At the end of Modules 1 to 3 modules 4 and 5, and 6 to 8 modules test follow-up examinations are performed. At the end of the course seminars presentation and discussion of the work done by students are made. Finally a test final exam is performed.

- **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:** Statement made by a 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.

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- **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 of the student 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 statements made during the course of a semester or after it.

### EVALUATION

#### ASSESSMENT METHODS * (Complete the table relating evaluation methods, skills and weight in the grade for the course.)

<table>
<thead>
<tr>
<th>Evaluation Methods</th>
<th>%</th>
<th>competences</th>
</tr>
</thead>
<tbody>
<tr>
<td>Final Exam</td>
<td>50</td>
<td>E13, E14, T1, T3 / CB6, CB7</td>
</tr>
<tr>
<td>Follow-up exams</td>
<td>25</td>
<td>E13, E14, T1, T3 / CB6, CB7</td>
</tr>
<tr>
<td>Project and presentation</td>
<td>20</td>
<td>E13, E14, T1, T3 / CB9, CB10</td>
</tr>
<tr>
<td>Participation</td>
<td>5</td>
<td>T1</td>
</tr>
<tr>
<td><strong>TOTAL</strong></td>
<td>100</td>
<td></td>
</tr>
</tbody>
</table>

#### LEARNING OUTCOMES (Explanation of the achievements of the student allowing skills assessment, relating them to the skills and methods of evaluation.)

- The student must demonstrate knowledge of the principles of Chemical Process.
- The student must demonstrate knowledge using the principles of development of synthesis processes on an industrial scale for the production of drugs or organic compounds of interest.
- The student must demonstrate the ability to select industrializable synthetic routes in a multidisciplinary environment individually or as a member of a team.
- The student must demonstrate understanding of the impact of development of synthesis processes on an industrial scale in the production of drugs and organic compounds of interest and the importance of working in a professional environment and ethically responsible

#### QUALIFICATION (Explanation of the computer system of the course grade.)

The grade of this course is obtained:

- **Final Exam**: 50%
- **Follow-up exams**: 25%
- **Papers and presentations**: 20%
- **Participation**: 5%

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Final exams (EF)
Follow-up exams (AS)
Project and presentation (T)
Participation (P)

The final grade is calculated using the results of the final examination (EF), the average test scores tracking (AS), the student’s work and its presentation (T) and class participation (P):

Grade = 50% EF + 25% AS + 20% T + 5% P

SKILLS ASSESSMENT (Define calculation expressions for each competency based assessment activities concerned.)

<table>
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<th>Observations</th>
</tr>
</thead>
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<tr>
<td>Knowledge and understanding that provide a basis or opportunity for originality in developing and / or applying ideas, often in a research context (CB6).</td>
<td>Final exam</td>
<td>50% 50% EF + AS</td>
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<td></td>
<td>Monitoring activities</td>
<td></td>
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<td>T</td>
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<td>Final exam</td>
<td>50% 50% EF + AS</td>
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<td>Final exam</td>
<td>50% 50% EF + AS</td>
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<td>Monitoring activities</td>
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<tr>
<td>Ability to communicate in English and use English as a working language (T1)</td>
<td>Papers and presentations</td>
<td>T</td>
</tr>
<tr>
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<td>Participation</td>
<td>P</td>
</tr>
</tbody>
</table>

BIBLIOGRAPHY (Recommended and accessible to the student.)

TEXTBOOKS:

* These characteristics should not be changed without the approval of the bodies responsible for top-level academic structures (subject, module and / or curriculum).
• ICH guidelines (http://www.ich.org)
• European Pharmacopoeia (http://www.pheur.org)
• US Pharmacopeia (http://www.usp.org)

REQUIRED MATERIAL:
• http://iqs.blackboard.com

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