COURSE: STRUCTURAL DETERMINATION

SUBJECT MATTER: Biotechnology for Health
MODULE: Optional Subjects
PROGRAM: Degree in Biotechnology

GENERAL FEATURES *
Type: ☐ Basic training, ☐ Compulsory, ☑ Elective
☐ Final Degree Project, ☐ Practicum
Duration: Semestral
Number of ECTS credits: 5
Language / s: Spanish, Catalan and English

DESCRIPTION

SHORT DESCRIPTION AND JUSTIFICATION (of the meaning of the course in relation to the studies. Between 100 and 200 words)

We present the main spectroscopic techniques that are currently used for the determination of the structure of organic compounds, with special attention to IR, NMR and EM. For each of the techniques, the physical foundation, the types of instruments used and their operation, the preparation of the necessary sample and the spectral parameters are explained. The spectral characteristics of the main types of organic molecules are detailed and knowledge is strengthened by specific exercises for each technique. Finally, problems that require the joint use of several of these techniques are discussed and solved, highlighting their complementary nature.

COMPETENCES (of the course placed in relation to the pre-assigned competences in the subject matter)

- Be able to understand and apply advanced knowledge of Structural Determination (IR, NMR, UV-Vis, MS) for application in the field of Biomolecular Sciences. (E3)
- That students develop those learning skills necessary to undertake further studies with a high degree of autonomy (CB5)
- Be able to assess the impact of their professional activity on the sustainable development of society (T3)
- Be able to incorporate contemporary aspects related to the exercise of their profession. (T5)
- Be able to integrate the knowledge and tools of Structural Determination (IR, NMR, UV-Vis, MS) for their application to different industrial sectors that use, develop or produce biotechnological products or processes (E6)

PREVIOUS REQUIREMENTS * (modules, subject matters, courses or knowledge necessary for the follow-up of the subject. State previous courses required to be completed)

According to the program planning and academic regulations.

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CONTENTS (List the content of the course, with up to two level detail)

0. Spectroscopy.

1. Mass spectrometry (MS).

2. UV-Vis Spectroscopy.

3. Infrared Spectroscopy (IR).
   Background and technique, harmonic oscillator, functions and eigenvalues, selection rules (IR and Raman rotation-vibrational) normal modes of vibration and characteristic frequencies. Instrumentation and sample preparation. Interpretation of spectra, functional groups. IR quantitative.

4. Nuclear Magnetic Resonance Spectroscopy (NMR)
   Foundation and technique. Spectral parameters, coupling, selection rules, first-order perturbations, chemical and magnetic equivalence (chirality), second order spectra, multiplets (Karplus diagrams), protons in heteroatoms, decoupling, relaxation time and NOE effect. Interpretation of $^{13}$C-NMR and $^1$H-NMR spectra, substituent effects and tables. Introduction to 2D-NMR: homonuclear correlation through bonds (COSY) and through space (NOESY), heteronuclear correlation through bonds (HSQC, HMQC).

5. Structural Elucidation Exercises by spectroscopic methods.

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METHODOLOGY

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

<table>
<thead>
<tr>
<th>Learning Activities</th>
<th>ECTS Credits</th>
<th>Competences</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lectures</td>
<td>0,7</td>
<td>T3, T5, E3</td>
</tr>
<tr>
<td>Case and Problem-Solving Sessions</td>
<td>0,7</td>
<td>T3, T5, E3, E6</td>
</tr>
<tr>
<td>Seminars</td>
<td>0,2</td>
<td>T3, T5, E3, E6</td>
</tr>
<tr>
<td>Practical and Lab Work</td>
<td>0,9</td>
<td>B5, T3, T5, E3, E6</td>
</tr>
<tr>
<td>Personal Study</td>
<td>2,4</td>
<td>T3, T5, E3, E6</td>
</tr>
<tr>
<td>Assessment Tasks (Exams, Continuous Assessment...)</td>
<td>0,1</td>
<td>B5, T3, T5, E3, E6</td>
</tr>
<tr>
<td><strong>TOTAL</strong></td>
<td><strong>5,0</strong></td>
<td><strong>B5, T3, T5, E3, E6</strong></td>
</tr>
</tbody>
</table>

TEACHING METHODOLOGY (justify the teaching methodology in relation to the competences and course contents. Between 100 and 200 words)

- **Lectures** - Presentation and explanation of contents by a teacher (possibly including demonstrations).
- **Case and Problem-Solving Sessions** - Resolution of exercises and problems, and exposition / discussion of cases by a teacher with the active participation of students.
- **Seminars** - Period of instruction carried out by a teacher with the aim of reviewing, discussing and resolving doubts about the materials and topics presented in the lectures and in the case and problem-solving sessions.
- **Practical and Lab** - Period where the student performs laboratory activities or similar (computer practices, projects, workshops, etc.) under the direct supervision of a teacher.
- **Personal study activities** - Personal work of the student necessary to acquire the competences of each subject matter, and to assimilate the knowledge exposed in lectures and case and problem-solving sessions, using the recommended reference materials. They also include the preparation of tasks related to the other activities, and the preparation of exams.
- **Assessment Tasks** - Oral and / or written tests made during the academic period of a course, or once it has finished (final exams, follow-up controls).

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ASSESSMENT

ASSESSMENT METHODS * (Complete the table relating assessment methods, competences, and weight percentage in the course qualification)

<table>
<thead>
<tr>
<th>Assessment methods</th>
<th>Weight</th>
<th>Competences</th>
</tr>
</thead>
<tbody>
<tr>
<td>Final Exam</td>
<td>50%</td>
<td>B5, T3, T5, E3, E6</td>
</tr>
<tr>
<td>Continuous Assessment Activities</td>
<td>25%</td>
<td>E3, T3, T5, E6</td>
</tr>
<tr>
<td>Lab or Field Work</td>
<td>20%</td>
<td>B5, E3, E6</td>
</tr>
<tr>
<td>Participation</td>
<td>5%</td>
<td>E3, E6</td>
</tr>
</tbody>
</table>

LEARNING OUTCOMES (Explanation of the student's achievements that allow the assessment of competences, relating them to the competences and the assessment methods)

1. Demonstrate understanding and ability to apply the knowledge of Structural Determination (IR, NMR, UV-Vis, EM) in the practice and performance of activities in the field of Biomolecular Sciences (E3)
2. Demonstrate having developed those learning skills necessary to undertake further studies with a high degree of autonomy (B5)
3. Demonstrate the ability to assess the impact of their professional activity on the sustainable development of society (T3)
4. Demonstrate ability to incorporate contemporary aspects related to the exercise of their profession (T5)
5. Demonstrate the ability to integrate the knowledge and tools of Structural Determination (IR, NMR, UV-Vis, EM) for their application to different industrial sectors that use, develop or produce biotechnological products or processes (E6)

QUALIFICATION (Explanation of the qualification system)

The first qualification of the student, always in continuous evaluation, is obtained by means of the weighted average of the different evaluation methods reflected in the previous table:
- 50% Final exam (theory + problems)
- 25% Average of tests and follow-up activities done in class time
- 20% Experimental work
- 5% Participation in class

For the recovery of the subject in subsequent calls, the best score between i) the one obtained in the recovery exam (theoretical-practical) and ii) its inclusion as a substitute for the final exam in the previous scale..

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ASSESSMENT OF THE COMPETENCES (Describe the grading system for each competence in relation with the assessment tasks)

For the evaluation of the E3 competence, the student's final grade will be used as an indicator. For the evaluation of the T3 / T5 competences, the mark of the exams and follow-up activities will be used as an indicator. For the evaluation of the B5 competence, the mark of the experimental work will be used as an indicator and for the E6, the experimental work and individual follow-up activities in the classroom will be used.

BIBLIOGRAPHY (Recommended and accessible to the student.)

TEXTBOOKS:

BASIC BIBLIOGRAPHY:

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Databases:

DOCUMENT HISTORY

PREVIOUS REVISIONS (Indicate date and author / s, first the most recent one)

CURRENT REVISION (Indicate date and author / s)
February 20, 2019, Dr. Jordi Teixidó i Closa

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