



## IDENTIFYING DATA

### Organic chemistry III

|                     |   |           |      |            |
|---------------------|---|-----------|------|------------|
| Subject             | Organic chemistry III   |           |      |            |
| Code                | V11G200V01704   |           |      |            |
| Study programme     | (*)Grao en Química  |           |      |            |
| Descriptors         | ECTS Credits  | Choose    | Year | Quadmester |
|                     | 9   | Mandatory | 4th  | 1st        |
| Teaching language   | Spanish   |           |      |            |
| Department          | Organic Chemistry   |           |      |            |
| Coordinator         | Álvarez Rodríguez, Rosana   |           |      |            |
| Lecturers           | Álvarez Rodríguez, Rosana<br>Fall Diop, Yagamare<br>Rodríguez de Lera, Angel<br>Tojo Suárez, Emilia   |           |      |            |
| E-mail              | rar@uvigo.es  |           |      |            |
| Web                 |   |           |      |            |
| General description | This subject will integrate all the previous knowledge of Organic Chemistry, in particular regarding organic synthesis and his consequences in the creation of new stereogenic elements. For this, will use the tools of rethrosynthetic analysis , paying particular attention to the analysis of synthetic proposals that take place with selectivity (chemo-, regio- and stereoselectivity). |           |      |            |

## Competencies

|      |  |
|------|--|
| Code |  |
| A1   | Students have demonstrated knowledge and understanding in a field of study that builds upon their general secondary education, and is typically at a level that, whilst supported by advanced textbooks, includes some aspects that will be informed by knowledge of the forefront of their field of study |
| A2   | Students can apply their knowledge and understanding in a manner that indicates a professional approach to their work or vocation, and have competences typically demonstrated through devising and sustaining arguments and solving problems within their field of study                                  |
| A4   | Students can communicate information, ideas, problems and solutions to both specialist and non-specialist audiences  |
| A5   | Students have developed those learning skills that are necessary for them to continue to undertake further study with a high degree of autonomy  |
| C2   | Demonstrate knowledge and understanding of essential facts, concepts, principles and theories: types of chemical reactions and its main characteristics  |
| C10  | Demonstrate knowledge and understanding of essential facts, concepts, principles and theories: properties of aliphatic, aromatic, heterocyclic and organometallic compounds  |
| C11  | Demonstrate knowledge and understanding of essential facts, concepts, principles and theories: nature and behavior of functional groups in organic molecules   |
| C12  | Demonstrate knowledge and understanding of essential facts, concepts, principles and theories: structural features of chemical elements and their compounds, including stereochemistry   |
| C13  | Demonstrate knowledge and understanding of essential facts, concepts, principles and theories: main synthetic routes in organic chemistry, including interconversions of functional groups and the formation of carbon-carbon and carbon-heteroatom bonds  |
| C19  | Apply knowledge and understanding to solve basic problems of quantitative and qualitative nature   |
| C20  | Evaluate, interpret and synthesize data and chemical information   |
| C23  | Present oral and written scientific material and scientific arguments to a specialized audience  |
| C24  | Recognize and analyze new problems and plan strategies to solve them   |
| C25  | Handle chemicals safely, considering their physical and chemical properties, including the evaluation of any specific risks associated with its use  |
| C26  | Perform common laboratory procedures and use instrumentation in synthetic and analytical work  |
| C27  | Monitor, by observation and measurement of physical and chemical properties, events or changes, and document and record them in a consistent and reliable way  |

|     |   |
|-----|---|
| C28 | Interpret data derived from laboratory observations and measurements in terms of their significance and relate them to the appropriate theory |
| D1  | Communicate orally and in writing in at least one of the official languages of the University   |
| D3  | Learn independently   |
| D4  | Search and manage information from different sources  |
| D5  | Use information and communication technologies and manage basic computer tools  |
| D7  | Apply theoretical knowledge in practice   |
| D8  | Teamwork  |
| D9  | Work independently  |
| D13 | Make decisions  |
| D14 | Analyze and synthesize information and draw conclusions   |
| D15 | Evaluate critically and constructively the environment and oneself  |
| D18 | Generate new ideas and show initiative  |

### Learning outcomes

| Expected results from this subject  | Training and Learning Results |  |   |
|---|-------------------------------|--|---|
| 1. Recognise structural elements in organic molecules.                    | A2                            | C2<br>C11<br>C12<br>C13<br>C23<br>C24        | D1<br>D3<br>D7<br>D9<br>D13<br>D14<br>D18       |
| 2. Propose retrosynthetic sequences of target molecules.                  | A1<br>A2<br>A5                | C2<br>C11<br>C12<br>C13<br>C24               | D1<br>D3<br>D4<br>D5<br>D7<br>D9<br>D13<br>D18  |
| 3. Analyse alternative retrosynthetic proposals.                          | A1<br>A2<br>A5                | C2<br>C10<br>C11<br>C12<br>C13<br>C20<br>C24 | D1<br>D3<br>D4<br>D5<br>D7<br>D9<br>D13<br>D18  |
| 4. Design synthetic sequences to target molecules.                        | A1<br>A2<br>A5                | C2<br>C10<br>C11<br>C12<br>C13<br>C20        | D1<br>D3<br>D4<br>D5<br>D7<br>D9<br>D13<br>D18  |
| 5. Value the use of structure-simplifying reactions.                      | A1<br>A2<br>A5                | C2<br>C10<br>C11<br>C12<br>C13<br>C20<br>C24 | D1<br>D3<br>D4<br>D7<br>D9<br>D13<br>D14<br>D18 |
| 6. Recognise relationships between functional groups of target molecules. | A1<br>A2<br>A5                | C2<br>C10<br>C11<br>C12<br>C13<br>C20<br>C24 | D1<br>D3<br>D4<br>D7<br>D9<br>D13<br>D18        |

7. Use properly the functional groups interconversions.

|    |     |     |
|----|-----|-----|
| A1 | C2  | D1  |
| A2 | C10 | D3  |
| A5 | C11 | D4  |
|    | C12 | D5  |
|    | C13 | D7  |
|    | C20 | D9  |
|    | C24 | D13 |
|    |     | D14 |
|    |     | D18 |

8. Propose synthesis of carbocyclic and heterocyclic compounds.

|    |     |     |
|----|-----|-----|
| A1 | C2  | D1  |
| A2 | C10 | D3  |
| A5 | C11 | D4  |
|    | C12 | D7  |
|    | C13 | D9  |
|    | C20 | D13 |
|    | C24 | D14 |
|    | C25 | D18 |
|    | C26 |     |
|    | C27 |     |
|    | C28 |     |

9. Know the reactivity of heterocyclic compounds.

|    |     |     |
|----|-----|-----|
| A1 | C2  | D1  |
| A2 | C10 | D3  |
| A5 | C11 | D4  |
|    | C12 | D7  |
|    | C13 | D9  |
|    | C20 | D13 |
|    | C24 | D14 |
|    | C26 | D18 |
|    | C27 |     |
|    | C28 |     |

10. Know the reactions that can provide selectivity (chemo-, regio- and stereoselectivity) in chemical transformations.

|    |     |     |
|----|-----|-----|
| A1 | C2  | D1  |
| A2 | C10 | D3  |
| A5 | C11 | D4  |
|    | C12 | D5  |
|    | C13 | D7  |
|    | C19 | D8  |
|    | C20 | D9  |
|    | C24 | D13 |
|    |     | D14 |
|    |     | D18 |

11. Handle appropriately the disconnections between unsaturated fragments.

|    |     |     |
|----|-----|-----|
| A1 | C2  | D1  |
| A2 | C10 | D3  |
| A5 | C11 | D4  |
|    | C12 | D5  |
|    | C13 | D7  |
|    | C20 | D9  |
|    | C24 | D13 |
|    |     | D14 |
|    |     | D18 |

12. Evaluate and propose the use of protective groups in organic synthesis.

|    |     |     |
|----|-----|-----|
| A1 | C2  | D1  |
| A2 | C10 | D3  |
| A5 | C11 | D4  |
|    | C12 | D7  |
|    | C13 | D9  |
|    | C20 | D13 |
|    | C24 | D14 |
|    |     | D18 |

13. Recognise and value the importance of organic synthesis in the advancement of society.

|    |     |     |
|----|-----|-----|
| A2 | C23 | D15 |
| A4 |     |     |
| A5 |     |     |

## Contents

Topic

|  |   |
|--|---|
| 1. THE DESIGN OF ORGANIC SYNTHESIS. RETROSYNTHETIC ANALYSIS  | 1.1. Introduction to target-oriented synthesis.<br>1.2. Retrosynthetic analysis. The synthon approach. Transforms and rethrons. Strategic disconnections. The synthesis tree.<br>i. Preliminary evaluation.<br>ii. Simplifying transforms.<br>iii. Powerful transforms.<br>iv. Interconversion, addition and removal of functional groups.<br>1.3. Computer-based synthetic strategies.   |
| 2. CRITERIA OF SELECTION OF DISCONNECTIONS   | 2.1. One- and two-group C-X disconnections (1,n).<br>i. Synthons and synthetic equivalents.<br>ii. Alternate polarities.<br>iii. Inversion of polarity.<br>iv. Functional groups interconversions.<br>v. Addition and removal of functional groups.<br>2.2. One- and two-group C-C disconnections (1,n).<br>i. One-group C-C disconnections.<br>ii. (1,n) C-C disconnections of difunctionalized compounds.<br>2.3. Tactics of skeletal transformations. Rearrangements and fragmentations. |
| 3. FUNCTIONAL GROUPS INTERCONVERSIONS  | 3.1. Interconversion of functional groups by substitution, addition and elimination.<br>3.2. Oxidation reactions.<br>i. Transition metals (*Cr and *Mn).<br>ii. Methods based in the generation of "activated DMSO".<br>iii. Hypervalent iodine reagents.<br>iv. Olefin epoxidation and dihydroxylation.<br>3.3. Reduction reactions.   |
| 4. CHEMOSELECTIVITY. PROTECTIVE GROUPS IN ORGANIC SYNTHESIS  | 4.1. Strategies for the selection of protective groups: orthogonal or of modulated sensitivity.<br>4.2. Description of protective groups.<br>i. Sensitive to acids or bases.<br>ii. Sensitive to fluoride.<br>iii. Sensitive to reduction and oxidation reagents.<br>iv. Other protective groups.   |
| 5. STEREOCHEMICAL STRATEGIES. STEREOSELECTIVITY  | 5.1. Description of Stereochemistry.<br>i. Symmetry and chirality. Stereogenic units.<br>ii. Topicity.<br>iii. Relative configuration. Descriptors.<br>5.2. *Stereochemistry in chemical reactions.<br>i. Product selectivity.<br>ii. Simple- and induced-distereoselectivity.<br>5.3. Disconnections based in chiral fragments.  |
| 6. DISCONNECTIONS OF UNSATURATED COMPOUNDS   | 6.1. Stereoselective olefin synthesis.<br>i. Carbanions stabilised by phosphorous: Wittig and HWE reactions.<br>ii. Carbanions stabilised by silicon: Peterson reaction.<br>iii. Carbanions stabilised by sulphur: Julia reaction.<br>iv. Claisen rearrangement.<br>v. Olefin metathesis.<br>6.2. Palladium-catalyzed reactions.<br>i. Heck reaction.<br>ii. Stille, Negishi and Suzuki cross-coupling.   |
| 7. FORMATION AND REACTIVITY OF CYCLIC COMPOUNDS. TOPOLOGICAL STRATEGIES  | 7.1. Formation of saturated carbocyclic and heterocyclic compounds.<br>i. Cyclization reactions. The Thorpe-Ingold effect.<br>ii. Baldwin Rules.<br>iii. Formation of carbocyclic compounds.<br>7.2. Formation of heterocyclic compounds.<br>i. (3+2) Cycloadditions.<br>ii. Condensation of dicarbonyl compounds.<br>7.3. Properties and reactivity of aromatic heterocyclic compounds.<br>7.4. Topological strategies in Retrosynthetic Analysis.   |
| LAB EXPERIMENT 1. Preparation of a-D-glucopyranoside pentaacetate  | One session   |
| LAB EXPERIMENT 2. Preparation of b-D-glucopyranoside pentaacetate  | Two sessions  |
| LAB EXPERIMENT 3. Reactivity of dimethylsulfoxonium methylide with conjugated and nonconjugated carbonyl compounds: synthesis of epoxides and cyclopropanes. | One session   |

|  |               |
|--|---------------|
| LAB EXPERIMENT 4. Microwave-assisted Diels-Alder reaction                                    | One session   |
| LAB EXPERIMENT 5. Preparation of an Ionic Liquid. Application in the synthesis of coumarines | Two sessions  |
| LAB EXPERIMENT 6. Suzuki reaction in water   | One session   |
| LAB EXPERIMENT 8. Total synthesis of a natural product: caffeic acid phenethyl ester (CAPE)  | Four sessions |

## Planning

|                      | Class hours | Hours outside the classroom | Total hours |
|----------------------|-------------|-----------------------------|-------------|
| Seminars             | 26          | 49                          | 75          |
| Laboratory practices | 45.5        | 32.5                        | 78          |
| Lecturing            | 13          | 17                          | 30          |
| Short answer tests   | 3           | 27                          | 30          |
| Essay questions exam | 2           | 10                          | 12          |

\*The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.

## Methodologies

|                      | Description   |
|----------------------|---|
| Seminars             | In this activity, which is scheduled to take place twice a week, the most complex topics of the subject will be discussed, and the exercises and problems previously proposed by the teaching staff will be solved.   |
| Laboratory practices | Each student will plan and execute the corresponding lab experiments in sessions lasting 3.5 hours. The students will be provided with the explanation of the lab session by the teaching staff. All the observations, calculations and notes for every experiment will be collected in a lab notebook, which will also include the discussion of the questions posed in the experiment description as well as the spectroscopic characterization of the synthesized compounds. |
| Lecturing            | The teaching staff will explain the general contents of the course paying particular attention to those considered key topics and of the greater difficulty. In anticipation of each master session, all the handouts and presentations will be made available in the TEMA teaching platform for downloading by the students.   |

## Personalized attention

| Methodologies        | Description   |
|----------------------|---|
| Lecturing            | The teaching staff will devote the necessary time to solve the requests and questions raised by the students related to the course syllabus, informing beforehand about his/her availability.     |
| Seminars             | The teaching staff will devote the necessary time to solve the requests and questions raised by the students related to the course syllabus, informing beforehand about his/her availability.     |
| Laboratory practices | The teaching staff will devote the necessary time to solve the requests and questions raised by the students related to the laboratory practice, particularly in the lab sessions and beforehand. |

| Tests                | Description  |
|----------------------|--|
| Short answer tests   | The teaching staff will devote the necessary time to solve the requests and questions raised by the students related to the short answer tests, informing beforehand about his/her availability. In addition, short answer test exams from previous years will be solved in seminars before the official tests take place. |
| Essay questions exam | The teaching staff will devote the necessary time to solve the requests and questions raised by the students related to the long answer tests, informing beforehand about his/her availability. In addition, long answer test exams from previous years will be solved in seminars before the official tests take place.   |

## Assessment

| Description | Qualification | Training and Learning Results |
|-------------|---------------|-------------------------------|
|             |               |                               |

|                      |  |    |                      |  |  |
|----------------------|--|----|----------------------|--|--|
| Seminars             | The resolution of problems and questions posed in the seminar classes, as well as the homework carried out by the students in those tasks of personal work entrusted by the teachers will be valued.<br>Results of the learning:<br>All the indicated, since the seminars will take place along the course.  | 20 | A1<br>A2<br>A4<br>A5 | C2<br>C10<br>C11<br>C12  | D1<br>D3<br>D4<br>D5   |
|                      |  |    |                      | C13<br>C19<br>C20<br>C23<br>C24  | D7<br>D8<br>D9<br>D13<br>D14<br>D15<br>D18                         |
| Laboratory practices | 1.- The work carried out in the laboratory: the assistance to each one of the sessions is compulsory. The attitude and skill of the student in the laboratory and the interpretation of the mechanisms and spectra will be valued.<br>2.- The laboratory notebook.<br>3.- Written exam: it will consist on theoretical and practical questions related to the lab experiments. It will take place in the official dates established by the Faculty.<br><br>To pass the lab course it is mandatory to have passed each one of the three parts evaluated. Those students who passed the lab course in the academic year 2014-2015 are entitled to keep that grade in the present academic year.<br><br>In the extraordinary exam the student will answer the written examination and will deliver a new laboratory notebook if required, keeping the qualifications obtained during the course in the others parts of the subject.<br>Results of the learning:<br>1. Recognise structural elements in the organic molecules.<br>2. Design alternative synthetic sequences.<br>3. Handle reactions of functional groups interconversions.<br>4. Propose synthesis of carbo- and heterocyclic molecules.<br>5. Recognise selective reactions.<br>6. Recognise the importance of organic synthesis to the advancement of society. | 30 | A1<br>A2<br>A4       | C25<br>C26<br>C27<br>C28   |  |
| Short answer tests   | A short answer exam will be carried out (10%).<br>Results of the learning:<br>1. Recognise structural elements of organic molecules.<br>2. Propose retrosynthetic sequences.<br>3. Analyse alternative retrosynthetic proposals.<br>4. Value the use of structurally-simplifying reactions.<br>5. Recognise relationships between functional groups.<br>6. Use properly functional groups interconversion reactions.   | 10 | A1<br>A2<br>A5       | C2<br>C10<br>C11<br>C12<br>C13<br>C20<br>C24   | D1<br>D3<br>D4<br>D5<br>D7<br>D9<br>D13<br>D14<br>D18              |
| Essay questions exam | A global proof for the evaluation of the competitions acquired in the subject.<br>For passing the subject the students will have to obtain a minimum of 50% in the written proofs (short and long answer). Therefore, the qualification of the remaining parts will only be added when the grade obtained in overall written proofs is equal or higher than two and a half points.<br>Results of the learning:<br>1. Recognise structural elements of organic molecules.<br>2. Propose retrosynthetic sequences.<br>3. Analyse alternative retrosynthetic proposals.<br>4. Value the use of structurally-simplifying reactions.<br>5. Recognise relationships between functional groups.<br>6. Use properly functional groups interconversion reactions.<br>7. Design synthetic sequences.<br>8. Propose synthesis of carbo- and heterocyclic molecules.<br>9. Know the reactivity of heterocyclic compounds.<br>10. Know selective reactions.<br>11. Propose disconnections in unsaturated compounds.<br>12. Know the use of protective groups in organic synthesis.  | 40 | A1<br>A2<br>A4<br>A5 | C2<br>C10<br>C11<br>C12<br>C13<br>C19<br>C20<br>C23<br>C24<br>C25<br>C26<br>C27<br>C28 | D1<br>D3<br>D4<br>D5<br>D7<br>D8<br>D9<br>D13<br>D14<br>D15<br>D18 |

### Other comments on the Evaluation

The participation of the students in any of the acts of evaluation of the subject will involve that they purchase the condition of "presented" and, therefore, they will have assigned a qualification. Acts of evaluation are considered the assistance to the classes of laboratory (three or but sessions), the realisation of the written exams and the handling of a minimum of 25% of the homework assigned by the teaching staff.

Evaluation of the July call:

>1) Grade obtained by the students during the course: maximum of 4 points, divided in the qualification obtained by the students along the course in the resolution of the problems, homework, etc (maximum of 1 point) and the realisation of the laboratory exams (maximum of 3 points).

2) Work carried out by the students: maximum of 1,5 points

for the resolution and handling of the exercises proposed by the teaching staff after the evaluation of January, that will be oriented to the acquisition of the necessary knowledge to pass the matter. This work will be handled in advance to the official date of the exam.

3) Written Tests: maximum of 4,5 points, which will evaluate the knowledge of the matter.

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### Sources of information

#### Basic Bibliography

#### Complementary Bibliography

Warren, S.; Wyatt, P., **Organic Synthesis: The Disconnection Approach**, 2nd, Wiley, 2008

Wyatt, P.; Warren, S., **Organic Synthesis: Strategy and Control**, 1st, Wiley, 2008

Zweifel, G. S.; Nantz, M. H., **Modern Organic Synthesis: An Introduction**, 1st, W H Freeman, 2007

Clayden, J.; Greeves, N.; Warren, S., **Organic Chemistry**, 2nd, Oxford University Press, 2012

Starkey, L. S., **Introduction to strategies for organic synthesis**, 1st, Wiley, 2012

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### Recommendations

#### Subjects that continue the syllabus

Pharmaceutical chemistry/V11G200V01903

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#### Subjects that it is recommended to have taken before

Chemistry, physics and biology: Integrated laboratory 1/V11G200V01103

Chemistry, physics and geology: Integrated laboratory 2/V11G200V01202

Organic chemistry I/V11G200V01304

Structural Determination/V11G200V01501

Organic chemistry II/V11G200V01504