



## Teaching Guide

| Teaching Guide      |                                                                                                                                                                                                                                                   |        |                         |           |
|---------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------|-------------------------|-----------|
| Identifying Data    |                                                                                                                                                                                                                                                   |        |                         | 2017/18   |
| Subject (*)         | Medicinal Chemistry                                                                                                                                                                                                                               |        | Code                    | 610G01040 |
| Study programme     | Grao en Química                                                                                                                                                                                                                                   |        |                         |           |
| Descriptors         |                                                                                                                                                                                                                                                   |        |                         |           |
| Cycle               | Period                                                                                                                                                                                                                                            | Year   | Type                    | Credits   |
| Graduate            | 2nd four-month period                                                                                                                                                                                                                             | Fourth | Optativa                | 4.5       |
| Language            | Spanish                                                                                                                                                                                                                                           |        |                         |           |
| Teaching method     | Face-to-face                                                                                                                                                                                                                                      |        |                         |           |
| Prerequisites       |                                                                                                                                                                                                                                                   |        |                         |           |
| Department          | Química                                                                                                                                                                                                                                           |        |                         |           |
| Coordinador         | García Romero, Marcos Daniel                                                                                                                                                                                                                      | E-mail | marcos.garcia1@udc.es   |           |
| Lecturers           | García Romero, Marcos Daniel                                                                                                                                                                                                                      | E-mail | marcos.garcia1@udc.es   |           |
|                     | Riveiros Santiago, Ricardo                                                                                                                                                                                                                        |        | ricardo.riveiros@udc.es |           |
| Web                 |                                                                                                                                                                                                                                                   |        |                         |           |
| General description | An introductory course in Medicinal Chemistry is offered. Basic concepts related to the structure and activity of drugs, mechanisms of action and metabolism are covered. Main strategies in the design and synthesis of drugs are also analyzed. |        |                         |           |

## Study programme competences / results

| Code | Study programme competences / results                                                                                                                                                                                  |
|------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| A1   | Ability to use chemistry terminology, nomenclature, conventions and units                                                                                                                                              |
| A9   | Knowledge of structural characteristics of chemical and stereochemical compounds, and basic methods of structural analysis and research                                                                                |
| A10  | Knowledge of chemical kinetics, catalysis and reaction mechanisms                                                                                                                                                      |
| A13  | Understanding of chemistry of main biological processes                                                                                                                                                                |
| A14  | Ability to demonstrate knowledge and understanding of concepts, principles and theories in chemistry                                                                                                                   |
| A15  | Ability to recognise and analyse new problems and develop solution strategies                                                                                                                                          |
| A16  | Ability to source, assess and apply technical bibliographical information and data relating to chemistry                                                                                                               |
| A17  | Ability to work safely in a chemistry laboratory (handling of materials, disposal of waste)                                                                                                                            |
| A18  | Risk management in relation to use of chemical substances and laboratory procedures                                                                                                                                    |
| A19  | Ability to follow standard procedures and handle scientific equipment                                                                                                                                                  |
| A20  | Ability to interpret data resulting from laboratory observation and measurement                                                                                                                                        |
| A21  | Understanding of qualitative and quantitative aspects of chemical problems                                                                                                                                             |
| A22  | Ability to plan, design and develop projects and experiments                                                                                                                                                           |
| A23  | Critical standards of excellence in experimental technique and analysis                                                                                                                                                |
| A24  | Ability to explain chemical processes and phenomena clearly and simply                                                                                                                                                 |
| A25  | Ability to recognise and analyse link between chemistry and other disciplines, and presence of chemical processes in everyday life                                                                                     |
| A26  | Ability to follow standard laboratory procedures in relation to analysis and synthesis of organic and inorganic systems                                                                                                |
| B1   | Learning to learn                                                                                                                                                                                                      |
| B2   | Effective problem solving                                                                                                                                                                                              |
| B3   | Application of logical, critical, creative thinking                                                                                                                                                                    |
| B4   | Working independently on own initiative                                                                                                                                                                                |
| B6   | Ethical, responsible, civic-minded professionalism                                                                                                                                                                     |
| B7   | Effective workplace communication                                                                                                                                                                                      |
| C1   | Ability to express oneself accurately in the official languages of Galicia (oral and in written)                                                                                                                       |
| C2   | Oral and written proficiency in a foreign language                                                                                                                                                                     |
| C3   | Ability to use basic information and communications technology (ICT) tools for professional purposes and learning throughout life                                                                                      |
| C4   | Self-development as an open, educated, critical, engaged, democratic, socially responsible citizen, equipped to analyse reality, diagnose problems, and formulate and implement informed solutions for the common good |
| C6   | Ability to assess critically the knowledge, technology and information available for problem solving                                                                                                                   |

|    |                                                                                                      |
|----|------------------------------------------------------------------------------------------------------|
| C7 | Acceptance as a professional and as a citizen of importance of lifelong learning                     |
| C8 | Understanding role of research, innovation and technology in socio-economic and cultural development |

| Learning outcomes                                                                            |                                                                  |                                  |                                        |
|----------------------------------------------------------------------------------------------|------------------------------------------------------------------|----------------------------------|----------------------------------------|
| Learning outcomes                                                                            | Study programme competences / results                            |                                  |                                        |
| Know the structure and mode of action of drugs and the relationship with biological activity | A1<br>A9<br>A13<br>A14<br>A15<br>A16<br>A21<br>A24<br>A25        | B1<br>B2<br>B3<br>B4<br>B6<br>B7 | C1<br>C2<br>C3<br>C4<br>C6<br>C7<br>C8 |
| Know the impact of drugs and the pharmaceutical companies in the society.                    | A13<br>A14<br>A16<br>A24<br>A25                                  | B1<br>B3<br>B4<br>B6<br>B7       | C1<br>C3<br>C4<br>C6<br>C7<br>C8       |
| Know basic principles and strategies used to design and synthesized drugs.                   | A1<br>A9<br>A10<br>A13<br>A14<br>A15<br>A16<br>A21<br>A24<br>A25 | B1<br>B2<br>B3<br>B4<br>B6<br>B7 | C1<br>C3<br>C4<br>C6<br>C7<br>C8       |
| Knowing how to work done in the laboratories of pharmaceutical companies                     | A17<br>A18<br>A19<br>A20<br>A22<br>A23<br>A26                    |                                  |                                        |

| Contents                                           |                                                                                                                                                                                                          |
|----------------------------------------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Topic                                              | Sub-topic                                                                                                                                                                                                |
| Chapter 1. Basic principles in Medicinal Chemistry | 1.1 Medicinal Chemistry : definition and basic concepts<br>1.2 Historical Perspective .<br>1.3 Pharmacokinetics and Pharmacodynamics<br>Drug Discovery 1.4<br>1.5 Drugs: nomenclature and classification |



|                                                                             |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
|-----------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Chapter 2. Molecular basis on pharmacological activity:<br>Pharmacodynamics | 2.1 Drug-receptor interactions . Molecular topology and biological activity<br>2.2 Proteins: structure and function. Protein Interactions<br>2.3 Enzymes: enzymatic catalysis. Michaelis - Menten equation . Enzyme inhibition :<br>Types<br>2.5 Cell receptors: structure and classification .<br>2.6 Nucleic Acids . Structure and functions. Drug interactions with nucleic acids<br>2.7 Interactions with lipid and carbohydrate                                                                                                                                                                          |
| Chapter 3. Phramacokinetics                                                 | 3.1 ADME processes.<br>3.2 Absorption of drugs. Modes of administration . Physicochemical properties of<br>drugs : Lipinsky rules . Bioavailability .<br>3.3 Distribution of drugs. Blood : composition and properties. Removal rate . Mid life.<br>Volume of distribution<br>3.4 Drug metabolism : metabolism in phase I and phase II<br>3.5 Elimination of drugs.                                                                                                                                                                                                                                           |
| Chapter 5. Drug discovery                                                   | 4.1 Steps in drug discovery. Biological target vs Phenotypic approach. Structural<br>diversity. Chemical space. Drug binding energy. High Throughput Screening ( HTS ).<br>Chemical libraries: combinatorial chemistry , parallel synthesis , solid phase synthesis<br>4.2 Strategies in drug discovery (lead discovery) . Screening modes . Drug screening<br>methods . Drug Design<br>4.3 Optimization of drugs (lead optimization) . Structure- actividadIdentificación<br>pharmacophore . Pharmacomodulation : modification of functional groups.<br>Optimization receptor binding and pharmacokinetics . |
| Chapter 7. Drug synthesis                                                   | Main synthetis methods for the synthesis of drugs                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |

| Planning                                                                                                                        |                                                                                          |                                         |                                  |             |
|---------------------------------------------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|-----------------------------------------|----------------------------------|-------------|
| Methodologies / tests                                                                                                           | Competencies /<br>Results                                                                | Teaching hours<br>(in-person & virtual) | Student?s personal<br>work hours | Total hours |
| Guest lecture / keynote speech                                                                                                  | A1 A9 A10 A13 A14<br>A15 A16 A21 A24<br>A25 B1 B2 B3 B4 B6<br>B7 C1 C2 C3 C4 C6<br>C7 C8 | 16                                      | 16                               | 32          |
| Seminar                                                                                                                         | A1 A9 A10 A13 A14<br>A15 A16 A21 A24<br>A25 B1 B2 B3 B4 B6<br>B7 C1 C3 C4 C6 C7<br>C8    | 7                                       | 28                               | 35          |
| Field trip                                                                                                                      | A17 A18 A19 A20<br>A21 A22 A23 A26                                                       | 6                                       | 0                                | 6           |
| Laboratory practice                                                                                                             | A17 A18 A19 A20<br>A21 A22 A23 B6 C2<br>C6 C7                                            | 3                                       | 3                                | 6           |
| Mixed objective/subjective test                                                                                                 | A1 A13 B2 B3 B4 B6<br>C1 C2                                                              | 4                                       | 28.5                             | 32.5        |
| Personalized attention                                                                                                          |                                                                                          | 1                                       | 0                                | 1           |
| (*)The information in the planning table is for guidance only and does not take into account the heterogeneity of the students. |                                                                                          |                                         |                                  |             |

| Methodologies |             |
|---------------|-------------|
| Methodologies | Description |



|                                 |                                                                                                                                                                                                                                                                         |
|---------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Guest lecture / keynote speech  | The contents will be presented. During the presentations the teacher can provide supplementary material to the literature with the aim that the explanations can be tracked effectively. The ability to create notes and search for information will also be developed. |
| Seminar                         | The contents of each chapter will be discussed in seminars by solving exercises and analysis of practical cases. Students will have early enough problem sets through the Moodle platform. We may request delivery of solved exercises.                                 |
| Field trip                      | As a practical activity visits to research centers and/or related companies with Medicinal Chemistry aims will be scheduled. Attendance at these activities is mandatory and the development of an individual activity report will be necessary                         |
| Laboratory practice             | Practices involving the use of programs and databases and / or experiments related for the synthesis of drugs is proposed.                                                                                                                                              |
| Mixed objective/subjective test | A test with questions related to the contents of the subject will be asked.                                                                                                                                                                                             |

## Personalized attention

| Methodologies                                                    | Description                                                                                                                        |
|------------------------------------------------------------------|------------------------------------------------------------------------------------------------------------------------------------|
| Seminar<br>Laboratory practice<br>Guest lecture / keynote speech | This activity will be headed to the individual assistance for explanations, doubts, as well as to the resolution of the exercises. |

## Assessment

| Methodologies                   | Competencies / Results                                                                   | Description                                                                                                              | Qualification |
|---------------------------------|------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------|---------------|
| Seminar                         | A1 A9 A10 A13 A14<br>A15 A16 A21 A24<br>A25 B1 B2 B3 B4 B6<br>B7 C1 C3 C4 C6 C7<br>C8    | The active participation of students in solving the problems of the bulletins and assignment submitted will be assessed. | 20            |
| Field trip                      | A17 A18 A19 A20<br>A21 A22 A23 A26                                                       | Attendance and the final report will be assessed.                                                                        | 5             |
| Laboratory practice             | A17 A18 A19 A20<br>A21 A22 A23 B6 C2<br>C6 C7                                            | Attendance and the final report will be assessed.                                                                        | 5             |
| Guest lecture / keynote speech  | A1 A9 A10 A13 A14<br>A15 A16 A21 A24<br>A25 B1 B2 B3 B4 B6<br>B7 C1 C2 C3 C4 C6<br>C7 C8 | Attendance and participation in class will be assessed                                                                   | 10            |
| Mixed objective/subjective test | A1 A13 B2 B3 B4 B6<br>C1 C2                                                              | The responses in the written exam will be evaluated.                                                                     | 60            |

## Assessment comments

The assistance to the field trip and to the laboratory practice is compulsory except for the students with part-time enrollment or academic exemption. These students should exchange these activities by tasks related that not require attendance. A student can obtain the qualification of "No presented" if do not realise activities with an upper computation to 50% in the evaluation or not to present to the mixed test. The students will have two opportunities, and those that do not surpass the subject in the first opportunity will conserve the qualification obtained in the seminars, field trip and laboratory practice, and will realise a second mixed test in the determinate dates by the calendar fixed by the Board of Faculty. The students that are evaluated in the second opportunity only will be able to opt to the "matrícula de honor" (highest qualification) if these have not been covered at the first opportunity. The process of education-learning, included the evaluation, refers to an academic course and starts every new academic course, including all the activities and procedures of evaluation programmed.

#### Sources of information

|                      |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
|----------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Basic</b>         | <ul style="list-style-type: none"> <li>- Stevens, E. (2014). Medicinal Chemistry, an Introduction.. Pearson Education. New York.</li> <li>- Patrick, G. L (2013). An Introduction to Medicinal Chemistry. 5th ed.. New York: Oxford University Press</li> <li>- Avendaño, C (2001). Introducción a la Química Farmacéutica. Madrid: McGraw-Hill</li> <li>- Thomas, Gareth (2007). Medicinal Chemistry: An introduction. Wiley</li> <li>- Delgado, A.; Minguillón, C.; Joglar, J. (2003). Introducción a la Química Terapéutica. Madrid: Díaz de Santos</li> <li>- Delgado, A.; Minguillón, C.; Joglar, J. (2002). Introducción a la síntesis de fármacos. Madrid: Síntesis</li> </ul> |
| <b>Complementary</b> |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |

#### Recommendations

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

Organic Chemistry 1/610G01026  
 Organic Chemistry 2/610G01027  
 Intermediate Organic Chemistry/610G01028  
 Advanced Organic Chemistry/610G01030

##### Subjects that are recommended to be taken simultaneously

Final Dissertation/610G01043

##### Subjects that continue the syllabus

##### Other comments

(\*)The teaching guide is the document in which the URV publishes the information about all its courses. It is a public document and cannot be modified. Only in exceptional cases can it be revised by the competent agent or duly revised so that it is in line with current legislation.