VNIVERSITAT DE VALÈNCIA

Course Guide
44712 Bioorganic chemistry and supramolecular chemistry

COURSE DATA

Data Subject	
Code	44712
Name	Bioorganic chemistry and supramolecular chemistry
Cycle	Master's degree
ECTS Credits	3.0
Academic year	2022 - 2023

Study (s)

Degree	Center	Acad. year	Period
2226 - M.D. in Organic Chemistry	Faculty of Chemistry	1	Annual

Subject-matter

Degree	Subject-matter	Character
2226 - M.D. in Organic Chemistry	8 - Bioorganic chemistry and supramolecular chemistry	Obligatory

Coordination

Name	Department
DEL POZO LOSADA, CARLOS	325 - Organic Chemistry

SUMMARY

The part of the subject corresponding to Bioorganic Chemistry deals with the study of the formation, structure and biological activity of secondary metabolites. These compounds are produced by living beings but even though they are not essential for their growth, development or reproduction, they have a function ecological. In these subjects the student is introduced in the field of different natural products grouped in base on the biogenetic route through which they are generated. The fundamental synthetic sequences are described, paying attention to the main bioorganic reactions involved. Likewise, attention is paid to the biological properties of natural products and their importance is discussed under a pharmacological, toxicological and ecological point of view, when relevant.

On the other hand, supramolecular chemistry can be defined as chemistry beyond the molecule and is based on the non-covalent interactions that can be established between charged molecules or species. For this reason, the study of the different types of interactions that can occur will be included. In addition, concepts widely used in the area of supramolecular chemistry such as molecular recognition, allosteric cooperativity, self-assembly or dynamic libraries will be discussed. Likewise, a study of the different devices that can be produced using these concepts as well as their possible applications both in the field of materials and in biological processes will be carried out.

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

There are no specified enrollment restrictions with other subjects of the curriculum.

Other requirements

Fundamental knowledge of Organic Chemistry is required for a correct follow-up of the studied topics.

OUTCOMES

2226 - M.D. in Organic Chemistry

- Students should apply acquired knowledge to solve problems in unfamiliar contexts within their field of study, including multidisciplinary scenarios.
- Students should be able to integrate knowledge and address the complexity of making informed judgments based on incomplete or limited information, including reflections on the social and ethical responsibilities associated with the application of their knowledge and judgments.
- Students should communicate conclusions and underlying knowledge clearly and unambiguously to both specialized and non-specialized audiences.
- Students should demonstrate self-directed learning skills for continued academic growth.
- Students should possess and understand foundational knowledge that enables original thinking and research in the field.
- Use different presentation formats (oral, written, slide presentations, boards, etc.) to communicate knowledge, proposals and positions.
- Be able to access to information tools in other areas of knowledge and use them properly.
- Saber participar en debates y discusiones, dirigirlos y coordinarlos y ser capaces de resumirlos y extraer de ellos las conclusiones más relevantes y aceptadas por la mayoría.
- Poseer habilidades sociales, un buen nivel de comunicación oral y escrita, así como capacidad para trabajar en equipo y con personas de diferentes procedencias.
- Competencias de gestión tales como la capacidad para la planificación y gestión de tiempo y recursos, así como para dirigir y tomar decisiones.
- Ser capaces de valorar la necesidad de completar su formación científica, en lenguas, en informática, asistiendo a conferencias o cursos y/o realizando actividades complementarias, autoevaluando la aportación que la realización de estas actividades supone para su formación integral.
- Conocer las rutas biosintéticas generales de los metabolitos secundarios y aplicar los conocimientos fundamentales de la reactividad orgánica a la comprensión de los mecanismos de las reacciones biosintéticas.

- Profundizar en el conocimiento de las propiedades fundamentales de las fuerzas intermoleculares y su importancia en química, biología y ciencia de materiales.
- Comprender la utilidad de la química supramolecular para la construcción de dispositivos moleculares y materiales moleculares nanoestructurados.

LEARNING OUTCOMES

With regard to Bioorganic Chemistry, the objectives to be obtained are summarized in the following points:

-To know the general biosynthetic pathways of secondary metabolites (acetate, shikimato,

mevalonate, nitrogen compounds).

-To use the fundamental knowledge of organic reactivity for understanding the mechanisms of biosynthetic reactions.

-To carry out chemical and biological identification of the different groups of metabolites according to their biogenetic origin.

-To recognize the most important uses and applications of natural products with particular emphasis on the research for new drugs

-To study natural products with heterocyclic structure and to realize their importance in biological processes.

As regards Supramolecular Chemistry, the objectives that are intended to be achieved can be summarized in the following points

-To know the fundamental properties of intermolecular forces and their importance in chemistry and biology.

-To learn how to apply the concepts of supramolecular chemistry to the design and synthesis of molecular receptors and simple molecular devices.

-To interpret chemical and biochemical processes whose operations are based on intermolecular interactions.

-To identify the intermolecular forces involved in the stabilization of multimolecular structures as well as distinguish their relative importance.

-To know the experimental methods used in the characterization of supramolecular systems.

-To understand the utility of supramolecular chemistry for the construction of molecular devices and nanostructured molecular materials.

- Design, selection and/or development products and chemical processes efficiently (ODS 7) that minimize their impact in the environment (ODS 14 and 15), taking advantage of the alternative row materials and generating the minor amount of residues possible (ODS 11)

DESCRIPTION OF CONTENTS

1. Acetate route: fatty acids and polyketides

Introduction. Primary and secondary metabolites. Aliphatic polyketides. Lipids and related compounds. Prostaglandins, thromboxanes and leukotrienes. Macrolides and polyethers. Aromatic polyketides.

2. Sikimato route: aromatic amino acids and phenylpropanoids

Aromatic amino acids and simple benzoic acids. Cinnamic acids. Coumarins. Mixed metabolites (shikimato + acetate): Flavonoids. Isoflavones.

3. Mevalonate route: terpenes and steroids.

Biosynthetic origin of terpenoid compounds. Monoterpenes (C10).. Sesquiterpenes (C15). Diterpenes (C20). Triterpenes (C30). Tetraterpenes (C40). Steroids: cholesterol.

4. Alkaloids: amino acid derivatives.

Alkaloids derived from tyrosine and phenylalanine. Tryptophan derived alkaloids. Alkaloids derived from ornithine and lysine. Alkaloids derived from nicotinic acid.

5. Definition and development of supramolecular chemistry

Host-guest relationship. Preorganization and complementarity. Kinetic and thermodynamic selectivity. Nature of supramolecular interactions. Host design.

6. Cation recognition

Crown ethers, lariat ethers and podands. Cryptands, Spherands, Calixarenos, Heterocoronas and mixed cryptands. Selectivity in the complexation of cations. Complexation of organic cations. Chiral recognition.

7. Anion recognition

Basic concepts in the design of receptors for anions. Receptors containing amines. Guanidinium derived receptors. Organometallic receptors. Neutral receptors.

8. Neutral molecules recognition

Cyclodextrins and their applications. Molecular Tweezers. Cyclophanes. Cryptophanes. Covalent cavities: Carcenanos and hemicarcenanos. The supramolecular chemistry of fullerenes.

9. Self-assembly

Self-assembly in synthetic systems: kinetic and thermodynamic considerations. Self-assembly in coordination compounds. Self-assembly in metallic networks. Self-assembly through hydrogen bonds. Catenanos and rotaxanes. Helicates. Molecular knots.

10. Extraction and transport

Extraction techniques. Methods for determining extraction constants. Applications. Deactivation of cations. Anion activation: Phase transfer catalysis. Techniques for the evaluation of complexation constants. Variables that affect complexation constants. Membrane transport. Transport mediated by carriers. Transport processes coupled.

11. Molecular devices

Switchers. Supramolecular photochemistry and electrochemistry. Information and signaling: chemical sensors. Molecular devices based on rotaxanes and catenans

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	15,00	100
Seminars	15,00	100
TOTAL	**30,00**	

TEACHING METHODOLOGY

The course is organized in such a way that student is the protagonist of his own learning and is structured as follows:

• From the beginning of the course the students will have all the pedagogical material corresponding to the course.

• Master classes (face-to-face) .

-In these classes the basic concepts of the subject will be introduced. The active participation of the student will be encouraged by making questions related to the application of concepts and knowledge previously acquired.

• Seminars.

- This teaching activity will be dedicated to the resolution of problems and issues with the active participation of the student.

• Works.

- Additionally, when the teacher considers it appropriate, small topics will be proposed. They will be developed by each group and will consist of the study and, where appropriate, oral presentation of a practical case, related to some of the topics in the program and described in a scientific publication. The maximum duration of the exhibition will be 15 minutes, which will be followed by a maximum of 20 minutes of discussion.

EVALUATION

Evaluation will be carried in a continuous way throughout the course and will consist of the following sections.

● Direct teacher evaluation. 10% of the score will come from the direct evaluation of the teacher in both theoretic and practice classes as well as in the tutorials. In this evaluation, different aspects will be taken into account, including:

- Assistance and reasoned and clear participation in discussions.

- Progress in the use of the language of bioorganic chemistry and supramolecular chemistry

- Problem solving and questioning.

- Critical spirit.

- Delivery of exercises and works.

● Evaluation of works done by the student. Both the content and the form and, where appropriate, the oral presentation and the answers to the questions asked by the other students will be taken into account. This section will correspond to 25% of the final score.

● Oral and written exams or tests. 65% of the score will be obtained from the results of the oral or written tests, which will be carried out in the periods established for it.

- Exams of traditional style including theoretical questions as well as problem related to the studied topics. These questions and problems will be of such a nature that they force the student to find relationships between different aspects of the topics explained in the course.

- Development of a work (oral presentation and defense or written memory) on any of the topics discussed throughout the course.

The final mark will be obtained as average of the marks obtained in Bioorganic Chemistry and Supramolecular Chemistry.

REFERENCES

Basic

- J. Mann, Secondary Metabolism, Clarendon Press, 1987, 2ª edición.
- P. M. Dewick, Medicinal Natural Products: A Biosynthetic Approach, Wiley 2002, 2ª edición; 2009, 3ª edición.
- K.B.G. Torssell, Natural Products Chemistry, J. Wiley & Sons, 1983.
- J. W. Steed, J. L. Atwood, Supramolecular Chemistry. John Wiley & Sons, 2009.
- P. J. Cragg, A Practical Guide to Supramolecular Chemistry, Wiley (Weinheim), 2005
- J.-M. Lehn, Supramolecular Chemistry. VCH (Weinheim), 1995

Additional

- D.L. Nelson y M.M. Cox, Lehninger Principles of Biochemistry, Worth Publishers, 2000, 3ª edición.
- M. Carda et al., Productos Naturales, Colección Material Docente, Publicaciones de la Universitat Jaume I, 1997.
- J. Mann et al., Natural Products. Their Chemistry and Biological Significance, Longman Scientific & Technical, 1994.
- K. E. Suckling, C. J. Suckling, Biological Chemistry. The Molecular Approach to Biological Systems, Cambridge University Press, 1980
- P. Gil Ruiz, Productos Naturales, Universidad Pública Navarra, 2002
- F. Pietra, Biodiversity and natural products diversity, Pergamon, Amsterdam, 2002
- J. A. Marco, Química de los Productos Naturales, Síntesis, 2006.
- J. A. Joule, K. Mills, Heterocyclic Chemistry, Wiley, 2010, 5ª edición.
- T. Eicher, S. Hauptmann, A. Speicher The Chemistry of Heterocycles, Wiley-VCH, 2005.
- P. D. Beer, P. A. Gale, D. K. Smith, Supramolecular Chemistry. Oxford University Press, 1999
- A. E. Kaifer, M. Gómez-Kaifer, Supramolecular Electrochemistry, VCH (Weinheim) 1999.
- A. Bianchi, K. Bowman-James, E. García-España (eds), Supramolecular Chemistry of Anions, (Editores), Wiley-VCH (New York), 1997.

- V. Balzani, F. Scandola, E. Harwood, Supramolecular Photochemistry, Wiley-VCH (New York) 1999.
- L. B. Feringa (ed), Molecular Switches, Wiley-VCH (New York) 2001