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
Academic year: 2026-27

STUDY (S)

Degree	Center	Acad. year	Period
2226 - Master's degree in Organic Chemistry	Facultat de Química	1	First quarter

SUBJECT-MATTER

Degree	Subject-matter	Character
2226 - Master's degree in Organic Chemistry	Bioorganic chemistry and supramolecular chemistry	COMPULSORY

COORDINATION

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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.

COMPETENCES / LEARNING OUTCOMES

2226 - Master's degree in Organic Chemistry

Be able to access to information tools in other areas of knowledge and use them properly.

Competencias de gestión tales como la capacidad para la planificación y gestión de tiempo y recursos, así como para dirigir y tomar decisiones.

Comprender la utilidad de la química supramolecular para la construcción de dispositivos moleculares y materiales moleculares nanoestructurados.

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.

Poseer habilidades sociales, un buen nivel de comunicación oral y escrita, así como capacidad para trabajar en equipo y con personas de diferentes procedencias.

Profundizar en el conocimiento de las propiedades fundamentales de las fuerzas intermoleculares y su importancia en química, biología y ciencia de materiales.

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.

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.

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.

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

PRESENCIAL ACTIVITIES

Activity	Hours
Theory	15,00
Seminar	15,00
Total hours	**30,00**

NON PRESENCIAL ACTIVITIES

Activity	Hours
Attendance at other activities	0,00
Individual or group project	10,00

Independent study and work	25,00
Preparation of lessons	0,00
Preparation for assessment activities	10,00
Resolution of case studies	0,00
Total hours	**45,00**

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. 15% 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 20% 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.

In the second call, the section on direct evaluation by the teacher will not be recoverable.

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