COURSE DATA

Data Subject	
Code	44713
Name	Industrial organic chemistry
Cycle	Master's degree
ECTS Credits	3.0
Academic year	2019 - 2020

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	9 - Industrial organic chemistry	Obligatory

Coordination

Name	Department
DEL POZO LOSADA, CARLOS	325 - Organic Chemistry

SUMMARY

In this subject it is intended that the student acquires a body of knowledge directly related to the world of chemical companies in general and agrocchemicals in particular. Nowadays, the training provided to the student during his university education cannot undertake a series of issues directly related to the industrial aspect of chemistry so this course aims to resolve this shortcoming.

The contents of the course are as follows:

- The organic chemical industry. The food industry.

- Industrial chemical processes and sustainability.

- Relative importance of organic products and important industrial sectors of organic chemistry.

- Origin of industrial products from raw materials to finished products: major transformation pathways of carbon.

- Major groups of pesticides and mechanisms of action

- Lead generation.

- Optimization of the lead: general aspects.

- Evaluation and development of the compound.

- Problematic of pesticide residues in the environment and food.

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

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

Other requirements

The study of this subject requires a good foundation in Organic Chemistry

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.
- Reconocer los valores de la química sostenible: utilización de fuentes renovables de materias primas, reducción de sustancias contaminantes y diseño de procesos sostenibles.
- 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.
- Profundizar en el conocimiento de las fuentes principales de productos químicos y su manipulación para su transformación posterior en materiales orgánicos de valor añadido.
- Ahondar en el conocimiento de la industria química orgánica, en particular del sector agroquímico, farmacéutico y medioambiental.

LEARNING OUTCOMES

The objectives to be achieved in this subject are summarized below:

- Be able to describe the main sources of chemicals and how they are handled for further processing in organic materials of value.

- Deepen sustainable chemistry, use of renewable sources of raw materials, reduction of pollutants and design of sustainable processes.

- Know general aspects of organic chemical, agrochemical and environmental sector and how they are treated from the academic and industrial perspective.

- Knowing the most important groups of current pesticides (focusing mainly on fungicides, insecticides and herbicides), their mode of action and the processes of generation and optimization followed until their commercial development.

- Know the problem of pesticide residues in the environment and food.

DESCRIPTION OF CONTENTS

1. The organic chemical industry: overview

Petrochemical fine chemicals. Chemical laboratory against industrial chemistry. The origin of industrial organic carbon: petroleum, natural gas, coal, natural products. Large petrochemical processes in relation to the organic chemical industry. Main organic raw materials: Preparation, main roads transformation. Possible alternatives to the current petrochemical. Research as a decisive factor in the organic chemical industry. Environmental aspects that condition the organic chemical industry. Sustainable chemistry.

2. Agrochemicals. Major groups of pesticides and Mechanisms of Action

Introduction to the modes of action of pesticides. Animal and plant cell. Mechanisms of action of insecticides. Synapse as the molecular target. Acetylcholinesterase inhibitors. Insecticides acting on the acetylcholine receptor. Modulators of the sodium channel. Antagonists chloride channel associated with GABA. Rianodine receptors.
Main modes of action of herbicides. Photosynthesis inhibitors. Herbicides affecting pigment synthesis. Inhibitors of fatty acid synthesis. Main mechanisms of action of fungicides. Sterol synthesis route. Inhibitors methionine synthesis. Fungicides acting on the electron transport chain. Mitotic inhibitors and cell division. Fungicides non-specific.

3. The agrochemical industry and development of new pesticides

Characteristics of the agrochemical industry. Need to develop new pesticides. Process research and development. Assays: In vitro vs. in vivo. The ideal product. Lead discovery. Sources of biologically active substances: High throughput screening. Serendipity. Crossed screening. Combinatorial chemistry. Innovative chemistry. Biorational design. Natural products. Patents competitors. Optimization of the lead: general aspects. Design new molecules. Chemical approaches. Design strategies. Agrokinetics properties. Physical properties. Selected examples of lead optimization (insecticides, fungicides and herbicides). Evaluation and development of the compound. Bioassays in the field. Formulations for agrochemicals. What are patents?. Toxicological studies.

4. The problem of pesticide residues in the environment and food

Socio-economic importance of pesticides. Pesticide residues in food. Maximum residue limits. EFSA and AESAN. Surveillance and control programs. Methods of Analysis of agrochemicals. Immunoanalitics approaches to the analysis of waste. Development and validation of immunoassays.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	16,00	100
Seminars	14,00	100
TOTAL	**30,00**	

TEACHING METHODOLOGY

The subject is raised so that the student is the protagonist of their own learning. Since the beginning of the course students will have all the necessary teaching materials and teaching is structured as follows:

• Lectures (plesential).- In these classes the basic concepts of the subject will be introduced. the active participation of students will be encouraged by raising issues related to the application of concepts and knowledge previously acquired by students.

• Seminars.- This educational activity will be devoted to solving problems and issues with active student participation.

• Works.- In addition, when the teacher deems appropriate, any work related to the program and described in a scientific publication will be proposed.

EVALUATION

The evaluation of the course will be conducted by the teacher throughout the course and will consist of the following sections.

● **Continuous evaluation**. 10% of the grade will come from direct assessment of the teacher in theoretical and problem classes and tutorials. In this assessment various aspects are taken into account, among which include:

- Assistance and reasoned and clear participation in the discussions raised.

- Progress in the use of language of the subject.

- Troubleshooting and raising doubts.

- Critical spirit.

- Delivery of exercises.

● **Oral expositions and debates.** It will take into account both content and form. This section will correspond to 30% of the final grade.

● **Exams and written tests.** 60% of the mark will be obtained from the results of the written tests.

- Exams of both theoretical issues and problems of the content related to the subject. These issues and problems will be such that will require the student to relate different aspects that appear on different topics of the subject or, if the teacher considers it appropriate, in different subject matter.

REFERENCES

Basic

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- H.H. Szmant, Organic Building Blocks of the Chemical Industry, Wiley 1989.
- H. A. Wittcoff, B. G. Reuben, Productos Químicos Orgánicos Industriales, Editorial Limusa, México, 1996.
- E. Primo Yúfera, Química Orgánica básica y aplicada. De la molécula a la industria, Editorial Reverté, Barcelona, 2007
- W. Krämer, U. Schirmer (ed.), Modern Crop Protection Compounds, 2nd edition, Wiley-VCH Verlag, Weinheim, 2012.
- L. G. Copping and H.G. Hewitt, Chemistry and Mode of Action of Crop Protection Agents, Royal Society of Chemistry, Redwood Books Ltd., Trowbridge, Wiltshire, 1998.

Additional

- C.R.A. Godfrey (ed.), Agrochemicals from Natural Products, Marcel Dekker, Inc., New York, 1995
- C.D.S. Tomlin (ed.), The Pesticide Manual: A World Compendium, 15th edition. British Crop Protection Council, Farnham, UK, 2009 (new edition in 2013).
- R. Beaudegnies, A.J.F. Edmunds, R.G. Hall, J. Schaetzer, S. Wendeborn, T.E.M. Fraser, T.R. Hawkes, G. Mitchell and G. Wibley, Bioorg. Med. Chem. 2009, 17(12), 4134-4152.
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- P.T. Anastas, and T.C. Williamson, Green Chemistry: Frontiers in Benign Chemical Syntheses and Processes, Oxford University Press, Oxford, 1998

ADDENDUM COVID-19

This addendum will only be activated if the health situation requires so and with the prior agreement of the Governing Council

• Second call evaluation

Due to the alarm state imposed by the sanitary situation, the second call evaluation will be performed in the not in person mode. The face to face theoretical classes and the evaluation of the first call was already finished when the alarm state was ordered.

To this end, the tools stipulated in the platform “Aula Virtual” will be employed. In the same token, the integrity of the exams will be verified with the software provided by the UVEG. The students will identify themselves by means of the password necessary to access the “Aula Virtual” platform.