

From Small Molecules to Nanomaterials

Code: 42423
ECTS Credits: 6

Degree	Type	Year	Semester
4313385 Industrial Chemistry and Introduction to Chemical Research	OT	0	1

The proposed teaching and assessment methodology that appear in the guide may be subject to changes as a result of the restrictions to face-to-face class attendance imposed by the health authorities.

Contact

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Use of Languages

Principal working language: english (eng)

Teachers

Ramón Alibés Arqués
Carles Jaime Cardiel
Rosa Maria Ortuño Mingarro
Adelina Vallribera Massó
Felix Busqué Sánchez
Jean-Didier Pierre Marechal
Rosa Maria Sebastián Pérez

Prerequisites

There are no special prerequisites to attend the Module 6 but the same as to access the Master. It is required to be in possession of an official Spanish University Degree or another Degree issued by a Higher Education Institution, belonging to another member state of the European Higher Education, or from third countries empowered to access a master's degree.

On the other hand, it is desirable to have advanced knowledge of English, level B1 of the Common Reference European Framework for Languages of the European Council.

Objectives and Contextualisation

The aim of the module is to learn and deepen the study of the properties and applications of specific relevant materials in research by focusing on supramolecular materials, nanomaterials and biomaterials. In this sense, the preparation, properties and applications of molecules based on their molecular weight and increasing structural complexity down to nanostructured materials will be studied. In this regard the following two sub blocks are splitted:

- Small molecules and dendrimers: synthesis, properties and utility. Chirality: molecular recognition and biological activity.
- Soft materials and metallic nanoparticles: synthesis, functionalization and applications

On the other hand, lecturing in English as well as evaluating the contents in English will allow the students to

be familiar with the chemistry terminology as well as to consolidate an essential language for their future careers both as in companies as in a university department or a research center.

Competences

- Apply materials and biomolecules to innovative fields of chemical industry and research.
- Correctly apply new information capture and organisation technologies to solve problems in professional activity.
- Define specialised concepts, principles, theories and facts in the different areas of Chemistry.
- Identify information in the scientific literature using the appropriate channels and integrating said information to approach and contextualise a research issue.
- Innovate in chemical synthesis and analysis methods related with different areas of Chemistry.
- Possess and understand knowledge that provides a basis or opportunity for originality in the development and/or application of ideas, often in a research context
- Student should possess an ability to learn that enables them to continue studying in a manner which is largely self-supervised or independent
- Students should know how to apply the knowledge acquired and the capacity to solve problems in new or little-known areas within broader (or multidisciplinary) contexts related to their area of study
- Students should know how to communicate their conclusions, knowledge and final reasoning that they hold in front of specialist and non-specialist audiences clearly and unambiguously
- Use scientific terminology in the English language to defend experimental results in the context of the chemistry profession.

Learning Outcomes

1. Apply the synthesis of small molecules in molecular biology and medicine
2. Assess the importance of chirality in molecular recognition and biological activity
3. Correctly apply new information capture and organisation technologies to solve problems in professional activity.
4. Describe the design and synthesis of drug transporters agents
5. Identify information in the scientific literature using the appropriate channels and integrating said information to approach and contextualise a research issue.
6. Possess and understand knowledge that provides a basis or opportunity for originality in the development and/or application of ideas, often in a research context
7. Prepare and functionalise metallic nanoparticles for their application to analysis and catalysis.
8. Prepare and use dendrimers in catalysis, biology, medicine and materials.
9. Student should possess an ability to learn that enables them to continue studying in a manner which is largely self-supervised or independent
10. Students should know how to apply the knowledge acquired and the capacity to solve problems in new or little-known areas within broader (or multidisciplinary) contexts related to their area of study
11. Students should know how to communicate their conclusions, knowledge and final reasoning that they hold in front of specialist and non-specialist audiences clearly and unambiguously
12. Use scientific terminology in the English language to defend experimental results in the context of the chemistry profession.

Content

- Modern organofluorinated chemistry. 3h Adelina Vallribera

General properties of fluorine and organofluorinated compounds. Applications in the field of materials chemistry. The role of fluoride in pharmaceuticals and medical chemistry. Synthetic methodologies for the introduction of fluorinated interest groups (F, CF₃, CF₂COOEt etc) en C_{sp}² i C_{sp}³.)

- Small molecules: synthesis and applications in molecular biology and medicine. 11 h. Ramon Alibés, Félix Busqué.

- Dendrimers. 5h. Rosi Sebastián

Dendrimers: General information (Characteristics, synthetic strategies). Main type of dendrimeric structures. Characterization. Applications (photochemistry, liquid crystals, metal nanoparticle stabilizers, catalysis, sensors, imaging, drug delivery)

- Introduction to polymeric materials. 5h. Carlos Jaime

Brief Introduction to Polymers. Synthesis of polymers: Step-growing polymerization - Condensation; Chain growth polymerization - Addition; Copolymerization. Polymer properties: Molecular weight; Morphology; Thermal properties; Electrical and optical properties; Rheology. Formulation: Composites, Fillers and Additives. Environmental issues: Polymers from renewable sources; Degradation and biodegradation of polymers. Characterization of polymers

- Nanomaterials and Analytical Chemistry. Chemical Sensing applications. 3 h Mar Puyol

Chemical signaling. Use of nanomaterials as high sensitive signal transducers. Spectroscopic and Electrochemical applications. Nanoparticles as support platforms of recognition elements: Bioassays and magnetic nanoparticles. Specific characteristics of nanomaterials for analytical applications: reproducibility (size distribution, shape), toxicity, solubility. From batch methods to scaled-down processes: Microreactors and microfluidic platforms.

- Drug / biomolecule delivery. 5h. Rosa Maria Ortuño

General concepts. Drug delivery: DD systems (DDS). Drug carriers. Drug Delivery by Soft Matter and Nanoparticles. Cell penetrating peptides (CPP). Applications: Drug / biomolecule carriers; CPP as contrast agent transporters; Target, image and drug delivery. Vectors for gene therapy. Theranostics and drug delivery: examples

- Computational Chemistry. 3h. Jean-Didier Marechal

Introduction. The importance of computing in designing small molecules. Basics of molecular modeling methods. Methods of quantum mechanics. Force field methods. Geometric scanning methods. Ligand-based methods. Structure-based methods. Examples of drug design.

Methodology

In general the following Teaching Methodologies will be followed in all the different subjects:

- Lectures
- Problem-solving classes
- Cooperative activities
- Seminars
- Oral presentations
- Tutoring

Annotation: Within the schedule set by the centre or degree programme, 15 minutes of one class will be reserved for students to evaluate their lecturers and their courses or modules through questionnaires.

Activities

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Lectures	38	1.52	4, 7, 8, 6, 2
Type: Autonomous			

Assessment

All subjects are compulsory attendance, and are evaluated separately by different evaluating procedures including writing exams, theoretical and practical tests, oral presentations, research papers understanding, in-class brief questions, written works, etc.

Regulations for the final mark of the Master:

- Every professor decides the number and typology of evaluation activities: oral presentations, written exams, delivery of discussed articles, small tests...
- The final mark of the module will be the sum of the mark of every professor multiplied by the percentage of his classes in the total teaching of the module.
- The marks of the written exams must be above 3.5 in order to average with other marks of the professor and/or the module.
- There will be a period in January to repeat written exams with marks under 5. Only students that have attended to 2/3 of the evaluation activities can retake the exams in January. In the case of exams under 3.5 it will be mandatory to the student, in case of exams between 3.5 and 5, it would be optional to the student.
- In the case that a student will not arrive to a 3.5 mark after the retaking exam in January, the coordinator of the module could proceed to average this mark with the rest of the module. However, this option can only be considered for two written exams in the whole master.
- The marks of other evaluations activities (i. e. oral presentations) will average with the rest of the marks of the professor/module independently of the value. There will not be option of repeating these other evaluation activities.
- An average mark of 5.0 is mandatory in order to pass a module.

Some previewed evaluation methods are detailed next. Written examinations will be grouped in two sessions and detailed in your schedule.

- Modern organofluorinated chemistry: written exam
- Dendrimers: Written examination covering the general concepts seen during course.
- Small molecules: Synthesis and applications in molecular biology and medicine: Written examination+ Presentation in pairs (10 min) based on previous work.
- Introduction to polymeric materials: Written examination
- Nanomaterials and Analytical Chemistry. Chemical Sensing applications: Questions about a research paper on the field (approx. 1h)
- Drug / biomolecule delivery: Written exam on the topics discussed during the course.
- Computational chemistry: online questionnaire at the end of the set of classes

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Manuscripts and reports	30%	4	0.16	3, 1, 4, 5, 7, 8, 10, 11, 9, 12, 2
Oral communications	40%	10	0.4	1, 4, 5, 7, 8, 11, 6, 12, 2
Practical and Teorical Writing Exams	30%	6	0.24	1, 4, 7, 8, 10, 12, 2

Bibliography

All recommended literature will be given during the sessions. Here some general indicators of some subjects:

- Dendrimers.

1. *Dendrimers: Towards Catalytic, Material and Biomedical Uses*. First Edition. Anne-Marie Caminade, Cédric-Olivier Turrin, Régis Laurent, Armelle Ouali and Béatrice Delavaux-Nicot , 2011, John Wiley & Sons, Ltd. Published 2011 by John Wiley & sons, Ltd. ISBN 9780470748817

2. *Dendrimer Chemistry*. Fritz Vögtle, Gabriele Richardt and Nicole Werner. 2009 WILEY-VCH Verlag GMBH & Co. KGaA, Weinheim. ISBN 978-3-527-32066-0

- Soft materials: polymeric coatings and gelators, Supramolecular structures.

1. *Introduction to Soft Matter: Synthetic and Biological Self-Assembling Materials*, I. W. Hamley, Wiley 2007.

2. *Polymer Chemistry*, C. E. Carraher, Jr. 7th Edition. CRC Press, 2011.

- Nanomaterials and Analytical Chemistry. Chemical Sensing applications.

1. *The Use of Magnetic Nanoparticles in Analytical Chemistry*. Jacob S. Beveridge, Jason R. Stephens, and Mary Elizabeth Williams. Annu. Rev. Anal. Chem. 2011. 4:251-73

2. *Chemical Functionalization of Carbon Nanomaterials. Chemistry and Applications*. Edited by Vijay Kumar Thakur and Manju Kumari Thakur. CRC Press 2015. Pages 664-681. ISBN: 978-1-4822-5394-8.

3. *Nanomaterials and Analytical Chemistry*. F. Valentini and G. Palleschi. Analytical Letters, (2008), 41:4, 479-520, DOI: 10.1080/00032710801912805

Software

- Computational Chemistry

Ucsf chimera

<http://www.cgl.ucsf.edu/chimera/>

Rdkit

<http://rdkit.org>