

MASTER

 **CHEM**
BIO & **MAT**

CHEMISTRY

at the Interface with

BIOLOGY *and*

MATERIALS Science

BROCHURE 2020/2021

Contact:

 master.chembio-mat@usc.es

 +34 881 815 746  +34 881 815 797

More information:

 <http://masterchembiomat.usc.es>

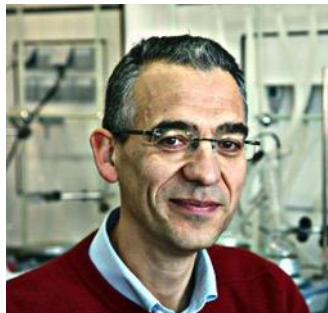
 [@ChemBio&Mat](https://twitter.com/ChemBio&Mat)

 [ChemBioMatMSc](https://www.instagram.com/ChemBioMatMSc)

Table of Contents

WELCOME LETTER	4
PROGRAMME	5
COURSES OVERVIEW	8
TEACHING STAFF 2020/2021.....	125
TEACHING TIMETABLE	146

Welcome letter



Dear Master Students,

With this letter we want to wish you our warmest welcome. We are delighted that you have chosen our master school to continuing with your education and formation. My name is Juan R. Granja and I have the pleasure of serving as the coordinator of this master for the 2020-2021 academic year that is now starting.

The ChemBio&Mat aims to provide the right environment and conditions to allow the best training and skills in several topics of Chemistry, and especially on those at the interface with molecular and cell biology and material science. We trust that with your dedication and effort, this master will open many opportunities for your scientific and/or professional future. One key prerequisite for your academic success is, of course, your own personal engagement. Work hand-in-hand with our teaching staff by preparing lectures and discussions ahead of time, and by carefully reviewing your notes afterwards. Please also take advantage of our academic support services.

All of us will support you in your venture. We expect that after taking our program you will be part of a body of exceptionally talented students that can be recognized for its academic abilities, ambition and creativity.

Probably, you have often heard that the CiQUS (Centre for Research in Biological Chemistry and Molecular Materials) is a special place at the USC. It is a research centre fully committed to scientific excellence and equipped with state-of-the-art research facilities. This unique scientific environment will contribute to make of this Master one of the bests.

Our academic program aims at providing future graduates with a multidisciplinary training in several topics of **chemistry, biomedicine and materials science**. Importantly, the program should also allow to acquire leading and problem-solving abilities and set you in an idoneal position to perform research tasks, start an academic career or enter the job market in areas like biotechnology, nanotechnology or energy.

This year is the COVID, that is affecting our mobility and social skills and unfortunately is limiting our teaching and learning capabilities. This infection is also a challenging for our university and for the scientific community. Improving our knowledge about chemical and biology involved in any kind of infection is mandatory to prevent future problems to our society. In addition, the challenges facing the 21st century society in areas as diverse as health, energy or sustainable development must be tackled from a multidisciplinary perspective; and undoubtedly, those with knowledge on molecular chemistry, biomedicine and physics will be in a better position to provide solutions. In this context, the proposed master's program will provide you with a rigorous and practical training in these disciplines, and a multi- and interdisciplinary vision of science and technology.

We look forward to working with you to provide transformative and innovative learning experiences. We are confident that you will find this a truly exciting time of intellectual stimulation and growth. I hope your one year and a half ahead is both challenging and successful.

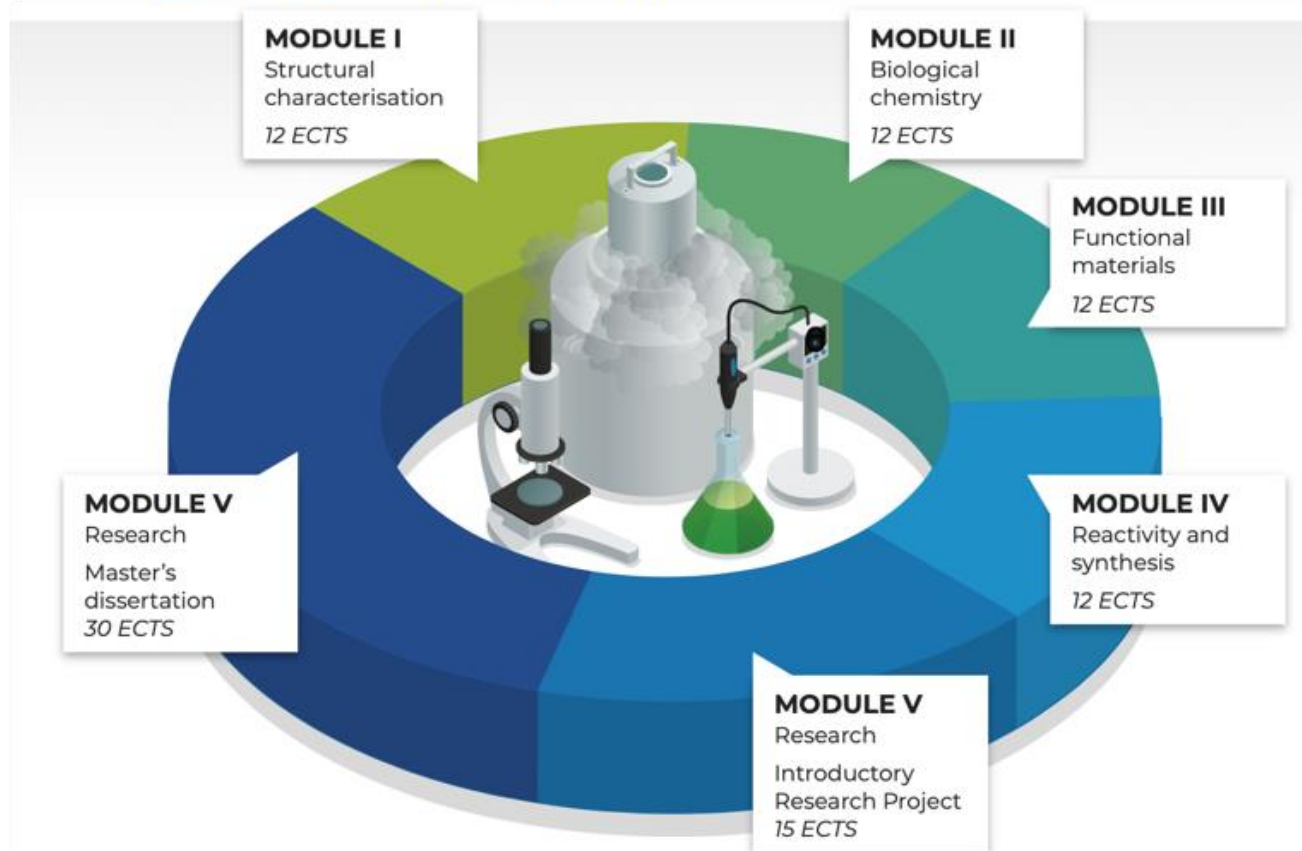
Again, welcome!

PROGRAMME

MASTER CHEM BIO&MAT

CHEMISTRY

at the Interface with
BIOLOGY *and*
MATERIALS Science



90 ECTS

It is a study programme organized in 5 areas (modules)



1.5 YEARS

Programme length: 3 semesters (18 months)



ENGLISH

All courses are taught in English



MULTIDISCIPLINARY

19 Research Groups at CiQUS working in 3 thematic areas: Biological & Medicinal Chemistry; Functional Materials and Synthetic Methodologies



INTERNATIONAL

The teaching staff includes up to 5 ERC grantees (8 ERC Projects) and other internationally renowned scientists



EXPERIMENTAL

Hands-on training in state-of-the-art experimental techniques. Research projects mean 50% (45 ECTS) of the study plan



MOBILITY

Opportunity to do an internship to conduct research in a different Partner institution or company



MENTORING

Academic and industrial supervisors for career advising and professional development

1ST SEMESTER (1ST YEAR - 30 ECTS)**2ST SEMESTER (1ST YEAR - 30 ECTS)****3RD SEMESTER (2ND YEAR - 30 ECTS)****MODULE I****STRUCTURAL CHARACTERISATION (12 ECTS)**

- Magnetic Resonance
- Microscopy
- Colloidal and Interface Characterisation
- Spectroscopic and Spectrometric Techniques

MODULE II**BIOLOGICAL CHEMISTRY (12 ECTS)**

- Biological and Cellular Chemistry
- Supramolecular Chemistry
- Experimental Techniques in Molecular Biology and Medicine (*Op.*)
- Biophysics (*Op.*)

MODULE III**FUNCTIONAL MATERIALS (12 ECTS)**

- Nanostructured Materials
- Molecular Materials
- Molecular Magnetism (*Op.*)
- Nanobiotechnology (*Op.*)

MODULE IV**REACTIVITY AND SYNTHESIS (12 ECTS)**

- Catalysis
- Chemical Synthesis
- Determination of Reaction Mechanisms (*Op.*)
- Computational Chemistry (*Op.*)

MODULE V**RESEARCH (48 ECTS)**

- Tutored Training Activities
- Introductory Research Project
- Master Dissertation



In spite of the uncertainty about the evolution of the COVID-19 pandemic, the Master in Chemistry at the Interface with Biology and Materials Science will be running during the the academic year 20-21.

Teaching will involve a blend of in-person and online lecturing, adapting to the circumstances at each moment. We will make sure that the quality of the training process is not compromised.

COURSES OVERVIEW

IDENTIFICATION FORM

Course Data

Course number	P1251101
Subject	<i>Magnetic Resonance</i>
Title	Chemistry at the interface with Biology and Materials Science (ChemBio&Mat) P1251V01
Course Level	Master
Credits	3.0
Module	I (Structural Characterization)
Academic Year	2019-2020

Titulation

Title	Center	Course	Semester
ChemBio&Mat	FACULTAD de QUÍMICA/CiQUS	1	First

Subject

Title	Course Title	Course type
ChemBio&Mat	Magnetic Resonance	Compulsory

Coordination

Name	Department	Contact
Víctor Sánchez Pedregal	Organic Chemistry	victor.pedregal@usc.es / 15710

SUMMARY

NMR spectroscopy is one of the most powerful analytical tools in organic and inorganic chemistry. It finds application in other fields of science, such as biology, medicine, or materials science, among others. Applications of NMR are not limited to structure determination. NMR spectroscopy is also used to study other molecular properties, like diffusion, reaction mechanism, dynamic processes or intermolecular interactions, for example. ESR spectroscopy is a technique used to study chemical species with unpaired electrons. This plays an important role in the understanding of organic and inorganic radicals, transition metal complexes, and some biomolecules. This course will give an overview of the theoretical principles and the most valuable methods for the research chemist.

PREREQUISITES

Relation with other topics of the Master

No enrollment restrictions have been specified with other subjects of the curriculum.

Other requirements

No enrollment restrictions have been specified with other subjects of the curriculum. Students are expected to have a basic knowledge of spectroscopy, in general, and magnetic resonance, in particular, at the undergraduate level.

COMPETENCES

Basic

- **CB6:** Possess and understand the knowledge that provides a basis or an opportunity for being creative and unique in the development and/or implementation of ideas, often in a research context.
- **CB7:** Students should know how to use the knowledge acquired and their problem-solving capacity in new or little-known environments within wider (or multidisciplinary) contexts related to their field of study.
- **CB8:** Students should be able to integrate knowledge and deal with the complexity of making judgements from information which – being incomplete or limited – includes reflections on the social and ethical responsibilities linked to the use of their knowledge or judgements.
- **CB9:** Students should know how to communicate their findings and the knowledge and underlying reasons underpinning them to specialised and non-specialised audiences in a clear and unambiguous way.
- **CB10:** Students should have the learning skills that allow them to carry on studying in such a way that should be mainly self-directed or autonomous.

General

- **CG2:** Know how to apply the scientific method and acquire skills for developing the necessary protocols for the design and critical assessment of chemical experiments.
- **CG3:** Be able to discuss and communicate ideas, in both oral and written form, to specialised and non-specialised audiences (congresses, conferences, etc.) in a clear and reasoned way.
- **CG5:** Have the skills that allow students to develop an autonomous method for studying and learning.
- **CG7:** Be able to work as part of multidisciplinary teams and collaborate with other professionals, both nationally and internationally.
- **CG8:** Be able to use scientific literature and develop the judgement needed for its interpretation and use.
- **CG11:** Be able to adapt efficiently to future doctoral studies in multidisciplinary areas.

Transversal

- **CT1:** Develop teamwork skills: cooperation, leadership and good listening skills. Adapt to multidisciplinary teams.
- **CT2:** Draft scientific and technical reports and defend them publicly.

- **CT4:** Apply the concepts, principles, theories and models related to Biological Chemistry and Molecular Materials to new or little-known environments within multidisciplinary contexts.
- **CT7:** Show critical and self-critical reasoning when seeking scientific rigour and quality. Handle IT tools and information and communication technology (ICT), as well as on-line access to databases.

Specific

- **CE4:** Know and understand the chemical tools and analytical techniques used for biological chemistry and molecular materials.
- **CE7:** Students should acquire knowledge on advanced techniques for the structural characterization of macromolecules, supramolecules and colloids which are relevant in the field of biological chemistry and molecular materials.
- **CE8:** Gain technical skill for carrying out the structural characterization of molecules, biomolecules, supramolecules and nanoparticles and interpreting the experimental data obtained.
- **CE10:** Know the potential of NMR and ESR techniques for the analysis of biomolecule dynamic processes (diffusion) in biological media, being able to process and interpret real spectra of these techniques.

OBJECTIVES OF TRAINING

The students, once passed the subject, should be able to:

- Know the basics of NMR and ESR spectroscopy, as well as the type of information they provide in the study of chemistry.
- Be able to process data and interpret NMR and ESR spectra, in order to deduce the structure and other properties of molecules and / or supramolecular complexes.
- Design their own solutions, selecting the most suitable spectroscopic methods for the study of each chemical problem.

COURSE CONTENTS

1. ESR spectroscopy. Acquisition of spectra and interpretation

Electron Spin Resonance spectroscopy. Introduction and theory. Range of application. Laboratory practicals: data acquisition and analysis.

2. One-dimensional NMR spectroscopy.

Multipulse 1D experiments: homonuclear decoupling, NOE, ¹³C, DEPT. Interpretation of 1D spectra.

3. Two-dimensional NMR spectroscopy.

Introduction to 2D NMR. Homonuclear (COSY, TOCSY, NOESY) and heteronuclear (HMQC, HSQC, HMBC) correlations. Interpretation of 2D spectra.

4. Processing of NMR spectra

Introduction to NMR data acquisition and processing. Laboratory practicals: the NMR spectrometer and processing software.

COURSE BIBLIOGRAPHY

1. Basic

- Field, L.D.; Sternhell, S.; Kalman, J.R. *Organic Structures from Spectra*, 5th ed., Wiley, **2013**. ISBN: 978-0-470-31926-0.
- Hesse, M.; Meier, H.; Zeeh, B. *Spectroscopic Methods in Organic Chemistry*, 2nd ed., Thieme, **2007**.
- Poole, Charles P. *Electron Spin Resonance: A Comprehensive Treatise on Experimental Techniques*, 2nd ed., Wiley, **1996**.

2. Complementary

- Günther, H. *NMR Spectroscopy*, 3rd. ed., **2013**. ISBN: 978-3-527-33000-3.
- Claridge, T.D.W. *High-Resolution NMR Techniques in Organic Chemistry*, 2nd ed., Tetrahedron Organic Chemistry, vol. 27, **2009**. ISBN-13: 978-0080548180.
- Silverstein, R.M.; Webster, F.X.; Kiemle, D.J. *Spectrometric Identification of Organic Compounds*, Wiley, **2005**. ISBN: 0-471-39362-2.
- Friebolin, H. *Basic One- and Two-Dimensional NMR Spectroscopy*, 5th ed., Wiley, **2011**. ISBN: 978-3-527-32782-9.
- Crews, P.; Rodriguez, J.; Jaspers, M. *Organic Structure Analysis*, 2nd ed., Oxford University Press, New York, **2009**. ISBN: 9780195336047.

STUDENT WORKLOAD

The training activities will be distributed according to the following table.

	Activity	hours	% presential
Presential classes	Lectures and conferences	4	100%
	Seminars and classroom exercises	6	100%
	Tutorials	1	100%
	Practical laboratory or computer classes	12	100%
	Oral presentations os students or lectures by guest speakers	2	100%
	Final exam	2	100%
Non Presential	Preparation and study of problems	10	0%
	Elaboration of individual work	35	0%
	Literature searching	3	0%
	TOTAL	75	

TEACHING METHODOLOGY

The Virtual Campus will be used for delivering the necessary material to the students, according to the professor criterion. This material will include: the course program, exercises and problems to be solved, copies of the classroom presentations, etc.

Along the course, the student should participate in various formative activities, with the aim of acquiring the established knowledge and skills.

- **Lectures.** Explanation of theoretical contents. The active participation of the students will be intended through the formulation of appropriate questions that they should try to answer.
- **Interactive classes encouraging student participation (seminars).** Discussion of exercises and problems, individually or in groups.
- Combined use of blackboard and fast and anonymous response methods in class (*clickers*) to know the degree of follow-up of the subject.
- Promoting **autonomous student learning**, through the work on topics proposed in class.
- Resolution of practical **exercises** (problems, multiple choice test, interpretation and processing of information, evaluation of scientific publications, etc.).
- **Oral** presentations of previously prepared topics, including discussion with classmates and teachers.

Recommendations for the study of the subject

- In the seminar classes we will mainly work on solving problems. The problems and the class schedule will be available to the students in the virtual classroom. Students should try to solve them autonomously in advance of the classes. The solutions will be analyzed in the classes.
- It is advised that students use the recommended bibliography. The faculty will advise the sections of each book that are most appropriate for each topic.
- In case of finding difficulties, students can raise their doubts both in the classes and in the tutorials.

ASSESSMENT SYSTEM

Guiding principles.

With the aim of encouraging the constant student work to favor the learning, a continuous evaluation will be applied. This methodology will inform the professor about the content's assimilation by the student as well as their ability to apply them to problem solving. The evaluation will be individual.

Along the course, on professor criterion, the students will have to solve some exercises and hand them in at the scheduled date. Performing short tests in classroom is also foreseen.

In order to evaluate the knowledge related to the master classes and the problem-solving ability of the students, one exam and/or individual oral presentation will be performed.

Final grade.

The grade of this subject will be determined by *CONTINUOUS ASSESSMENT* (30%) and a *FINAL EXAM* (70%).

The access to the final exam is conditioned to the participation in at least 80% of the compulsory attendance activities (practicals, seminars and tutorials).

FINAL EXAM (70%). There will be a single theoretical-practical final exam that will cover all the contents of the subject. To pass the subject, it is mandatory to achieve a grade of at least 4 out of 10 in the final exam (4/10). Otherwise the score of the elements of the continuous assessment will not be added, the final grade being that obtained in the exam.

CONTINUOUS ASSESSMENT (30%). Along the course, the students will do a series of activities (problems, presentation of works, participation in seminars, etc.) that will be evaluated.

CALCULATION OF THE FINAL GRADE.

In case of passing the final mark of the final exam (4/10), the final grade of the subject will be obtained as the following weighted average:

$$CF = (0.7 * Ex) + (0.3 * EC)$$

CF: Final mark of the subject (0 - 10)
Ex: Exam rating (0 - 10)
EC: Continuous Evaluation (0 - 10)

The subject will be passed if the final grade is **at least 5/10**.

In the case of not passing the subject at the 'first opportunity', the student will be evaluated again of the final exam at the 'second opportunity', keeping the grade of the continuous evaluation. Repeating students will have the same attendance regime for classes as those who take the subject for the first time.

COMMENTS

CONTINGENCY PLAN

According to the document "Guidelines for the development of safe classroom teaching, academic year 2020-2021", two possible new scenarios are contemplated for the teaching methodology and the evaluation system in case it is not possible to develop the adapted normality scenario :

Scenario 2: distancing (with partial restrictions on physical presence).

- The expository teaching will be non-face-to-face and the seminars and practical laboratory and computer classroom. However, the distance measures imposed may mean that it is necessary to reduce the size of the practice groups and, therefore, the number of contact hours (up to a maximum of 50% of the practical hours of the subject) that must be complemented with non-contact activities.
- The tutorials will preferably be virtual.
- The final tests will preferably be telematic.

Scenario 3: closure of the facilities (impossibility of teaching face-to-face).

- Teaching will be completely virtual, with synchronous or asynchronous mechanisms.
- The tutorials will be exclusively virtual.

- The final tests will be exclusively telematic.

For virtual teaching, Moodle platforms will be used for the final test and continuous assessment and MS Teams for expository classes, seminars and tutorials.

FACULTY DATA

Faculty	Contact	Semester	Day	Time	Class
Francisco Rivadulla Fdz.	15724	1st	Tue/Thu 21/09 to 15/09	16:00/17:30	Maths (3 rd floor)
Víctor M. Sánchez Pedregal	15710			16:00/17:30	
Marc Fonts Molins					
Andrés Seoane					

IDENTIFICATION FORM

Course Data

Course number	P1251106
Subject	Microscopy
Title	Chemistry at the interface with Biology and Materials Science (ChemBio&Mat) P1251V01
Course Level	Master
Credits	3.0
Module	I (Structural Characterization)
Academic Year	2019-2020

Titulation

Title	Center	Course	Semester
ChemBio&Mat	FACULTAD de QUÍMICA/CiQUS	1	First

Subject

Title	Course Title	Course type
ChemBio&Mat	Microscopy	Compulsory

Coordination

Name	Department	Contact
José M. Martínez Costas	Biochemistry	jose.martinez.costas@usc.es

SUMMARY

Microscopy, either optical, electronic or x-ray is an essential technique for the characterization of biological processes and structures, as well as for the detailed determination of the structural characteristics of new materials.

PREREQUISITES

Relation with other topics of the Master

No enrollment restrictions have been specified with other subjects of the curriculum.

Other requirements

No enrollment restrictions have been specified with other subjects of the curriculum. Broad knowledge of general biology aspects is preferred.

COMPETENCES

Basic

- **CB6:** Possess and understand the knowledge that provides a basis or an opportunity for being creative and unique in the development and/or implementation of ideas, often in a research context.
- **CB7:** Students should know how to use the knowledge acquired and their problem-solving capacity in new or little known environments within wider (or multidisciplinary) contexts related to their field of study.
- **CB9:** Students should know how to communicate their findings and the knowledge and underlying reasons underpinning them to specialised and non-specialised audiences in a clear and unambiguous way.
- **CB10:** Students should have the learning skills that allow them to carry on studying in such a way that should be mainly self-directed or autonomous.

General

- **CG1:** Know how to use the knowledge acquired for practical problem solving in the field of research and innovation, in the multidisciplinary context of biological chemistry and molecular materials.
- **CG3:** Be able to discuss and communicate ideas, in both oral and written form, to specialised and non-specialised audiences (congresses, conferences, etc.) in a clear and reasoned way.
- **CG4:** Be able to understand the social and ethical responsibilities linked to the use of knowledge or judgements in research, development and innovation in the field of biological chemistry and molecular materials.
- **CG5:** Have the skills that allow students to develop an autonomous method for studying and learning.
- **CG6:** Have leadership, creativity, initiative and entrepreneurship abilities.
- **CG7:** Be capable of working in multidisciplinary teams and collaborating with other specialists, both nationally and internationally.
- **CG8:** Be able to use scientific literature and develop the judgement needed for its interpretation and use.
- **CG10:** Be able to develop the different research stages (from the conception of an idea and the literature search through to target setting, experiment design, analysis of the results and drawing conclusions).

Transversal

- **CT1:** Develop teamwork skills: cooperation, leadership and good listening skills. Adapt to multidisciplinary teams.
- **CT2:** Draft scientific and technical reports and defend them publicly.
- **CT3:** Perform day-to-day research or professional activity in an independent and efficient manner.

- **CT4:** Apply the concepts, principles, theories and models related to Biological Chemistry and Molecular Materials to new or little-known environments within multidisciplinary contexts.
- **CT5:** Appreciate the value of good quality and continuous improvement by acting rigorously, responsibly and ethically.
- **CT6:** Be capable of adapting to changes by being self-motivated when applying new and advanced technologies and other relevant developments.
- **CT7:** Show critical and self-critical reasoning when seeking scientific rigour and quality. Handle IT tools and information and communication technology (ICT), as well as on-line access to databases.

Specific

- **CE4:** Know and understand the chemical tools and analytical techniques used for biological chemistry and molecular materials.
- **CE5:** Know how to analyze and use the data obtained autonomously in complex laboratory experiments by relating them to the suitable chemical, physical or biological techniques
- **CE7:** Students should acquire knowledge on advanced techniques for the structural characterization of macromolecules, supramolecules and colloids which are relevant in the field of biological chemistry and molecular materials.
- **CE8:** Gain technical skill for carrying out the structural characterization of molecules, biomolecules, supramolecules and nanoparticles and interpreting the experimental data obtained.
- **CE9:** Use advanced instrumentation related to research on biological chemistry and molecular materials.

OBJECTIVES OF TRAINING

- Know the different types of microscopy techniques and their theoretical basis.
- Know the different methods and requirements for the preparation of samples for different types of microscopy.
- Get clear notions about the differences between different microscopy techniques and its uses.

COURSE CONTENTS

1. The optical microscope

Structure and basic operation. Preparation of samples. Phase contrast. Visualization of living cells.

2. Fluorescence microscopy.

FRAP and FRET. 3D optical sectioning: deconvolution and confocal microscopy. Visualization of unique molecules by TIRF. Super-resolution microscopy: types. Treatment and preparation of samples for fluorescence microscopy.

3. Transmission (TEM) and scanning electron microscope (SEM)

Operation basics. Preparation of samples for TEM. Contrast and negative staining. 3D reconstruction by tomography. Cryo-microscopy and determination of structures by single particle reconstruction.

4. Scanning probe microscopy.

Bases and types. Preparation of samples. Application to materials.

COURSE BIBLIOGRAPHY

1. Basic

- Molecular Biology of the Cell, B. Alberts et al, Garland Science, 2014

2. Complementary

–

STUDENT WORKLOAD

The training activities will be distributed according to the following calendar.

	Activity	hours	% presential
Presential classes	Lectures and conferences	3	100%
	Seminars and classroom exercises	4	100%
	Tutorials	1	100%
	Practical classes	14	100%
	Oral presentations	2	100%
	Final exam	3	100%
Non Presential	Preparation and study of problems	10	0%
	Elaboration of individual work	35	0%
	Literature searching and so on	3	0%
	TOTAL	75	

TEACHING METHODOLOGY

- Interactive classes encouraging student participation.
- Combined use of computer and blackboard methods.

- Work in the laboratory: preparation of samples and management / demonstration of different types of microscopes with prepared samples.
- Promotion of self-learning of the student proposing challenges and posing questions.
- Resolution of practical exercises (problems, questions type test, interpretation and processing of information, evaluation of scientific publications, etc.).
- Oral presentations of previously prepared topics, including discussion with classmates and teachers.

ASSESSMENT SYSTEM

General considerations

- The evaluation process will be used to know if the student has acquired the scheduled skills and to review the teaching methodology.
- Written exam on theoretical and practical basic contents of the subject.
- Continuous evaluation associated with active participation and autonomous learning.

Evaluation weights: Minimum weighting (MiW)- Maximum weight (MaW)

Written Exam: 50%-70%

Oral presentations: 10%-30%

Other Activities: 20%-40%

Tutoring: 0%-10%

In scenario 1, all exams and tests will be in classroom, while in scenarios 2 and 3 they will be conducted online through the Moodle Quizzes and Microsoft's "Teams" software.

For cases of fraudulent performance of exercises or tests, the provisions of the "Regulations for the evaluation of students academic performance and qualifications review" will apply.

COMMENTS

CONTINGENCY PLAN

changes in teaching methodology and assessment methods are envisaged depending on the evolution of the SARS-Cov2 pandemic and changes between scenarios 1, 2 and 3.

FACULTY DATA

Faculty	Contact	Semester	Day	Time	Class
José M. Martínez Costas	15733	1st	Theory/seminars	16:00/17:30	Fac. Chemistry
Pablo A. del Pino			Tues/Thurs 22/09 to 29/10 Practical	9-14	Maths (3 rd floor) CIQUS

IDENTIFICATION FORM

Course Data

Course number	P1251103
Subject	Colloidal Characterization and Interfaces
Title	Chemistry at the interface with Biology and Materials Science (ChemBio&Mat) P1251V01
Course Level	Master
Credits	3.0
Module	I (Structural Characterization)
Academic Year	2019-2020

Titulation

Title	Center	Course	Semester
ChemBio&Mat	FACULTAD de QUÍMICA/CiQUS	1	First

Subject

Title	Course Title	Course type
ChemBio&Mat	Supramolecular Chemistry	Compulsory

Coordination

Name	Department	Contact
M. Arturo López Quintela	Physical Chemistry	malopez.quintela@usc.es/13044

SUMMARY

The physicochemical characterization of nanostructured materials is a very important task for knowing the properties of these materials. During this course we will study some basic experimental techniques related to the colloidal and interfacial properties of the nanomaterials, as well as their chemical composition and thermal stability.

PREREQUISITES

Relation with other topics of the Master

No enrollment restrictions have been specified with other subjects of the curriculum.

Other requirements

No enrollment restrictions have been specified with other subjects of the curriculum. Broad knowledge of general physical chemistry is required, especially in aspects related to colloidal chemistry, interfaces and transport properties.

COMPETENCES

Basic

- **CB6:** Possess and understand the knowledge that provides a basis or an opportunity for being creative and unique in the development and/or implementation of ideas, often in a research context.

General

- **CG1:** Know how to use the knowledge acquired for practical problem solving in the field of research and innovation, in the multidisciplinary context of biological chemistry and molecular materials.
- **CG3:** Be able to discuss and communicate ideas, in both oral and written form, to specialised and non-specialised audiences (congresses, conferences, etc.) in a clear and reasoned way.
- **CG5:** Have the skills that allow students to develop an autonomous method for studying and learning.
- **CG9:** Be capable of handling chemical substances safely and work in a chemical laboratory without risks.

Transversal

- **CT3:** Perform day-to-day research or professional activity in an independent and efficient manner.
- **CT4:** Apply the concepts, principles, theories and models related to Biological Chemistry and Molecular Materials to new or little-known environments within multidisciplinary contexts.

Specific

- **CE4:** Know and understand the chemical tools and analytical techniques used for biological chemistry and molecular materials.
- **CE5:** Know how to analyze and use the data obtained autonomously in complex laboratory experiments by relating them to the suitable chemical, physical or biological techniques.
- **CE6:** Know the physicochemical bases of biological processes.
- **CE7:** Students should acquire knowledge on advanced techniques for the structural characterization of macromolecules, supramolecules and colloids which are relevant in the field of biological chemistry and molecular materials.

- **CE8:** Gain technical skill for carrying out the structural characterization of molecules, biomolecules, supramolecules and nanoparticles and interpreting the experimental data obtained.

OBJECTIVES OF TRAINING

The main learning objectives of this course are:

- To know the basic experimental techniques for the physicochemical characterization of nanostructured systems.
- To obtain an integrated and multidisciplinary view of the area, in the context of other scientific areas.
- To obtain a general view of the experimental methods and techniques more widely used for studying nanostructured materials
- To know the possible applications of this scientific area.

COURSE CONTENTS

- Determine the composition of nanomaterials.
- Determine the hydrodynamic size of colloids by dynamic light scattering.
- Determine the zeta potential by “Laser Doppler Anemometry”.
- Determine the electrophoretic mobility by gel electrophoresis.
- Determine the thermal stability of colloids by thermogravimetric analysis.
- Determine the quantum efficiency of luminescent nanoparticles.

COURSE BIBLIOGRAPHY

1. Basic

- P. Atkins, J. de Paula & J. Keeler: “Physical Chemistry”, 11th Edition; Oxford University Press, 2017
- I. N. Levine: “Physical Chemistry”, 6th Edition; McGraw-Hill, 2013
Previous editions are also valid.

2. Complementary

- F. MacRitchie: “Chemistry at Interfaces”; Academic Press, 1990.
- D. Myers: Surfaces: “Interfaces and Colloids: Principles and Applications”; VCH, 1999.
- D. Berti & G. Palazzo: “Colloidal Foundations of Nanoscience”; Elsevier, 2014.
- R.J. Hunter: “Foundations of Colloid Science”, 2nd Edition; Oxford University Press, 2001.
- G.T. Barnes & I.R. Gentle: “Interfacial Science: an Introduction”, 2nd Edition; Oxford University Press, 2011.

- John P. Sibilias: “A Guide to Materials Characterization and Chemical Analysis”. VCH Publishers, 1998.
- M.E. Brown: “Introduction to Thermal Analysis. Techniques and applications”; Chapman and Hall, 1998.

In addition, complementary information (research articles, webpages, texts) will be recommended in each part of the matter.

STUDENT WORKLOAD

The training activities will be distributed according to the following table.

	Activity	hours	% presential
Presential classes	Lectures and conferences	3	100%
	Seminars and classroom exercises	4	100%
	Tutorials	1	100%
	Practical classes	14	100%
	Oral presentations	2	100%
	Final exam	3	100%
Non Presential	Preparation and study of problems	10	0%
	Elaboration of individual work	35	0%
	Literature searching and so on	3	0%
	TOTAL	75	

TEACHING METHODOLOGY

The Virtual Campus will be used for delivering the necessary material to the students, according to the professor criterion. This material will include: the course program, exercises and problems to be solved, copies of the classroom presentations, etc.

Along the course, the student should participate in various formative activities, with the aim of acquiring the established knowledge and skills.

Master classes: Explanation of theoretical contents supplemented by audiovisual aids. The active participation of the students will be intended, through the formulation of appropriate questions that they should try to answer.

Seminars: There will be two classroom hours before the partial exams dedicated to review concepts and/or clarify doubts.

Use of fast and anonymous response methods in class (clickers) to know the degree of follow-up of the subject.

Presentation of individual works on some topics related to the subject, including the debate with his classmates and teachers.

Group and individual tutoring.

ASSESSMENT SYSTEM

General considerations:

- The evaluation process will not only serve to determine whether the learner has acquired the programmed competencies but also to review the teaching methodology.
- Written test on basic theoretical and practical contents of the subject.
- Continuous evaluation associated with active participation and autonomous learning.

SYSTEM OF EVALUATION; WEIGHTING

Final examination: 70 %

Oral exhibition: 10 %

Homework / activities / oral exhibition: 20 %

The continuous assessment will have a weight of 30 % in the qualification of the subject and will consist of two components: resolution of problems and practical cases (20 %), oral exhibition (works, reports, problems and practical cases) (10 %). The seminars and the tutorships will include exercises and face-to-face realized works and delivered to the teacher.

The final examination will have a weight of 70 % and will cover all the contents of the subject.

The learning evaluation system will be implemented in the subject in different ways depending on the possible teaching scenarios in which we are.

Scenario 1: normality adapted (without restrictions to physical presence).

The continuous evaluation will preferably be telematic (Virtual Campus or Microsoft TEAMS). The final exam will be face-to-face.

Scenario 2: Distancing (with partial restrictions on physical presence)

Both the continuous evaluation and the final exam will preferably be telematic (Virtual Campus or Microsoft TEAMS).

Scenario 3: closure of the premises (impossibility of teaching in person)

Both the continuous evaluation and the final exam will be exclusively telematic (Virtual Campus or Microsoft TEAMS).

COMMENTS

The teaching will be mainly given in English.

"Contingency Plan"

Adaptations corresponding to the teaching methodology and assessment systems sections foreseen for scenarios 2 and 3 for the purposes of future degree monitoring and accreditation processes.

Methods of teaching:

Scenario 1: normality adapted (without restrictions to physical presence).

*The expositive and interactive teaching will be fundamentally face-to-face, although in an exceptional and justified way the telematics teaching (using Microsoft TEAMS) can be combined with the classroom

teaching up to a maximum of 10%.

*The tutorials can be carried out partially in a telematic way (Virtual Campus or Microsoft TEAMS)

*Final tests will be in person.

Scenario 2: Distancing (with partial restrictions on physical presence)

*Expository teaching may be carried out in its entirety in a telematic way (in teaching spaces where distancing is not possible) using Microsoft TEAMS, or combine 50% with the classroom in those teaching spaces where distance is possible. In interactive teaching, seminars and laboratories, it will be possible to combine physical and telematic presence, up to a maximum of 50% of the hours of the subject in telematic mode, when the distancing so requires.

*Tutorials will preferably be telematic (Virtual Campus or Microsoft TEAMS).

*The final tests will preferably be of a telematic nature (Virtual Campus or Microsoft TEAMS).

Scenario 3: closure of the premises (impossibility of teaching in person)

*The teaching will be completely telematic (Virtual Campus or Microsoft TEAMS), with synchronous mechanisms (in the usual timetables of class) or asynchronous.

*Tutorials will be exclusively telematic (Virtual Campus or Microsoft TEAMS).

*The final tests will be exclusively of a telematic nature (Virtual Campus or Microsoft TEAMS).

Assessment systems

Scenario 1: normality adapted (without restrictions to physical presence).

The continuous evaluation will preferably be telematic (Virtual Campus or Microsoft TEAMS). The final exam will be face-to-face

Scenario 2: Distancing (with partial restrictions on physical presence)

Both the continuous evaluation and the final exam will preferably be telematic (Virtual Campus or Microsoft TEAMS).

Scenario 3: closure of the premises (impossibility of teaching in person)

Both the continuous evaluation and the final exam will be exclusively telematic (Virtual Campus or Microsoft TEAMS).

FACULTY DATA

Faculty	Contact	Semester	Day	Time	Class
M. Arturo López Quintela	13044	1st	Tue/Thu	17:30/19:00	Maths (3 rd floor)
Carlos Vázquez Vázquez	13011		12/11 to 17/12		
Pablo del Pino González	15711				

IDENTIFICATION FORM

Course Data

Course number	P1251106
Subject	<i>Spectroscopic and Spectrometric Techniques</i>
Title	Chemistry at the interface with Biology and Materials Science (ChemBio&Mat) P1251V01
Course Level	Master
Credits	3.0
Module	I (Structural Characterization)
Academic Year	2019-2020

Titulation

Title	Center	Course	Semester
ChemBio&Mat	FACULTAD de QUÍMICA/CiQUS	1	First

Subject

Title	Course Title	Course type
ChemBio&Mat	<i>Spectroscopic and Spectrometric Techniques</i>	Compulsory

Coordination

Name	Department	Contact
Eugenio Vázquez	Organic Chemistry	email/Extension

SUMMARY

The extraordinary sensitivity, simplicity and speed of optical spectroscopic techniques makes them ideally suited for addressing a broad range of questions in molecular and cellular biophysics. Spectroscopic properties such as absorbance, fluorescence and chiroptical properties provide information about the identity, concentration, energy, conformation or dynamics of molecules and can be sensitive to tiny changes in molecular structure or in the properties of their surroundings. Because they usually are not destructive, spectrophotometric techniques can be used with samples that must be recovered after an experiment. They also can provide analytical methods that avoid the need for radioisotopes or hazardous reagents. When combined with genetic engineering and microscopy, they provide windows to the locations, dynamics and turnover of particular molecules in living cells. Altogether, spectroscopic techniques include some of the most powerful weapons in the analytical arsenal, and a basic working knowledge of their scope and applications is fundamental for the development of modern chemistry.

PREREQUISITES

Relation with other topics of the Master

No enrollment restrictions have been specified with other subjects of the curriculum.

Other requirements

No enrollment restrictions have been specified with other subjects of the curriculum. Broad knowledge of general organic and inorganic chemistry is required, especially in its synthetic and structural aspects.

COMPETENCES

Basic

- **CB6:** Possess and understand the knowledge that provides a basis or an opportunity for being creative and unique in the development and/or implementation of ideas, often in a research context.
- **CB7:** Students should know how to use the knowledge acquired and their problem-solving capacity in new or little known environments within wider (or multidisciplinary) contexts related to their field of study.
- **CB9:** Students should know how to communicate their findings and the knowledge and underlying reasons underpinning them to specialised and non-specialised audiences in a clear and unambiguous way.
- **CB10:** Students should have the learning skills that allow them to carry on studying in such a way that should be mainly self-directed or autonomous.

General

- **CG1:** Know how to use the knowledge acquired for practical problem solving in the field of research and innovation, in the multidisciplinary context of biological chemistry and molecular materials.
- **CG2:** Know how to apply the scientific method and acquire skills for developing the necessary protocols for the design and critical assessment of chemical experiments.
- **CG3:** Be able to discuss and communicate ideas, in both oral and written form, to specialised and non-specialised audiences (congresses, conferences, etc.) in a clear and reasoned way.
- **CG5:** Have the skills that allow students to develop an autonomous method for studying and learning.
- **CG8:** Be able to use scientific literature and develop the judgement needed for its interpretation and use.

Transversal

- **CT3:** Work autonomously and efficiently in the daily practice of research or professional activity.
- **CT4:** Apply the concepts, principles, theories and models related to Biological Chemistry and Molecular Materials to new or little-known environments within multidisciplinary contexts.
- **CT5:** Appreciate the value of good quality and continuous improvement by acting rigorously, responsibly and ethically.
- **CT6:** Be able to adapt to changes, having the initiative to apply new technologies and advanced technologies, as well as other relevant developments
- **CT7:** Show critical and self-critical reasoning when seeking scientific rigour and quality. Handle IT tools and information and communication technology (ICT), as well as on-line access to databases.

Specific

- **CE1:** Know the impact of chemistry, biological chemistry and molecular materials on the industry, environment, health, agrofood and renewable energies.
- **CE2:** Be able to critically confront experimental data and theoretical hypotheses.
- **CE3:** Know the rules on risk prevention in the laboratory and in the industry related to chemistry.
- **CE4:** Know and understand the chemical tools and analytical techniques used in biological chemistry and molecular materials.
- **CE5:** Know how to analyze and use the data obtained autonomously in complex laboratory experiments and relate them to the appropriate chemical, physical or biological techniques.
- **CE8:** Acquire technical skills to carry out the structural characterization of molecules, biomolecules, supramolecules and nanoparticles and in the interpretation of the experimental data obtained.

OBJECTIVES OF TRAINING

- Learn the basis of spectroscopic and spectrometric techniques and the structural information that can be obtained from them.
- Obtain an overview of the methods and experimental spectroscopic and spectrometric techniques used in biological chemistry and molecular materials.
- Work safely and with competence with a variety of spectroscopic and spectrometric techniques.
- Ability to interpret spectroscopic and spectrometric results to gain structural information.
- Be able to propose the molecular structure of organic and inorganic compounds through the use of spectroscopic techniques and mass spectrometry.
- Know the possible applications of this field of science.

COURSE CONTENTS

1. Absorption spectroscopy: UV-Vis and Circular Dichroism (CD)

Introduction to electronic spectroscopy and basics of UV and CD spectroscopy. The Lambert-Beer Law; absorbance and Scattering; empirical rules in CD; chirality in metal complexes and CD; conformation of biomolecules and CD.

2. Fluorescence spectroscopy

Basics of fluorescence spectroscopy: Energy levels and Jablonsky diagrams; quantum yield; fluorescence lifetime; excitation and emission spectra; Stoke's shift; Kasha's rule; fluorescence quenching; fluorescence anisotropy; resonance energy transfer; excimers and exciplexes; environmental effects in fluorescence; intrinsic fluorophores in biology; fluorescence sensing.

3. Mass spectrometry

Overview of mass spectrometry techniques; instrumentation: methodology

4. Applications of Spectroscopy

Determination of binding constants in supramolecular processes.

COURSE BIBLIOGRAPHY

1. Basic

- John Greaves, John Roboz. *Mass Spectrometry for the Novice*, CRC Press – Taylor & Francis Group, Boca Raton, USA (2014). **ISBN:** 978-1-420-09418-3.
- Bernard Valeur. *Molecular Fluorescence*, 2nd Edition. Wiley-VCH, Weinheim, Germany (2012). **ISBN:** 978-3-527-32837-6.
- Joseph R. Lakowicz. *Principles of Fluorescence Spectroscopy*, 3rd Edition. Springer, NY, USA (2006). **ISBN-10:** 0-387-31278-1.
- Nagao Kobayashi, Atsuya Muranaka, John Mack. *Circular Dichroism and Magnetic Circular Dichroism Spectroscopy for Organic Chemists*. Royal Society of Chemistry, Cambridge, UK (2012). **ISBN:** 978-1-84755-869-5.

2. Complementary

Papers on the application of Circular Dichroism for the study of peptides and proteins:

- N. J. Greenfield, Analysis of the kinetics of folding of proteins and peptides using circular dichroism. *Nat. Protoc.* **1**, 2891–2899 (2006).
- N. J. Greenfield, Using circular dichroism spectra to estimate protein secondary structure. *Nat. Protoc.* **1**, 2876–2890 (2006).
- N. J. Greenfield, Determination of the folding of proteins as a function of denaturants, osmolytes or ligands using circular dichroism. *Nat. Protoc.* **1**, 2733–2741 (2006).
- N. J. Greenfield, Using circular dichroism collected as a function of temperature to determine the thermodynamics of protein unfolding and binding interactions. *Nat. Protoc.* **1**, 2527–2535 (2006).
- N. C. Garbett, P. A. Ragazzon, J. B. Chaires, Circular dichroism to determine binding mode and affinity of ligand-DNA interactions. *Nat. Protoc.* **2**, 3166–3172 (2007).

Fluorescence Spectroscopy:

- I. L. Medintz, H. T. Uyeda, E. R. Goldman, H. Mattoussi, Quantum dot bioconjugates for imaging, labelling and sensing. *Nat. Mater.* **4**, 435–446 (2005).
- J. W. Lichtman, J.-A. Conchello, Fluorescence microscopy. *Nat. Methods.* **2**, 910–919 (2005).
- U. Resch-Genger, M. Grabolle, S. Cavaliere-Jaricot, R. Nitschke, T. Nann, Quantum dots versus organic dyes as fluorescent labels. *Nat. Methods.* **5**, 763–775 (2008).
- L. D. Lavis, Chemistry Is Dead. Long Live Chemistry! *Biochemistry.* **56**, 5165–5170 (2017).
- G. Hong, A. L. Antaris, H. Dai, Near-infrared fluorophores for biomedical imaging. *Nature Biomedical Engineering.* **1**, 0010 (2017).
- P. Wu, L. Brand, Resonance energy transfer: methods and applications. *Anal. Biochem.* **218**, 1–13 (1994).

STUDENT WORKLOAD

The training activities will be distributed according to the following table.

	Activity	hours	% presential
Presential classes	Lectures and conferences	3	100%
	Seminars and classroom exercises	4	100%
	Tutorials	1	100%
	Practical classes	16	100%
	Oral presentations	0	100%
	Final exam	3	100%
Non Presential	Preparation and study of problems	10	0%
	Elaboration of individual work	35	0%
	Literature searching and so on	3	0%
	TOTAL	75	

TEACHING METHODOLOGY

The Virtual Campus will be used for delivering the necessary material to the students, according to the professor criterion. This material will include: the course program, exercises and problems to be solved, etc.

Along the course, the student should participate in various formative activities, with the aim of acquiring the established knowledge and skills.

Master classes: Explanation of theoretical contents supplemented by audiovisual aids. The active participation of the students will be intended, through the formulation of appropriate questions that they should try to answer.

Practical classes: The core of this course are these practical laboratory experiments in which the students will use the instruments in designed experiments to illustrate the fundamentals of each technique.

Seminars: There will be four classroom hours before the partial exams dedicated to review concepts and/or clarify doubts.

Group and individual tutoring.

ASSESSMENT SYSTEM

A continuous evaluation will be applied. The evaluation will be individual. The students will have to solve some exercises and hand them in at the scheduled date. Performing short tests in classroom is also foreseen and the participation in the class will be also be considered for final grading (25%).

In order to evaluate the knowledge related to the master classes and the practical problem-solving ability of the students, they will handle written reports after each laboratory experiment. (75%).

The students who did not pass the continuous evaluation will have the opportunity to perform a second-chance exam. To pass the course, it will be mandatory obtaining 5 points out of 10.

FACULTY DATA

Faculty	Contact	Semester	Day	Time	Class
M. Eugenio Vázquez	15738	1st	Mon/Wend 21/09 to 19/10	19:00/20:30	Maths (3 rd floor)

IDENTIFICATION FORM

Course Data

Course number	P1251105
Subject	Biological and Cellular Chemistry
Title	Chemistry at the interface with Biology and Materials Science (ChemBio&Mat)
Course Level	Master
Credits	3.0
Module	II (Biological Chemistry)
Academic Year	2019-2020

Titulation

Title	Center	Course	Semester
ChemBio&Mat	FACULTAD de QUÍMICA/CiQUS	1	First

Subject

Title	Course Title	Course type
ChemBio&Mat	Biological and Cellular Chemistry	Compulsory

Coordination

Name	Department	Contact
José Luis Mascareñas	Organic Chemistry	joseluis.mascarenas@usc.es

SUMMARY

This subject deals with the understanding of how the main biological macromolecules organize within the cell, and with the discussion of relevant biological and chemical tools for specific manipulations. There will be a specific emphasis in nucleic acids and proteins.

PREREQUISITES

Relation with other topics of the Master

No enrollment restrictions have been specified with other subjects of the curriculum.

Other requirements

No enrollment restrictions have been specified with other subjects of the curriculum. Broad knowledge of general organic and inorganic chemistry is required, especially in its synthetic and structural aspects.

COMPETENCES

Basic

- **CB6:** Possess and understand the knowledge that provides a basis or an opportunity for being creative and unique in the development and/or implementation of ideas, often in a research context.
- **CB7:** Students should know how to use the knowledge acquired and their problem-solving capacity in new or little known environments within wider (or multidisciplinary) contexts related to their field of study.
- **CB9:** Students should know how to communicate their findings and the knowledge and underlying reasons underpinning them to specialised and non-specialised audiences in a clear and unambiguous way.
- **CB10:** Students should have the learning skills that allow them to carry on studying in such a way that should be mainly self-directed or autonomous.

General

- **CG1:** Know how to use the knowledge acquired for practical problem solving in the field of research and innovation, in the multidisciplinary context of biological chemistry and molecular materials.
- **CG3:** Be able to discuss and communicate ideas, in both oral and written form, to specialised and non-specialised audiences (congresses, conferences, etc.) in a clear and reasoned way.
- **CG4:** Be able to understand the social and ethical responsibilities linked to the use of knowledge or judgements in research, development and innovation in the field of biological chemistry and molecular materials.
- **CG5:** Have the skills that allow students to develop an autonomous method for studying and learning.
- **CG6:** Have leadership, creativity, initiative and entrepreneurship abilities.
- **CG7:** Be capable of working in multidisciplinary teams and collaborating with other specialists, both nationally and internationally.
- **CG8:** Be able to use scientific literature and develop the judgement needed for its interpretation and use.
- **CG10:** Be able to develop the different research stages (from the conception of an idea and the literature search through to target setting, experiment design, analysis of the results and drawing conclusions).

Transversal

- **CT1:** Develop teamwork skills: cooperation, leadership and good listening skills. Adapt to multidisciplinary teams.
- **CT2:** Draft scientific and technical reports and defend them publicly.
- **CT3:** Perform day-to-day research or professional activity in an independent and efficient manner.

- **CT4:** Apply the concepts, principles, theories and models related to Biological Chemistry and Molecular Materials to new or little-known environments within multidisciplinary contexts.
- **CT5:** Appreciate the value of good quality and continuous improvement by acting rigorously, responsibly and ethically.
- **CT6:** Be capable of adapting to changes by being self-motivated when applying new and advanced technologies and other relevant developments.
- **CT7:** Show critical and self-critical reasoning when seeking scientific rigour and quality. Handle IT tools and information and communication technology (ICT), as well as on-line access to databases.

Specific

- **CE1:** Know the impact of chemistry, biological chemistry and molecular materials on the industry, environment, health, agrofood and renewable energies.
- **CE4:** Know and understand the chemical tools and analytical techniques used for biological chemistry and molecular materials.
- **CE7:** Students should acquire knowledge on advanced techniques for the structural characterization of macromolecules, supramolecules and colloids which are relevant in the field of biological chemistry and molecular materials.
- **CE8:** Gain technical skill for carrying out the structural characterization of molecules, biomolecules, supramolecules and nanoparticles and interpreting the experimental data obtained.
- **CE9:** Use advanced instrumentation related to research on biological chemistry and molecular materials.
- **CE11:** Be familiar with the basics of biological and cellular chemistry.
- **CE12:** Understand the weak interaction forces that control supramolecular processes and know how to apply them for obtaining new materials and biological functions.

OBJECTIVES OF TRAINING

- Understand the concept of biological chemistry and its relationship with chemical synthesis and cell biology
- Understand the chemical and molecular bases of cells.
- Know and understand the different tools used in biological chemistry
- Obtain a comprehensive and multidisciplinary vision of the area, in the context of other branches of the science.
- Get an overview of the most commonly used experimental methods and techniques in biological and cellular chemistry.
- Know the possible applications of this scientific field.

COURSE CONTENTS

5. Basic architecture of the cell

Compartments and intracellular traffic

6. Biomolecules

Basic aspects of cell chemistry

7. Synthesis of biomolecules

Bioconjugation and bioorthogonal chemistry.

8. Tools in biological chemistry

Sensors, transport peptides, photoactivatable compounds, molecular switches, enzymatic inhibitors, etc.

COURSE BIBLIOGRAPHY

3. Basic

- 1.- Molecular Biology of the Cell, B. Alberts et al, Garland Science, 2014
- 2.- Introduction to Bioorganic Chemistry and Chemical Biology. Vranken, D-V; Weiss, G.A. Garland Science 2012
- 3.- Nucleic Acids in Chemistry and Biology. Blackburn, M.: Gait, M.J.; Loakes, D.; Williams, D.M. (Editors). Royal Society of Chemistry, 2006
- 4.- Peptides: Synthesis, Structures and Application. Gutte, B. Academic Press,.1995

4. Complementary

- 5.- Introduction to Protein Structure. Brändén, C-I; Tooze, J. Garland Science 1999.
- 6.- Glycochemistry, Principles, Synthesis and Applications. Ed. Peng G. Wang, C. R. Betozzi. Marcel Dekker, New York, 2001.
- 7.- Concepts and Models in Bioinorganic Chemistry. Karls, R
- 8.- Metal Complex-DNA Interactions. Hadjiliadis, N.; Sletten, E. (Editors), Wiley, 2009.
- 9.- The Molecular and Supramolecular Chemistry of Carbohydrates. A chemical introduction to glicoscience. D. Serge. Oxford Science publications, 1997
- 10.- Introduction to Glycobiology. Taylor, M.E.; Drickamer, K. Oxford University press. 2011

STUDENT WORKLOAD

The training activities will be distributed according to the following table.

	Activity	hours	% presential
Presential classes	Lectures and conferences	14	100%
	Seminars and classroom exercises	4	100%
	Tutorials	1	100%
	Practical classes	0	100%
	Oral presentations	2	100%
	Final exam	3	100%
Non Presential	Preparation and study of problems	10	0%
	Elaboration of individual work	36	0%
	Literature searching and so on	5	0%
	TOTAL	75	

TEACHING METHODOLOGY

- Interactive classes encouraging student participation.
- Combined use of computer methods, and the blackboard.
- Use of fast and anonymous response methods in class (clickers) to evaluate the subject following-up.
- Promotion of student self-learning by proposing challenges and posing questions.
- Resolution of practical exercises (problems, tests, interpretation and information processing, evaluation of scientific publications, etc.).
- Oral presentations of previously prepared topics, including debates with their classmates and teachers.

ASSESSMENT SYSTEM

General considerations

- The evaluation process will be used to know if the student has acquired the scheduled skills and to review the teaching methodology.
- Written exam on theoretical and practical basic contents of the subject.
- Continuous evaluation associated with active participation and autonomous learning.

Evaluation weights: Minimum weighting (MiW)- Maximum weight (MaW)

Written Exam: 50%-70%

Oral presentations: 15%-40%

Other Activities: 15%-25%

Tutoring: 0%-10%

COMMENTS

CONTINGENCY PLAN

METHODOLOGY

Contingency plan for remote teaching activities:

They would be carried out synchronously / asynchronously and always according to the schedule established by the center, through the different telematic means available at the USC, preferably the Virtual Campus and Ms Teams.

Due to the nature and content of this subject, as well as the methodology used, the main difference between face-to-face teaching and remote teaching is (Scenario 1: in classroom teaching. Scenario 2: Expository classes and tutorials will be in classroom between 0% -50% of the classes, while the seminars will be in classroom between 50% -100% of the classes. Scenario 3: 100% telematic).

To carry out tutorials, as well as to maintain direct communication both between the students themselves and between them and the teacher, they can be done through the Virtual Campus forum, through Ms. Teams or by email.

EVALUATION SYSTEM

In cases of fraudulent performance of exercises or tests, the provisions of the *“Regulations for evaluating student academic performance and reviewing grades”* will apply.

The evaluation system will be exactly the same regardless of the type of teaching used (in classroom or virtual), with the only difference that the evaluation activities will be carried out, as established by the competent authorities, either in person in the classroom or remotely through the telematic means available at the USC. (Scenario 1: Final in classroom exam. Scenario 2 and 3: Final telematic exam).

FACULTY DATA

Faculty	Contact	Semester	Day	Time	Class
José Luis Mascareñas	15737	1st	Mon, Wed, Fri	17:30-19:00 h Dec18, 16-19h	Maths room (3rd floor)
José M. Martínez Costas	15733				
Javier Montenegro	15791				

IDENTIFICATION FORM

Course Data

Course number	P1251106
Subject	<i>Supramolecular chemistry</i>
Title	Chemistry at the interface with Biology and Materials Science (ChemBio&Mat) P1251V01
Course Level	Master
Credits	3.0
Module	II (Biological Chemistry)
Academic Year	2019-2020

Titulation

Title	Center	Course	Semester
ChemBio&Mat	FACULTAD de QUÍMICA/CiQUS	1	First

Subject

Title	Course Title	Course type
ChemBio&Mat	Supramolecular Chemistry	Compulsory

Coordination

Name	Department	Contact
Eugenio Vázquez	Organic Chemistry	email/Extension

SUMMARY

In the last years supramolecular chemistry has developed as one of the interdisciplinary areas that play a relevant role in different areas, such as biology, chemical biology or material sciences. From the fundamental point of view, the variety of non-covalent interactions that are able to induce interactions between different molecules will be evaluated. The formation of discrete aggregates (supermolecules) or large organizations (supramolecules) to create new properties that go beyond the molecule. In general, supramolecular processes are reversible and therefore they are dynamic and can be modulated by external inputs (media conditions, redox process, molecule signal and so on). This dynamic character allows the development of a variety of applications, including novel catalytic methods or molecular motors.

PREREQUISITES

Relation with other topics of the Master

No enrollment restrictions have been specified with other subjects of the curriculum.

Other requirements

No enrollment restrictions have been specified with other subjects of the curriculum. Broad knowledge of general organic and inorganic chemistry is required, especially in its synthetic and structural aspects.

COMPETENCES

Basic

- **CB6:** Possess and understand the knowledge that provides a basis or an opportunity for being creative and unique in the development and/or implementation of ideas, often in a research context.
- **CB7:** Students should know how to use the knowledge acquired and their problem-solving capacity in new or little-known environments within wider (or multidisciplinary) contexts related to their field of study.
- **CB9:** Students should know how to communicate their findings and the knowledge and underlying reasons underpinning them to specialised and non-specialised audiences in a clear and unambiguous way.
- **CB10:** Students should have the learning skills that allow them to carry on studying in such a way that should be mainly self-directed or autonomous.

General

- **CG1:** Know how to use the knowledge acquired for practical problem solving in the field of research and innovation, in the multidisciplinary context of biological chemistry and molecular materials.
- **CG2:** Know how to apply the scientific method and acquire skills for developing the necessary protocols for the design and critical assessment of chemical experiments.
- **CG3:** Be able to discuss and communicate ideas, in both oral and written form, to specialised and non-specialised audiences (congresses, conferences, etc.) in a clear and reasoned way.
- **CG5:** Have the skills that allow students to develop an autonomous method for studying and learning.
- **CG8:** Be able to use scientific literature and develop the judgement needed for its interpretation and use.

Transversal

- **CT1:** Develop teamwork skills: cooperation, leadership and good listening skills. Adapt to multidisciplinary teams.
- **CT2:** Draft scientific and technical reports and defend them publicly.
- **CT4:** Apply the concepts, principles, theories and models related to Biological Chemistry and Molecular Materials to new or little-known environments within multidisciplinary contexts.

- **CT5:** Appreciate the value of good quality and continuous improvement by acting rigorously, responsibly and ethically.
- **CT7:** Show critical and self-critical reasoning when seeking scientific rigour and quality. Handle IT tools and information and communication technology (ICT), as well as on-line access to databases.

Specific

- **CE1:** Know the impact of chemistry, biological chemistry and molecular materials on the industry, environment, health, agrofood and renewable energies.
- **CE11:** Be familiar with the basics of Supramolecular Chemistry, the most significant types of supramolecular entities, characterization methods, their modifications and their application to Science and Technology.
- **CE12:** Understand the weak interaction forces that control supramolecular processes and know how to apply them for obtaining new materials and biological functions.

OBJECTIVES OF TRAINING

- Understand the basic concepts on which supramolecular chemistry is based.
- Know and understand the different strategies of design and synthesis in supramolecular chemistry.
- Obtain an integral and multidisciplinary vision of the area, in the context of other branches of science.
- Obtain an overview of the experimental methods and techniques most commonly used to study supramolecular processes.
- Learn the possible applications of this field of science.

COURSE CONTENTS

1. Supramolecular Chemistry: Non covalent interactions

Introduction to the supramolecular chemistry, history and basic fundamentals. Weak interactions, strength and properties.

2. Methods for the characterization of supramolecular processes. Determination of binding constants

Evaluation of methods of characterization: AFM, STM, NMR, EM and so on. Properties and limitations. Methods for determination of association constant.

3. Molecular recognition of neutral and charged species: Design of receptors

Properties of molecular recognition. Design and properties of receptor design. Recognition of neutral molecules. Recognition of cationic and anionic components.

4. Self-assembly and supramolecular topology. Supramolecular dynamic chemistry

Self-assembling, properties and design. Kinetic and thermodynamic parameters in the formation of supramolecules. Methods for the preparation of linear, 2D and 3D structures. Design of dynamic process based on supramolecular chemistry. Covalent bonds in dynamic process and as kinetic traps. Self-organization: Gels and liquid crystal.

5. Coordination and organometallic chemistry in supramolecular chemistry

Supramolecular process based on metal coordination, new topologies. Organometallic complexes in supramolecular processes. Metal-metal interaction in supramolecular processes.

6. Applications of supramolecular processes

Transport processes. Catalysis and self-replication. Fluorescence sensors. Switchers and molecular wires. Molecular machines.

COURSE BIBLIOGRAPHY

1. Basic

- Steed, J. W.; Turner, D. R.; Wallace, K. J. *Core Concepts in Supramolecular Chemistry and Nanochemistry*. John Wiley & Sons, Ltd, **2007**. ISBN: 978-0-470-85866-0.
- Steed, J. W.; Atwood, J. A. *Supramolecular Chemistry*. 2nd Ed., John Wiley & Sons, Ltd, Chichester, **2009**. ISBN: 978-0-470-51234-0.
- Cragg, P. J. *Supramolecular Chemistry. From Biological Inspiration to Biomedical Applications*. Springer, **2010**. ISBN: 978-90-481-2581-4.
- Gale, P. A.; Steed, J. W. (Eds). *Supramolecular chemistry: from molecules to nanomaterials*. John Wiley & Sons Ltd, New York, **2012**. ISBN: 978-0-470-74640-0.

2. Complementary

- Nobuhiko Yui (Ed.). *Supramolecular Design for Biological Applications*. CRC Press, **2002**. ISBN: 0-8493-0965-4.
- Hans-Jörg Schneider (Ed.). *Supramolecular Systems in Biomedical Fields (Monographs in Supramolecular Chemistry)*. RSC Publishing. **2013**. ISBN: 978-1-84973-658-9.
- Tatsuya Nabeshima (Ed.). *Synergy in Supramolecular Chemistry*. CRC Press, **2015**. ISBN: 978-1-4665-9504-0.

STUDENT WORKLOAD

The training activities will be distributed according to the following table.

	Activity	hours	% presential
Presential classes	Lectures and conferences	14	100%
	Seminars and classroom exercises	4	100%
	Tutorials	1	100%
	Practical classes	0	100%
	Oral presentations	2	100%
	Final exam	3	100%
Non Presential	Preparation and study of problems	10	0%
	Elaboration of individual work	36	0%
	Literature searching and so on	5	0%
	TOTAL	75	

TEACHING METHODOLOGY

The Virtual Campus will be used for delivering the necessary material to the students, according to the professor criterion. This material will include: the course program, exercises and problems to be solved, copies of the classroom presentations, etc.

Along the course, the student should participate in various formative activities, with the aim of acquiring the established knowledge and skills.

Master classes: Explanation of theoretical contents supplemented by audiovisual aids. The active participation of the students will be intended, through the formulation of appropriate questions that they should try to answer.

Seminars: There will be two classroom hours before the partial exams dedicated to review concepts and/or clarify doubts.

Use of fast and anonymous response methods in class (clickers) to know the degree of follow-up of the subject.

Presentation of individual works on some topics related to the subject, including the debate with his classmates and teachers.

Group and individual tutoring.

ASSESSMENT SYSTEM

With the aim of encouraging the constant student work to favor the learning, a continuous evaluation will be applied. This methodology will inform the professor about the content's assimilation by the student as well as their ability to apply them to problem solving. The evaluation will be individual.

Along the course, on professor criterion, the students will have to solve some exercises and hand them in at the scheduled date. Performing short tests in classroom is also foreseen. (30%)

In order to evaluate the knowledge related to the master classes and the problem-solving ability of the

students, one exam and/or individual oral presentation will be performed. (70%)

The students who did not pass the continuous evaluation will have the opportunity to perform a second-chance exam. To pass the course, it will be mandatory obtaining 5 points out of 10.

COMMENTS

CONTINGENCY PLAN

METHODOLOGY

Contingency plan for remote teaching activities:

They would be carried out synchronously / asynchronously and always according to the schedule established by the center, through the different telematic means available at the USC, preferably the Virtual Campus and Ms Teams.

Due to the nature and content of this subject, as well as the methodology used, the main difference between face-to-face teaching and remote teaching is (Scenario 1: in classroom teaching. Scenario 2: Expository classes and tutorials will be in classroom between 0% -50% of the classes, while the seminars will be in classroom between 50% -100% of the classes. Scenario 3: 100% telematic).

To carry out tutorials, as well as to maintain direct communication both between the students themselves and between them and the teacher, they can be done through the Virtual Campus forum, through Ms. Teams or by email.

EVALUATION SYSTEM

In cases of fraudulent performance of exercises or tests, the provisions of the *“Regulations for evaluating student academic performance and reviewing grades”* will apply.

The evaluation system will be exactly the same regardless of the type of teaching used (in classroom or virtual), with the only difference that the evaluation activities will be carried out, as established by the competent authorities, either in person in the classroom or remotely through the telematic means available at the USC. (Scenario 1: Final in classroom exam. Scenario 2 and 3: Final telematic exam).

FACULTY DATA

Faculty	Contact	Semester	Day	Time	Class
Juan R. Granja	15746	1st	Tues/Wed/Thurs 12/11 to 17/12	Tues/Thurs 16:00/17:30	Maths (3 rd floor)
Miguel Vázquez				Wed 19:00/20:30 Dec 17, 16:00/19:00	

IDENTIFICATION FORM

Course Data

Course number	P1251201
Subject	<i>Experimental Techniques in Molecular Biology and Biomedicine</i>
Title	Chemistry at the interface with Biology and Materials Science (ChemBio&Mat) P1251V01
Course Level	Master
Credits	3.0
Module	II (Biological Chemistry)
Academic Year	2019-2020

Titulation

Title	Center	Course	Semester
ChemBio&Mat	FACULTAD de QUÍMICA/CiQUS	1	Second

Subject

Title	Course Title	Course type
ChemBio&Mat	Experimental Techniques in Molecular Biology and Biomedicine	Optional

Coordination

Name	Department	Contact
José M. Martínez Costas	Biochemistry and Molecular Biology	jose.martinez.costas@usc.es

SUMMARY

Living organisms represent not only the most complex chemical systems, but also a source of inspiration and problems to solve for chemists. In this subject, we will explore some of the most basic and useful techniques in the fields of Molecular Biology and Biomedicine, with a focus in their potential use for chemists. With an essentially applied and hands-on approach, we will learn how to manipulate and edit nucleic acids carrying your favorite gene, how to produce a protein of interest or how to grow cell lines and work with a living model organism.

PREREQUISITES

Relation with other topics of the Master

No enrollment restrictions have been specified with other subjects of the curriculum.

Other requirements

No enrollment restrictions have been specified with other subjects of the curriculum. Broad knowledge of general biology aspects is preferred.

COMPETENCES

Basic

- **CB6:** Possess and understand the knowledge that provides a basis or an opportunity for being creative and unique in the development and/or implementation of ideas, often in a research context.
- **CB7:** Students should know how to use the knowledge acquired and their problem-solving capacity in new or little known environments within wider (or multidisciplinary) contexts related to their field of study.
- **CB8:** Students should be able to integrate knowledge and deal with the complexity of making judgements from information which – being incomplete or limited – includes reflections on the social and ethical responsibilities linked to the use of their knowledge or judgements.
- **CB9:** Students should know how to communicate their findings and the knowledge and underlying reasons underpinning them to specialised and non-specialised audiences in a clear and unambiguous way.
- **CB10:** Students should have the learning skills that allow them to carry on studying in such a way that should be mainly self-directed or autonomous.

General

- **CG1:** Know how to use the knowledge acquired for practical problem solving in the field of research and innovation, in the multidisciplinary context of biological chemistry and molecular materials.
- **CG2:** Know how to apply the scientific method and acquire skills for developing the necessary protocols for the design and critical assessment of chemical experiments.
- **CG3:** Be able to discuss and communicate ideas, in both oral and written form, to specialised and non-specialised audiences (congresses, conferences, etc.) in a clear and reasoned way.
- **CG4:** Be able to understand the social and ethical responsibilities linked to the use of knowledge or judgements in research, development and innovation in the field of biological chemistry and molecular materials.
- **CG5:** Have the skills that allow students to develop an autonomous method for studying and learning.
- **CG6:** Have leadership, creativity, initiative and entrepreneurship abilities.
- **CG7:** Be capable of working in multidisciplinary teams and collaborating with other specialists, both nationally and internationally.
- **CG8:** Be able to use scientific literature and develop the judgement needed for its interpretation and use.

- **CG10:** Be able to develop the different research stages (from the conception of an idea and the literature search through to target setting, experiment design, analysis of the results and drawing conclusions).

Transversal

- **CT1:** Develop teamwork skills: cooperation, leadership and good listening skills. Adapt to multidisciplinary teams.
- **CT2:** Draft scientific and technical reports and defend them publicly.
- **CT3:** Perform day-to-day research or professional activity in an independent and efficient manner.
- **CT4:** Apply the concepts, principles, theories and models related to Biological Chemistry and Molecular Materials to new or little-known environments within multidisciplinary contexts.
- **CT5:** Appreciate the value of good quality and continuous improvement by acting rigorously, responsibly and ethically.
- **CT6:** Be capable of adapting to changes by being self-motivated when applying new and advanced technologies and other relevant developments.
- **CT7:** Show critical and self-critical reasoning when seeking scientific rigour and quality. Handle IT tools and information and communication technology (ICT), as well as on-line access to databases.

Specific

- **CE1:** Know the impact of chemistry, biological chemistry and molecular materials on the industry, environment, health, agrofood and renewable energies.
- **CE4:** Know and understand the chemical tools and analytical techniques used for biological chemistry and molecular materials.
- **CE5:** Know how to analyze and use the data obtained autonomously in complex laboratory experiments by relating them to the suitable chemical, physical or biological techniques
- **CE6:** Know the physicochemical bases of biological processes.
- **CE7:** Students should acquire knowledge on advanced techniques for the structural characterization of macromolecules, supramolecules and colloids which are relevant in the field of biological chemistry and molecular materials.
- **CE8:** Gain technical skill for carrying out the structural characterization of molecules, biomolecules, supramolecules and nanoparticles and interpreting the experimental data obtained.
- **CE9:** Use advanced instrumentation related to research on biological chemistry and molecular materials.
- **CE11:** Be familiar with the basics of biological and cellular chemistry.
- **CE12:** Understand the weak interaction forces that control supramolecular processes and know how to apply them for obtaining new materials and biological functions.
- **CE20:** Know how to plan and carry out new laboratory experiments in an autonomous and independent manner.

OBJECTIVES OF TRAINING

- Know the basic and advanced techniques in the fields of molecular biology, cell and research with laboratory animals.
- Know the possible applications of the different techniques of manipulation of the coding capacity of the cell in industry and research.
- Understand the bases of the methodology of research with animals in laboratory.
- Understand the relevance that the choice of organism may have in the research and / or production

COURSE CONTENTS

1. Useful microorganisms Molecular Biology and Biotechnology

Types of microbiological cultures. Basic microbiology techniques (2.5h, including 1h laboratory).

2. Cell culture

Types of cultures and growth media. Cell lines. Stem cells, cell cloning. 2D and 3D cultures (1.5h).

3. Genetic Engineering techniques

Molecular cloning. Manipulation and purification of nucleic acids (4.5h, including 1.5h laboratory).

4. Polymerase chain reaction (PCR)

PCR basics. Useful variations of PCR and practical applications (2.5h, including 1h laboratory).

5. Expression of recombinant proteins

Basics of protein expression. Fusion proteins. Protein expression in bacteria. Protein expression in eukaryotes. In vitro expression methods. Creation of cell lines expressing a protein of choice. (4h, including 1h laboratory)

6. Protein purification

Basic techniques for protein purification and analysis. Quality control of purified proteins. Functional assays (5h, including 2h laboratory).

7. Control of gene expression

Systems to regulate or control gene expression. Up-regulation, down-regulation and gene knock-outs. Genome edition of cultured cells. RNA interference and CRISPR (2h).

8. Animal models

Introduction to model organisms. Clonic animals. Genetically modified animals. Transgenics animals. Handling and imaging of live animals: techniques and applications (2h).

COURSE BIBLIOGRAPHY

1. Basic

- 1.- Molecular Biology of the Cell, 5th ed, B. Alberts et al., Garland Science, 2014.
- 2.- Wilson and Walker's Principles and Techniques of Biochemistry and Molecular Biology, 8th ed, A. Hofmann and S. Clokie, Cambridge University Press 2018.
- 3.- Molecular Biotechnology: Principles and Applications of Recombinant DNA, 5th ed, B.R. Glick and C.L. Patten, ASM Press 2017.

2. Complementary

- Specific scientific manuscripts will be provided for the relevant topics
- Molecular Cloning: A laboratory manual, 4th ed, M. Green and J. Sambrook, CSH Press 2012.

STUDENT WORKLOAD

The training activities will be distributed according to the following table.

	Activity	hours	% presential
Presential classes	Lectures and conferences	12	100%
	Seminars and classroom exercises	3	100%
	Tutorials	1	100%
	Practical classes	7	100%
	Oral presentations	0	0%
	Final exam	2	100%
Non Presential	Preparation and study of problems	10	0%
	Elaboration of individual work	36	0%
	Literature searching and so on	5	0%
	TOTAL	75	

TEACHING METHODOLOGY

- Interactive classes encouraging student participation.
- Combined use of computer and blackboard methods.
- Use of fast and anonymous response methods in class (clickers) to know the degree of following-up of the subject.
- Promotion of self-learning of the student by proposing challenges and posing questions.
- Resolution of practical exercises (problems, questions type test, interpretation and processing of information, evaluation of scientific publications, etc.).
- Oral presentations of previously prepared topics, including the debate with their classmates and teachers.
- Work in the laboratory: sample preparation and observation.

ASSESSMENT SYSTEM

- The evaluation process will not only serve to know if the student has acquired the programmed competences but also to review the teaching methodology.
- Written test on theoretical and practical basic contents of the subject.
- Continuous evaluation associated with active participation and autonomous learning.

Weightings between evaluation methods: minimum weighting (MiW) - maximum weighting (MaW)

Written exam: 50% -70%

Oral presentations: 10% -20%.

Lab work / activities: 15% -30%

Tutoring: 0% -10%

FACULTY DATA

Faculty	Contact	Semester	Day	Time	Class
José M. Martínez Costas jose.martinez.costas@usc.es	15733	2nd	M/T/W/T/F 25,27 Jan; 2,4,8,10,	19:00/20:30	Math (3rd floor)*
Miguel González Blanco miguel.gonzalez.blanco@usc.es	15386		12,18,22,24 Feb		

* Laboratory classes will be conducted at laboratory P3L6 in CIQUS

IDENTIFICATION FORM

Course Data

Course number	P1
Subject	Biophysic
Title	Chemistry at the interface with Biology and Materials Science (ChemBio&Mat)
Course Level	Master
Credits	3.0
Module	II (Biological Chemistry)
Academic Year	2020-2021

Titulation

Title	Center	Course	Semester
ChemBio&Mat	FACULTAD de QUÍMICA/CiQUS	1	second

Subject

Title	Course Title	Course type
ChemBio&Mat	Biophysic	Optative

Coordination

Name	Department	Contact
Francisco Rivadulla	Physical Chemistry	f.rivadulla@usc.es

SUMMARY

This subject deals with the understanding of how applies approaches and methods traditionally used in physics to study biological phenomena. Biophysics covers all scales of biological organization, from molecular to macroscopic level. Biophysical research shares significant overlap with biochemistry, molecular biology, physical chemistry, nanotechnology, bioengineering, computational biology, biomechanics, systems biology and so on.

PREREQUISITES

Relation with other topics of the Master

No enrollment restrictions have been specified with other subjects of the curriculum.

Other requirements

No enrollment restrictions have been specified with other subjects of the curriculum. Broad knowledge of general organic and inorganic chemistry is required, especially in its synthetic and structural aspects.

COMPETENCES

Basic

- **CB6:** Possess and understand the knowledge that provides a basis or an opportunity for being creative and unique in the development and/or implementation of ideas, often in a research context.
- **CB7:** Students should know how to use the knowledge acquired and their problem-solving capacity in new or little known environments within wider (or multidisciplinary) contexts related to their field of study.
- **CB8:** Students should be able to integrate knowledge and deal with the complexity of making judgements from information which – being incomplete or limited – includes reflections on the social and ethical responsibilities linked to the use of their knowledge or judgements.
- **CB9:** Students should know how to communicate their findings and the knowledge and underlying reasons underpinning them to specialised and non-specialised audiences in a clear and unambiguous way.
- **CB10:** Students should have the learning skills that allow them to carry on studying in such a way that should be mainly self-directed or autonomous.

General

- **CG2:** Know how to apply the scientific method and acquire skills for developing the necessary protocols for the design and critical assessment of chemical experiments.
- **CG3:** Be able to discuss and communicate ideas, in both oral and written form, to specialised and non-specialised audiences (congresses, conferences, etc.) in a clear and reasoned way.
- **CG5:** Have the skills that allow students to develop an autonomous method for studying and learning.
- **CG7:** Be capable of working in multidisciplinary teams and collaborating with other specialists, both nationally and internationally.
- **CG8:** Be able to use scientific literature and develop the judgement needed for its interpretation and use.
- **CG11:** Be able to adapt efficiently to future doctoral studies in multidisciplinary areas.

Transversal

- **CT1:** Develop teamwork skills: cooperation, leadership and good listening skills. Adapt to multidisciplinary teams.
- **CT2:** Draft scientific and technical reports and defend them publicly.
- **CT4:** Apply the concepts, principles, theories and models related to Biological Chemistry and Molecular Materials to new or little-known environments within multidisciplinary contexts.

- **CT7:** Show critical and self-critical reasoning when seeking scientific rigour and quality. Handle IT tools and information and communication technology (ICT), as well as on-line access to databases.

Specific

- **CE2:** Be capable of comparing experimental data and theoretical assumptions in a critical manner.
- **CE4:** Know and understand the chemical tools and analytical techniques used for biological chemistry and molecular materials.
- **CE6:** Know the physicochemical bases of biological processes.
- **CE7:** Students should acquire knowledge on advanced techniques for the structural characterization of macromolecules, supramolecules and colloids which are relevant in the field of biological chemistry and molecular materials.
- **CE8:** Gain technical skill for carrying out the structural characterization of molecules, biomolecules, supramolecules and nanoparticles and interpreting the experimental data obtained.

OBJECTIVES OF TRAINING

- Understand the physical basis of biological processes.
- Know the role of Thermodynamics in biological processes.
- Know the most usual physical techniques in the study of biological processes.
- Understand the phenomena of transport through cell membranes.
- Obtain a comprehensive and multidisciplinary vision of this area of knowledge and its relationship with other fields of Chemistry.

COURSE CONTENTS

1. Molecular structure and biological systems

Free energy, entropy, temperature and Boltzmann distribution as factors that determine the structure of macromolecules and processes of biological interest.

2. Energetic and Dynamics of Biological Systems

Self-assembling. Thermodynamics of Systems Far from Equilibrium

3. Physical factors of the environment

Friction processes in fluids: suspension and sedimentation. Viscosity and Reynolds number. Movement in biological systems. Diffusion: description of the simple solutions of the diffusion equation in biological systems and their consequences on molecular transport in cells.

4. The kinetics of biological systems

The kinetics of biological processes: enzymatic and polymerization reactions.

5. Transport in biological systems

Adsorption. The electric double layer model. Electric transport and membrane action potentials. Passive Transport of Substances Across Membranes. Channels and Carriers. Active Transport

COURSE BIBLIOGRAPHY

1. Basic

- 1.- Biophysics A Physiological Approach. Patrick F. Dillon, Cambridge Univ. Press 2012
- 2.- Fundamentals of Biophysics. Andrey B. Rubin. Scrivener Publishing. Wiley. 2014
- 3.- Biophysics: an introduction. Cotterill, R. John Wiley&sons, 2003.

2. Complementary

STUDENT WORKLOAD

The training activities will be distributed according to the following table.

	Activity	hours	% presential
Presential classes	Lectures and conferences	15	100%
	Seminars and classroom exercises	4	100%
	Tutorials	1	100%
	Practical classes	0	100%
	Oral presentations	2	100%
	Final exam	2	100%
Non Presential	Preparation and study of problems	10	0%
	Elaboration of individual work	36	0%
	Literature searching and so on	5	0%
	TOTAL	75	

TEACHING METHODOLOGY

- Interactive classes encouraging student participation.
- Combined use of computer methods, and the blackboard.
- Use of fast and anonymous response methods in class (clickers) to evaluate the subject following-up.
- Promotion of student self-learning by proposing challenges and posing questions.
- Resolution of practical exercises (problems, tests, interpretation and information processing, evaluation of scientific publications, etc.).
- Oral presentations of previously prepared topics, including debates with their classmates and teachers.

ASSESSMENT SYSTEM

General considerations

- The evaluation process will be used to know if the student has acquired the scheduled skills and to review the teaching methodology.
- Written exam on theoretical and practical basic contents of the subject.
- Continuous evaluation associated with active participation and autonomous learning.

Evaluation weights: Minimum weighting (MiW)- Maximum weight (MaW)

Written Exam: 50%-70%

Oral presentations: 25%-40%

Other Activities: 10%-40%

Tutoring: 0%-10%

FACULTY DATA

Faculty	Contact	Semester	Day	Time	Class
Fran Rivadulla	15724	2nd	Thu/Thurs Wed17m and Mo1	16-17:30h March8: 16-19h	Maths room (Third floor)

IDENTIFICATION FORM

Course Data

Course number	P1251107
Subject	Nanostructured Materials
Title	Chemistry at the interface with Biology and Materials Science (ChemBio&Mat) P1251V01
Course Level	Master
Credits	3.0
Module	Module III: Functional Materials
Academic Year	2019-2020

Titulation

Title	Center	Course	Semester
ChemBio&Mat	FACULTAD de QUÍMICA/CiQUS	1	First

Subject

Title	Course Title	Course type
ChemBio&Mat	Nanostructured Materials	Compulsory

Coordination

Name	Department	Contact
Massimo Lazzari	Physical Chemistry	massimo.lazzari@usc.es/15723

SUMMARY

The emphasis in this course is to introduce nanoscience and nanotechnology, with a special attention for nanostructured materials, their chemical and fundamental properties, as well as fabrication methodologies. Preparation and applications of nanostructured soft materials will also be discussed.

PREREQUISITES

Relation with other topics of the Master

No enrollment restrictions have been specified with other subjects of the curriculum.

Other requirements

No enrollment restrictions have been specified with other subjects of the curriculum. Broad knowledge of material science is required.

COMPETENCES

Basic

- **CB6:** Possess and understand the knowledge that provides a basis or an opportunity for being creative and unique in the development and/or implementation of ideas, often in a research context.
- **CB7:** Students should know how to use the knowledge acquired and their problem-solving capacity in new or little known environments within wider (or multidisciplinary) contexts related to their field of study.

General

- **CG1:** Know how to use the knowledge acquired for practical problem solving in the field of research and innovation, in the multidisciplinary context of biological chemistry and molecular materials.
- **CG3:** Be able to discuss and communicate ideas, in both oral and written form, to specialised and non-specialised audiences (congresses, conferences, etc.) in a clear and reasoned way.
- **CG7:** Be able of working in multidisciplinary teams and collaborating with other specialists, both nationally and internationally.
- **CG8:** Be able to use scientific literature and develop the judgement needed for its interpretation and use.

Transversal

- **CT1:** Develop teamwork skills: cooperation, leadership and good listening skills. Adapt to multidisciplinary teams.
- **CT6:** Be capable of adapting to changes by being self-motivated when applying new and advanced technologies and other relevant developments.

Specific

- **CE13:** Know the magnitudes that determine materials' properties at the nanoscale.
- **CE15:** Students should be familiarized with nanotechnology methods and usefulness for studying processes of medical and biological interest.

OBJECTIVES OF TRAINING

- a global and multidisciplinary vision of nanomaterials
- know the commercial and potential applications of nanostructured materials.

COURSE CONTENTS

1. Introduction to nanoscience and nanotechnology

2. Fundamentals of nanomaterials

Classification, size effects on optical, electrical, catalytic, magnetic and thermal properties, etc.

3. Synthesis of nanomaterials

1-D / 2-D nanomaterials and 3-D nanomaterials.

4. Self-assembly

Principles and applications.

5. Nanostructured soft materials

Biologically based nanomaterials (biopolymers, nanoscale biological assemblies, biomimetic materials), polymeric-based nanostructured materials (polymer composites and nanocomposites), (block copolymers: preparation and applications), organic/inorganic hybrid materials.

COURSE BIBLIOGRAPHY

1. Basic

- Essentials in Nanoscience and Nanotechnology, N. Kumar and S. Kumbhat, 2016 John Wiley & Sons.
- Advanced Nanomaterials, K. E. Geckeler, H. Nishide, 2010 John Wiley & Sons.
- Fundamentals, Properties, and Applications of Polymer Nanocomposites, J. H. Koo, 2016 Cambridge University Press.
- Introduction to Soft Matter: Synthetic and Biological Self-Assembling Materials. HAMLEY, I. W., Ed. John Wiley & Sons, Chichester, UK, 2007.
- Nanostructured Materials, Processing, Properties and Applications. 2nd Edition, C. C. Koch Elsevier. 2007.
- Physical Properties of Materials. M.A. White, 2n Edition, CRC Press, 2011.

2. Complementary

- Design of Nanostructures: Self-Assembly of Nanomaterials, H. B. Bohidar, K. Rawat, 2016 John Wiley & Sons.
- Nanobiomaterials, Nanostructured Materials for Biomedical Applications. 1st Edition. R. Narayan, Woodhead Publishing, 2017.

STUDENT WORKLOAD

The training activities will be distributed according to the following table.

	Activity	hours	% presential
Presential classes	Lectures and conferences	14	100%
	Seminars and classroom exercises	4	100%
	Tutorials	1	100%
	Practical classes	0	100%
	Oral presentations	2	100%
	Final exam	3	100%
Non Presential	Preparation and study of problems	10	0%
	Elaboration of individual work	36	0%
	Literature searching and so on	5	0%
	TOTAL	75	

TEACHING METHODOLOGY

Attendance to these classes is compulsory and non-attendance will have a negative effect on the summative assessment. The methodology consists in:

- Large-group lectures: teaching sessions conducted by a lecturer covering different aspects (theory, problems and/or examples, course guidelines...). The topics covered in the lectures will be based on the contents of the recommended bibliography in the syllabus of the course.
- Interactive classes (Seminars): classes in which specific topics and eventual exercises are proposed and discussed. In some of the seminars, assessment activities will be carried out. The marks obtained in these activities will be part of the student assessment.
- Tutorials: Students attend tutorials scheduled by the lecturer. This activity will involve discussion of questions or difficulties related to the course contents. This class may include assessment activities.
- Presentations by students on topics previously proposed, including discussion with fellows.

ASSESSMENT SYSTEM

Scenario 1.

1. Student assessment will have two components:

1.1. Summative assessment (50 %), consisting of:

- Seminars work (40 %)
- Presentation and Tutorial work (10 %)

1.2. Final Exam (50 %)

2. Assessment of seminars, presentation by students and tutorials will be based on the results of the different assessment activities carried out during the course.

3. The final examination consists in a series of questions aiming to assess students' knowledge and competencies.

4. The final mark will be the result of equation:

$$\text{Final mark} = \max(0.5 \times N1 + 0.5 \times N2, N2)$$

where:

N1 = Summative assessment mark

N2 = Final exam mark

Competence assessment

seminars: CB7, CG3, CG8, CT1, C13, C15

presentations and tutorials: CB6, CB7, CG3, CG7, CG8, CT1, CT7, C13

final exam: CB6, CG3, C13, C15

Scenario 2 and 3.

See the contingency plan in the Observations section.

COMMENTS

Contingency plan toward a possible change of scenario

1) Objectives: no changes

2) Contents: no changes

3) Bibliography: no changes

4) Competencies: no changes

5) Metodology:

Scenario 1

No changes

Scenario 2

Lectures will be online, maintaining the usual timetable, except in the case of unexpected occurrences that would be communicated to the students

Seminar classes and Presentations by students: part of teaching will be carried out online

If the measures adopted by the health authorities allow it, lectures will be carried out online (through Teams) and the interactive ones will be face-to-face, respecting the official hours of the sessions approved by the center.

If the limitation of capacity dictated by the health authorities does not allow all the students to attend the interactive face-to-face classes, these will be broadcast in streaming.

When scheduling the subject activity, the face-to-face assessment tests will be prioritized over the interactive classes.

The tutorials may be face-to-face or telematic and require an appointment

Scenario 3

Teaching will be online and classes will be held synchronously during official class time. Students will be notified in advance if, for unforeseen causes, some classes will be held asynchronously.

Tutorials will be face-to-face and require an appointment.

6) assessment activities

Scenario 1.

No changes.

Scenario 2 and 3.

Assessment activities that cannot be carried out in person, if they cannot be postponed, will be carried out online through institutional tools through Office 365 and Moodle. In this case, the adoption of a series of measures that require the student to have a microphone and a camera will be required until adequate evaluation software is available. Students can be called for an interview to comment or explain part or all of the test. The duration of the telematic activities will be a maximum of 1 hour for continuous assessment tests and 2 hours for the final exam.

In the case of fraudulent activity in exams or tests, the “*Normativa de evaluación do rendemento académico dos estudantes e de revisión de cualificacións*” will apply.

7) Study time and individual work: no changes

8) Recommendations for the study of the subject: no changes.

FACULTY DATA

Faculty	Contact	Semester	Day	Time	Class
Massimo Lazzari	15723	1st	Mon/Wend/Fry 16/11 to 16/12	16:00/17:30	Maths (3 rd floor)
Beatriz Pelaz	15908			Dec16, 16:00/19:00h	

IDENTIFICATION FORM

Course Data

Course number	P1251108
Subject	Molecular Materials
Title	Chemistry at the interface with Biology and Materials Science (ChemBio&Mat)
Course Level	Master
Credits	3.0
Module	III (Functional Materials)
Academic Year	2019-2020

Titulation

Title	Center	Course	Semester
ChemBio&Mat	FACULTAD de QUÍMICA/CiQUS	1	First

Subject

Title	Course Title	Course type
MolMat	Molecular Materials	Compulsory

Coordination

Name	Department	Contact
Diego Peña	Organic Chemistry	diego.pena@usc.es

SUMMARY

This course will introduce the student to the field of molecular materials with a chemical perspective and special emphasis on the structure/properties relation. Within the course we will study representative structures such as fullerenes, carbon nanotubes, graphene and 2D materials, and advanced polymers among other materials. Some of the most remarkable properties and applications of these molecular materials will be discussed during the course.

PREREQUISITES

Relation with other topics of the Master

No enrollment restrictions have been specified with other subjects of the curriculum.

Other requirements

No enrollment restrictions have been specified with other subjects of the curriculum. Broad knowledge of general organic, inorganic and physical chemistry is required.

COMPETENCES

Basic

- **CB6:** Possess and understand the knowledge that provides a basis or an opportunity for being creative and unique in the development and/or implementation of ideas, often in a research context.
- **CB7:** Students should know how to use the knowledge acquired and their problem-solving capacity in new or little known environments within wider (or multidisciplinary) contexts related to their field of study.
- **CB8:** Students should be able to integrate knowledge and deal with the complexity of making judgements from information which – being incomplete or limited – includes reflections on the social and ethical responsibilities linked to the use of their knowledge or judgements.
- **CB10:** Students should have the learning skills that allow them to carry on studying in such a way that should be mainly self-directed or autonomous.

General

- **CG1:** Know how to use the knowledge acquired for practical problem solving in the field of research and innovation, in the multidisciplinary context of biological chemistry and molecular materials.
- **CG5:** Have the skills that allow students to develop an autonomous method for studying and learning.
- **CG8:** Be able to use scientific literature and develop the judgement needed for its interpretation and use.
- **CG11:** Be able to adapt efficiently to future doctoral studies in multidisciplinary areas

Transversal

- **CT1:** Develop teamwork skills: cooperation, leadership and good listening skills. Adapt to multidisciplinary teams.
- **CT2:** Draft scientific and technical reports and defend them publicly.
- **CT3:** Perform day-to-day research or professional activity in an independent and efficient manner.
- **CT4:** Apply the concepts, principles, theories and models related to Biological Chemistry and Molecular Materials to new or little-known environments within multidisciplinary contexts.
- **CT5:** Appreciate the value of good quality and continuous improvement by acting rigorously, responsibly and ethically.
- **CT7:** Show critical and self-critical reasoning when seeking scientific rigour and quality. Handle IT tools and information and communication technology (ICT), as well as on-line access to databases.

Specific

- **CE1:** Know the impact of chemistry, biological chemistry and molecular materials on the industry, environment, health, agro-food and renewable energies.
- **CE15:** Students should be familiarized with nanotechnology methods and usefulness for studying processes of medical and biological interest.
- **CE16:** Know the most relevant catalysis processes in the field of biological chemistry and molecular materials

OBJECTIVES OF TRAINING

- Understand the basic concepts in the field of molecular materials.
- Know most representative structures in the field.
- Understand the structure/property relations in molecular materials.
- Learn about active research lines and most promising applications in the field.

COURSE CONTENTS

1. Introduction to molecular materials

Introduction to characterization techniques, fabrication of thin films and liquid crystals. Optoelectronic properties and organic semiconductors. Introduction to on-surface science.

2. Representative structures of molecular materials

Polycyclic aromatic compounds. Fullerenes and carbon nanotubes. Graphene and 2D materials. Conjugated polymers. Foldamers and helical polymers. Dendrimers. Molecular machines. Nanoparticles and atomic clusters. Porous materials.

3. Devices and applications

Field-effect transistors. Light-emitting diodes. Photovoltaic cells. Sensors.

COURSE BIBLIOGRAPHY

- Molecular Electronics: From Principles to Practice. M. C. Petty, John Wiley & Sons, 2007
- Dekker Encyclopedia of Nanoscience and Nanotechnology. J. A. Schwarz, C. I. Contescu, Karol Putyera (eds.). New York: Marcel Dekker, 2004
- Handbook of Conducting Polymers. T. A. Skotheim, J. R. Reynolds (eds), 3rd ed., Boca Raton: CRC Press, 2007.
- Carbon-Rich Compounds. M. M. Haley, R. R. Tykwinski (eds), Wiley VCH, 2006.

- Fullerenes: principles and applications. F. Langa, J.-F. Nierengarten (eds), Royal Society of Chemistry, 2008.
- Carbon Nanotubes: Synthesis, Structure, Properties and Applications. M. S. Dresselhaus, G. Dresselhaus, P. Avouris (eds), Springer-Verlag, 2001.
- Organic Optoelectronic Materials. Y. Li (ed), Springer, 2015
- Organic Photovoltaics: Materials, Device Physics, and Manufacturing Technologies. C. Brabec, U. Scherf, V. Dyakonov, (eds), 2nd ed., Weinheim: Wiley-VCH, 2014
- Organic Photovoltaics: Mechanism, Materials and Devices. S.-S. Sun, N. S. Sariciftci, (eds.) Boca Raton: Taylor & Francis, cop. 2005
- Light-Emitting Diodes. E. F. Schubert, Cambridge: Cambridge University Press, 2003
- Introduction to Liquid Crystals Chemistry and Physics. P. J. Collings, London: Taylor & Francis, 2001

STUDENT WORKLOAD

The training activities will be distributed according to the following table.

	Activity	hours	% presential
Presential classes	Lectures and conferences	14	100%
	Seminars and classroom exercises	4	100%
	Tutorials	1	100%
	Practical classes	0	100%
	Oral presentations	2	100%
	Final exam	3	100%
Non Presential	Preparation and study of problems	10	0%
	Elaboration of individual work	36	0%
	Literature searching and so on	5	0%
	TOTAL	75	

TEACHING METHODOLOGY

The Virtual Campus will be used for delivering the necessary material to the students, according to the professor criterion. This material will include: the course program, exercises and problems to be solved, copies of the classroom presentations, etc.

Along the course, the student should participate in various formative activities, with the aim of acquiring the established knowledge and skills.

Lectures: Explanation of theoretical contents supplemented by audiovisual aids. The active participation of the students will be intended, through the formulation of appropriate questions that they should try to answer.

Seminars: Dedicated to problem resolution. Encourage the self-learning through scientific articles and challenges

Tutorial: Dedicated to review concepts and/or clarify doubts.

Presentation of individual works on some topics related to the subject, including the debate with his classmates and teachers.

ASSESSMENT SYSTEM

In order to evaluate the knowledge related to the master classes and the problem-solving ability of the students, one exam and will be performed (70%).

With the aim of encouraging the constant student work to favor the learning, a continuous evaluation will be applied (30%). This may include to solve some exercises and hand them in at the scheduled date and demonstrate skills related with oral presentations of selected articles.

To pass the course, it will be mandatory obtaining 5 points out of 10.

According to the document "Guidelines for the development of safe face-to-face teaching, academic year 2020-2021", two new possible scenarios are contemplated if the teaching activities cannot be developed in the classical "normal" scenario.

The new scenarios are included in the observations section under the title of the Contingency Plan.

In cases of fraudulent conduct of exercises or tests, the provisions of the *"Regulations for assessing the academic performance of students and reviewing grades"* shall apply.

COMMENTS

CONTINGENCY PLAN

According to the document "Guidelines for the development of safe classroom teaching, academic year 2020-2021", two possible new scenarios are contemplated for the teaching methodology and the evaluation system in case it is not possible to develop the adapted normality scenario :

Scenario 2: distancing (with partial restrictions on physical presence).

- The expository teaching will be non-face-to-face and the seminars and practical laboratory and computer classroom. However, the distance measures imposed may mean that it is necessary to reduce the size of the practice groups and, therefore, the number of contact hours (up to a maximum of 50% of the practical hours of the subject) that must be complemented with non-contact activities.
- The tutorials will preferably be virtual.
- The final tests will preferably be telematic.

Scenario 3: closure of the facilities (impossibility of teaching face-to-face).

- Teaching will be completely virtual, with synchronous or asynchronous mechanisms.
- The tutorials will be exclusively virtual.
- The final tests will be exclusively telematic.

For virtual teaching, Moodle platforms will be used for the final test and continuous assessment and MS Teams for expository classes, seminars and tutorials.

FACULTY DATA

Faculty	Contact	Semester	Day	Time	Class
Diego Peña	15718	1st	Mon/Wend/Fry	16:00/17:30	Maths (3 rd floor)
Félix Freire			21/09 to 26/10	Feb26, 16:00/19:00	

IDENTIFICATION FORM

Course Data

Course number	P1251203
Subject	<i>Molecular Magnetism</i>
Title	Chemistry at the interface with Biology and Materials Science (ChemBio&Mat) P1251V01
Course Level	Master
Credits	3.0
Module	III (Functional Materials)
Academic Year	2019-2020

Titulation

Title	Center	Course	Semester
ChemBio&Mat	FACULTAD de QUÍMICA/CiQUS	1	Second

Subject

Title	Course Title	Course type
ChemBio&Mat	Molecular Magnetism	Optative

Coordination

Name	Department	Contact
Francisco Rivadulla	Physical-Chemistry	f.rivadulla@usc.es ; 15724

SUMMARY

Most magnetic materials are inorganic, mostly based on transition-metal alloys or crystalline oxides. However, in the last two decades organic and molecular materials have become also increasingly present in magnetic studies, particularly after the long-range magnetic order increased until high temperatures (particularly above liquid nitrogen). The possibility of applying synthetic chemistry techniques to form a very large variety of molecules in which transition-metal ions are used to provide the magnetic moment, and organic ligand groups mediate the interactions, open enormous possibilities to study. This strategy produced magnetic materials with a large variety of structures: chains (1D), layers (2D), and networks (3D), some of which show ordering at room temperature and high coercivity. Recently, single molecule magnets (0D), small magnetic clusters, were prepared, showing macroscopic quantum tunneling of their magnetization, which may find important applications in quantum computation.

PREREQUISITES

Relation with other topics of the Master

No enrollment restrictions have been specified with other subjects of the curriculum.

Other requirements

No enrollment restrictions have been specified with other subjects of the curriculum. Broad knowledge of general physical and inorganic chemistry is required.

COMPETENCES

Basic and General

- **CE1** To know the impact of chemistry, biological chemistry and molecular materials in the industry, the environment, health, agri-food and renewable energies.
- **CE2** To be able to critically compare the experimental data and the theoretical hypotheses.
- **CE6** To know the physicochemical bases of biological processes.

Transversal

- **CT4** To apply the concepts, principles, theories or models related to Biological Chemistry and Molecular Materials to new or little known environments, within contexts multidisciplinary.

Specific

- **CG1** To know how to apply the knowledge acquired to solve practical problems in the field of research and innovation in the multidisciplinary context of chemistry biological and molecular materials.
- **CG3** Being able to discuss and communicate their ideas, orally and in writing, to audiences specialized and non-specialized (congresses, etc.) in a clear and reasoned way.
- **CG8** Manage advanced scientific literature from primary sources and acquire the tools needed develop their critical interpretation, with the ability to establish the state of art ("state of the art") of novel thematic lines in the fields of chemistry biological and molecular materials.

OBJECTIVES OF TRAINING

The main objectives are that the student acquires the following competences:

- Acquisition of the basic knowledge necessary for the analysis of properties of the molecular-based magnets and their design.
- Knowledge of recent advances in molecular magnetism in the field of spintronics and quantum computing.

COURSE CONTENTS

1. - Definitions, units and basic concepts

Magnetization, magnetic susceptibility, experimental measurement techniques, types of magnetic behavior, Curie's law (Curie-Weiss), fundamental and Hamiltonian equations of spin.

2. Magnetism of isolated and interacting ions

Zeeman effect, spinorbit coupling, magnetic anisotropy, etc.

3. Cooperative magnetism

Types of long-range ordering (ferromagnetism, antiferromagnetism, ferrimagnetism and metamagnetism) and in unordered systems (superparamagnetism and spin glasses).

4. Molecular-based magnets

Mono molecular, ionic and chain based molecular magnets. Synthesis and basic magnetic properties.

5. Applications of molecular magnets.

Molecular spintronics and quantum computing based on molecular magnets.

COURSE BIBLIOGRAPHY

1. Basic

- Cristiano Benelli and Dante Gatteschi. Introduction to Molecular Magnetism: From Transition Metals to lanthanides. 2015 Wiley-VCH Verlag GmbH & Co. KGaA, Boschstr. 12, 69469 Weinheim, Germany.

2. Complementary

- Kahn, Olivier, Molecular magnetism. VCH Publishers, Inc. 220 East 23rd Street New York N.Y, ISBN 1-56081-566-3

STUDENT WORKLOAD

The training activities will be distributed according to the following table.

	Activity	hours	% presential
Presential classes	Lectures and conferences	12	100%
	Seminars and classroom exercises	6	100%
	Tutorials	1	100%
	Practical classes	0	100%
	Oral presentations	2	100%
	Final exam	3	100%
Non Presential	Preparation and study of problems	10	0%
	Elaboration of individual work	36	0%
	Literature searching and so on	5	0%
	TOTAL	75	

TEACHING METHODOLOGY

The Virtual Campus will be used for delivering the necessary material to the students, according to the professor criterion. This material will include: the course program, exercises and problems to be solved, copies of the classroom presentations, etc.

Along the course, the student should participate in various formative activities, with the aim of acquiring the established knowledge and skills.

Master classes: Explanation of theoretical contents supplemented by audiovisual aids. The active participation of the students will be intended, through the formulation of appropriate questions that they should try to answer.

Seminars: There will be two classroom hours before the partial exams dedicated to review concepts and/or clarify doubts.

Presentation of individual works on some topics related to the subject, including the debate with his classmates and teachers.

Group and individual tutoring.

ASSESSMENT SYSTEM

With the aim of encouraging the constant student work to favor the learning, a continuous evaluation will be applied. This methodology will inform the professor about the content's assimilation by the student as well as their ability to apply them to problem solving. The evaluation will be individual.

Along the course, on professor criterion, the students will have to solve some exercises and hand them in at the scheduled date. Performing short tests in classroom is also foreseen. (40%)

In order to evaluate the knowledge related to the master classes and the problem-solving ability of the students, one exam and/or individual oral presentation will be performed. (60%)

The students who did not pass the continuous evaluation will have the opportunity to perform a second-chance exam. To pass the course, it will be mandatory obtaining 5 points out of 10.

The continuous evaluation grade will only be obtained through "active" participation in the activities that make up said evaluation (class presentations, class problem solving, ...), in order to demonstrate that the knowledge set for each of the such activities.

The final exam will include theoretical questions and problems related to the subject included in the subject's program, regardless of whether the subject was worked in the expository, interactive or practical classes. The exam will be graded on a total of 10 points.

In cases of fraudulent performance of exercises or tests, the provisions of the *"Regulations for evaluating student academic performance and reviewing grades"* will apply.

SCENARIO 2. Distance (with partial restrictions on physical attendance)

The evaluation system does not undergo any modification with respect to what has already been indicated in the section corresponding to scenario 1. The same percentages of continuous evaluation and exam are maintained to obtain the final grade for the course.

The "active" participation in the activities that make up the continuous evaluation will depend on the attendance to the face-to-face sessions, the involvement and participation during the telematic sessions and the deliveries made through the virtual Classroom.

The final exam of the subject will be done electronically using the Virtual Classroom Questionnaires tool combined with simultaneous session in MS Teams. The contents that will be evaluated in the exam will be the same as those indicated for scenario 1.

SCENARIO 3. Closure of facilities (impossibility of teaching face-to-face)

The evaluation system does not undergo any modification with respect to what has already been indicated in the section corresponding to scenario 1. The same percentages of continuous evaluation and exam are maintained to obtain the final grade for the course.

The "active" participation in the activities that make up the continuous evaluation will depend on the involvement and participation during the telematic sessions and the deliveries made through the virtual Classroom.

The final exam of the subject will be done electronically using the Virtual Classroom Questionnaires tool combined with simultaneous session in MS Teams. The contents that will be evaluated in the exam will be the same as those indicated for scenario 1.

COMMENTS

Classes will be taught in English

FACULTY DATA

Faculty	Contact	Semester	Day	Time	Class
Francisco Rivadulla	15724	2nd	25,27 Jan; 2,4,8,10,	16:00/17:30	Maths (3 rd floor)
Maria Jiménez			12,18,22,24Feb; 1,3 Mar	Mar3, 16:00/19:00	

IDENTIFICATION FORM

Course Data

Course number	P1251204
Subject	Nanobiotechnology
Title	Chemistry at the interface with Biology and Materials Science (ChemBio&Mat) P1251V01
Course Level	Master
Credits	3.0
Module	III (Functional Materials)
Academic Year	2019-2020

Titulation

Title	Center	Course	Semester
ChemBio&Mat	FACULTAD de QUÍMICA/CiQUS	1	Second

Subject

Title	Course Title	Course type
ChemBio&Mat	Nanobiotechnology	Optional

Coordination

Name	Department	Contact
Pablo del Pino	Condensed Matter Physics	pablo.delpino@usc.es/15711

SUMMARY

Nanobiotechnology is the application of nanotechnologies in biological fields. The nanotechnologies are commonly fed by multidisciplinary, application-driven collaborations among chemists, physicists, biologists, among others. One result is the hybrid field of nanobiotechnology that uses biological starting materials, biological design principles or has biological or medical applications.

While biotechnology deals with metabolic and other physiological processes of biological subjects including microorganisms, in combination with nanotechnology, nanobiotechnology provides many useful tools in the study of life. Although the integration of nanomaterials with biology has led to the development of diagnostic devices, contrast agents, analytical tools, therapy, and drug-delivery vehicles, bionanotechnology research is still in its infancy.

PREREQUISITES

Relation with other topics of the Master

No enrollment restrictions have been specified with other subjects of the curriculum.

Other requirements

No enrollment restrictions have been specified with other subjects of the curriculum. Broad knowledge of general organic and inorganic chemistry is required, especially in its synthetic and structural aspects.

COMPETENCES

Basic

- **CB9:** Students should know how to communicate their findings and the knowledge and underlying reasons underpinning them to specialised and non-specialised audiences in a clear and unambiguous way.

General

- **CG3:** Be able to discuss and communicate ideas, in both oral and written form, to specialised and non-specialised audiences (congresses, conferences, etc.) in a clear and reasoned way.
- **CG7:** Be capable of working in multidisciplinary teams and collaborating with other specialists, both nationally and internationally

Transversal

- **CT1:** Develop teamwork skills: cooperation, leadership and good listening skills. Adapt to multidisciplinary teams.
- **CT4:** Apply the concepts, principles, theories and models related to Biological Chemistry and Molecular Materials to new or little-known environments within multidisciplinary contexts.

Specific

- **CE4:** Know and understand the chemical tools and analytical techniques used for biological chemistry and molecular materials.
- **CE6:** Know the physicochemical bases of biological processes.
- **CE12:** Know the weak interaction forces that dominate the supramolecular processes and that can apply them to obtain new materials and biological functions.
- **CE13:** Know the magnitudes that determine the properties of materials at the nanoscale.
- **CE15:** Know the methods and the utility of the nanotechnology for the study of the processes of medical and biological interest.

OBJECTIVES OF TRAINING

- Understand the basic concepts on which nanobiotechnology is based.

- Acquire and understand the different design and synthesis strategies of biofunctional nanomaterials.
- Obtain a comprehensive and multidisciplinary vision of the area, in the context of other scientific areas.
- Get an overview of the most commonly used experimental methods and techniques to study nanomaterials in the biological and medical context.
- Know the possible applications of nanobiotechnology.

COURSE CONTENTS

1. The "nano" scale in biology and medicine

Introduction to the nanobiotechnologies, history and basic fundamentals. Bio-nano-interactions, strength and properties.

2. Bio-applications of plasmonic nanoparticles in biosensing, imaging and therapy

Plasmonic nanomaterials synthesis and bio-functionalization; plasmon resonance; surface enhanced Raman spectroscopy (SERS); dark-field microscopy; photothermal effect; bionanoplasmonics.

3. Bio-applications of magnetic nanoparticles in biosensing, imaging and therapy

Superparamagnetism; monodomain magnetic nanoparticles; magnetic bionanosensing; magnetic resonance imaging; magnetic fluid hyperthermia.

4. Bio-applications of photoluminescent nanoparticles in biosensing and imaging

Bioimaging; labeling in vitro and in vivo; QDs, upconverting NPs; resonance energy transfer.

5. Bio-applications of polymeric nanostructures in biosensing, therapy and imaging

Drug delivery; nanomedicines based on polymeric scaffolds; theragnostic agents

6. Encapsulation of drugs in nanostructures

Loading efficiency and drug loading; drug leaking and stability; preserving the activity of drugs; interactions of drug and nanostructures (loading mechanisms).

7. Stimuli-controlled release of drugs

Ultrasounds; light; magnetic fields; biological environments/triggers.

8. In vitro studies: nanotoxicology, the protein corona and the interactions of nanoparticles with cells

Quantification of NP-uptake by cells and cell viability tests; unspecific absorption of proteins by NPs; correlation of NP-uptake, viability and protein corona.

9. In vivo studies: pharmacokinetics and biodistribution, vectorization and clinical applications

Active and passive targeting; cancer nanomedicines; clinical trials; current challenges for nanomedicine translation.

COURSE BIBLIOGRAPHY

1. Basic

- Nanobiotechnology: Concepts, Applications and Perspectives (2004); Edited by Christof M. Niemeyer & Chad A. Mirkin; ISBN: 978-3-527-30658-9

2. Complementary

- State of the art literature will be provided.

STUDENT WORKLOAD

The training activities will be distributed according to the following table.

	Activity	hours	% presential
Presential classes	Lectures and conferences	14	100%
	Seminars and classroom exercises	4	100%
	Tutorials	1	100%
	Practical classes	0	100%
	Oral presentations	2	100%
	Final exam	3	100%
Non Presential	Preparation and study of problems	10	0%
	Elaboration of individual work	36	0%
	Literature searching and so on	5	0%
	TOTAL	75	

TEACHING METHODOLOGY

The Virtual Campus will be used for delivering the necessary material to the students, according to the professor criterion. This material will include: the course program, exercises and problems to be solved, copies of the classroom presentations, etc.

Along the course, the student should participate in various formative activities, with the aim of acquiring the established knowledge and skills.

Master classes: Explanation of theoretical contents supplemented by audiovisual aids. The active participation of the students will be intended, through the formulation of appropriate questions that they should try to answer.

Seminars: There will be two hours of class before the partial exams dedicated to review concepts and/or clarify doubts.

Use of fast and anonymous response methods in class (clickers) to know the degree of follow-up of the subject.

Presentation of individual works on some topics related to the subject, including the debate with classmates and professor.

Group and individual tutoring.

ASSESSMENT SYSTEM

With the aim of encouraging the constant student work to favor the learning, a continuous evaluation will be applied. This methodology will inform the professor about the content's assimilation by the student as well as their ability to apply them to problem solving. The evaluation will be individual.

Along the course, on professor criterion, the students will have to solve some exercises and hand them in at the scheduled date. Performing short tests in classroom is also foreseen. (30%)

In order to evaluate the knowledge related to the master classes and the problem-solving ability of the students, one exam and/or individual oral presentation will be performed. (70%)

The students who did not pass the continuous evaluation will have the opportunity to perform a second-chance exam. To pass the course, it will be mandatory obtaining 5 points out of 10.

COMMENTS

Revise basic biochemistry and physics concepts

CONTINGENCY PLAN

Scenery 1: adapted normality (no restrictions to physical attendance).

Lectures and interactive lessons will be given under physical attendance modality. Exceptionally, on-line attendance will be implemented up to a 10% of the subject hours. For laboratory classes, this maximum limit might reach 25%.

Tutorships might be partially given on-line.

Final exams will be under physical attendance modality.

Scenery 2: social distancing (partial restrictions to physical attendance).

Lectures might be given totally on-line (when social distancing not possible at classroom) or combined with 50% physical attendance when social distancing is possible. As for interactive lessons (seminars and laboratories), physical and on-line attendance might combine up to a 50% on-line, if required.

Tutorships will preferentially be on-line.

Final exams will preferentially be on-line.

Scenery 3: closed facilities (no physical attendance).

All classes will be on-line, either under synchronous or asynchronous formats.

Tutorships will exclusively be on-line.

Final exams will exclusively be on-line.

For the three sceneries, on-line classes will be given with MS Teams and Moodle.

In case of exercises or test realized by dishonest means, the "Evaluation rules of students' academic performance and qualifications" will be of application.

FACULTY DATA

Faculty	Contact	Semester	Day	Time	Class
Pablo del Pino	15746	2nd		17:30/19:00	Math (3 rd Floor)
Eduardo Fernández-Megía	15727			March8: 16:00/19:30	

IDENTIFICATION FORM

Course Data

Course number	P1251106
Subject	Catalysis
Title	Chemistry at the interface with Biology and Materials Science (ChemBio&Mat) P1251V01
Course Level	Master
Credits	3.0
Module	Module IV: Reactivity and Synthesis
Academic Year	2019-2020

Titulation

Title	Center	Course	Semester
ChemBio&Mat	FACULTAD de QUÍMICA/CiQUS	1	First

Subject

Title	Course Title	Course type
ChemBio&Mat	Catalysis	Compulsory

Coordination

Name	Department	Contact
Moisés Gulías	Organic Chemistry	moises.gulias@usc.es

SUMMARY

A large majority of the industrial chemicals are made through catalytic processes. The presence of a catalyst offers an alternative, and more energetically favorable mechanism to the non-catalytic reactions and enables to carry out many reactions under milder conditions. They are also in connection with the principles of atom economy and green chemistry. Remarkably catalyst design allows to improve the control over chemo- regio- and stereoselectivity of the processes.

Catalysts come in a multitude of forms, varying from small organic molecules or organometallic complexes to large structures such as zeolites or enzymes. They also operate under a different variety of mechanisms. In this course a review the main types of catalytic transformations and the main principles behind these transformations.

PREREQUISITES

Relation with other topics of the Master

No enrollment restrictions have been specified with other subjects of the curriculum.

Other requirements

No enrollment restrictions have been specified with other subjects of the curriculum. Broad knowledge of general organic and inorganic chemistry is required, especially in its synthetic and structural aspects.

COMPETENCES

Basic

- **CB6:** Possess and understand the knowledge that provides a basis or an opportunity for being creative and unique in the development and/or implementation of ideas, often in a research context.
- **CB7:** Students should know how to use the knowledge acquired and their problem-solving capacity in new or little known environments within wider (or multidisciplinary) contexts related to their field of study.
- **CB9:** Students should know how to communicate their findings and the knowledge and underlying reasons underpinning them to specialized and non-specialized audiences in a clear and unambiguous way.
- **CB10:** Students should have the learning skills that allow them to carry on studying in such a way that should be mainly self-directed or autonomous.

General

- **CG1:** Know how to use the knowledge acquired for practical problem solving in the field of research and innovation, in the multidisciplinary context of biological chemistry and molecular materials.
- **CG3:** Be able to discuss and communicate ideas, in both oral and written form, to specialized and non-specialized audiences (congresses, conferences, etc.) in a clear and reasoned way.
- **CG4:** Be able to understand the social and ethical responsibilities linked to the use of knowledge or judgements in research, development and innovation in the field of biological chemistry and molecular materials.
- **CG6:** Have leadership, creativity, initiative and entrepreneurship abilities
- **CG8:** Be able to use scientific literature and develop the judgement needed for its interpretation and use.
- **CG9:** Be capable of handling chemical substances safely and work in a chemical laboratory without risks.

Transversal

- **CT1:** Develop teamwork skills: cooperation, leadership and good listening skills. Adapt to multidisciplinary teams.
- **CT3:** Perform day-to-day research or professional activity in an independent and efficient manner

- **CT4:** Apply the concepts, principles, theories and models related to Biological Chemistry and Molecular Materials to new or little-known environments within multidisciplinary contexts.
- **CT6:** Be capable of adapting to changes by being self-motivated when applying new and advanced technologies and other relevant developments.
- **CT7:** Show critical and self-critical reasoning when seeking scientific rigour and quality. Handle IT tools and information and communication technology (ICT), as well as on-line access to databases.

Specific

- **CE1:** Know the impact of chemistry, biological chemistry and molecular materials on the industry, environment, health, agrofood and renewable energies.
- **CE3:** Know the rules on risk prevention in the laboratory and within the chemistry-related industry.
- **CE5:** Know how to analyze and use the data obtained autonomously in complex laboratory experiments by relating them to the suitable chemical, physical or biological techniques.
- **CE16:** Know the most relevant catalysis processes in the field of biological chemistry and molecular materials.
- **CE17:** Be able to establish relationships between structure and reactivity.
- **CE19:** Know how to carry out, submit and defend individually, and once all curriculum credits are obtained, a comprehensive research project on Biological Chemistry and Molecular Materials which synthesizes the skills learnt in the Masters course.
- **CE20:** Know how to plan and carry out new laboratory experiments in an autonomous and independent manner.

OBJECTIVES OF TRAINING

- Understand the importance of catalysis and its general principles.
- Know and understand the different types of catalysis, included metallic-, organo-, bio- and surface catalysis; and the main characteristics and mechanisms they are based on.
- Obtain an overview of how to apply catalysis for the synthesis of organic molecules
- Learn the advanced applications of this field of science in chemical industry and drug discovery.

COURSE CONTENTS

1. Catalysis, types and physical and chemical principles related to the kinetics of the catalytic reactions

Catalysis, definition, types. Catalysis and *Green Chemistry*. The chemical Industry. Kinetics. The rate Equation and power rate laws. Reactions of different orders. Temperature dependence of the rate.

2. Principles and fundamentals of the heterogeneous catalysis

Introduction to the principles of the heterogeneous catalysis. Description of the main types of heterogeneous catalysts. Introductory review of most important heterogeneous catalytic reactions and processes.

3. Homogeneous catalysis. Catalysis with organometallic complexes

Introduction to the factors which influence the homogenous organometallic catalysis. Main mechanistic steps in organometallic reactions. Cross-coupling reactions: Suzuki, Negishi, Kumada, etc.. Reactions of η^3 -allyl complexes. Reactions of metal-carbene complexes. Reactions of η^2 -alkyne and alkene complexes. C-H functionalization reactions.

4. Homogeneous catalysis. Catalysis with organic molecules (organocatalysis) chemistry

Asymmetric Synthesis. Relevance and different approaches.

Asymmetric Organocatalysis: definition, historical perspective.

Modes of activation: Non-covalent and covalent organocatalysis; C-C and C-heteroatom bond forming reactions

Dual and / or cooperative catalysis: Organo + Photoredox catalysis, Organo + transition metal catalysis

5. Principles and fundamentals of the biocatalysis

Introduction. Enzymes, classification (oxidoreductases, lyases, isomerases, ...). Most relevant applications and case studies

6. Relevant synthetic applications of the catalytic processes.

Applications of synthetic catalytic processes in fine chemical industry and drug discovery. Case studies

COURSE BIBLIOGRAPHY

1. Basic

- *Catalysis: An Integrated Textbook for Students*, Ulf Hanefeld (Ed), Leon Lefferts (Ed), Wiley: 2018.

2. Complementary

- *Concepts of Modern Catalysis and Kinetics*, I. Chorkendorff (Ed), J. W. Niemantsverdriet (Ed). John Wiley & Sons, **2003**

- *Homogeneous Catalysts: Activity - Stability "C Deactivation*; John C. Chadwick (Ed), Piet W. N. M. van Leeuwen (Ed), Wiley-VCH, **2011**
- *Homogeneous Catalysis for Unreactive Bond Activation*, Zhang©\Jie Shi (Ed), Wiley-VCH, **2014**
- *Bridging Heterogeneous and Homogeneous Catalysis: Concepts, Strategies, and Applications*, Li Can Liu Yan (Ed), Wiley-VCH, 2014
- *Enantioselective Organocatalysis: Reactions and Experimental Procedures*, P. I. Dalko, Ed., Wiley-VCH: Weinheim, **2007**
- *Stereoselective Organocatalysis, Bond Formation Methodologies and Activation Modes*, Rios, R. (Ed.), Wiley-VCH, **2013**
- *Applications of Transition Metal Catalysis in Drug Discovery and Development: An Industrial Perspective*, M. L. Crawley (ED.), B. M. Trost (Ed.) John Wiley and Sons, **2012**
- *Organometallics as Catalysts in the Fine Chemical Industry*, Beller, M., Blaser, H.-U. (Eds.) Topics in Organometallic Chemistry, Springer-Verlag Berlin, **2012**

STUDENT WORKLOAD

The training activities will be distributed according to the following table.

	Activity	hours	% presential
Presential classes	Lectures and conferences	14	100%
	Seminars and classroom exercises	4	100%
	Tutorials	1	100%
	Practical classes	0	100%
	Oral presentations	2	100%
	Final exam	3	100%
Non Presential	Preparation and study of problems	10	0%
	Elaboration of individual work	36	0%
	Literature searching and so on	5	0%
	TOTAL	75	

TEACHING METHODOLOGY

The Virtual Campus will be used for delivering the necessary material to the students, according to the professor criterion. This material will include: the course program, exercises and problems to be solved, copies of the classroom presentations, etc.

Along the course, the student should participate in various formative activities, with the aim of acquiring the established knowledge and skills.

Master classes: Explanation of theoretical contents supplemented by audiovisual aids. The active participation of the students will be intended, through the formulation of appropriate questions that they should try to answer.

Seminars: There will be two classroom hours before the partial exams dedicated to review concepts and/or clarify doubts.

Use of fast and anonymous response methods in class (clickers) to know the degree of follow-up of the subject.

Presentation of individual works on some topics related to the subject, including the debate with his classmates and teachers.

Group and individual tutoring.

ASSESSMENT SYSTEM

With the aim of encouraging the constant student work to favor the learning, a continuous evaluation will be applied. This methodology will inform the professor about the content's assimilation by the student as well as their ability to apply them to problem solving. The evaluation will be individual.

In order to evaluate the knowledge related to the master classes and the problem-solving ability of the students, one exam and/or individual oral presentation will be performed. [60 % of the final mark]. Evaluated competences: CG1, CB6, CT3, CE1, CE3, CE5, CE16, CE17, CE19 and CE20]

Individual oral presentation will be performed. [25 % of the final mark]. Evaluated competences: CG2, CG3, CG6, CB9, CT1 and CE1]

Along the course, on professor criterion, the students will have to solve some exercises and hand them in at the scheduled date. Performing short tests in classroom is also foreseen. [15 % of the final mark]. Evaluated competences: CG2, CG5, CB10, CB7, CT1, CT3, CT4, CT6 and CT7

"In cases of fraudulent performance of exercises or tests, the provisions of the "Regulations for evaluating the academic performance of students and reviewing grades" will apply.

The evaluation system will be exactly the same regardless of the type of teaching used (in classroom or virtual), with the only difference that the evaluation activities will be carried out, as established by the competent authorities, either in the classroom or remotely through the telematic means available at the USC.

COMMENTS

Contingency plan for remote teaching activities in the event that in classroom presentations are suspended:

They would be carried out synchronously / asynchronously and always according to the schedule established by the center, through the different telematic means available at the USC, preferably the Virtual Campus and Ms Teams.

To carry out tutorials, as well as to maintain direct communication both between the students themselves and between them and the teacher, they can be done through the Virtual Campus forum, through Ms. Teams or by email.

"In cases of fraudulent performance of exercises or tests, the provisions of the" Regulations for evaluating the academic performance of students and reviewing grades "will apply.

The evaluation system will be exactly the same regardless of the type of teaching used (face-to-face or virtual), with the only difference that the evaluation activities will be carried out, as established by the

competent authorities, either face-to-face in the classroom or remotely through the telematic means available at the USC.

FACULTY DATA

Faculty	Contact	Semester	Day	Time	Class
Moisés Gulías Costa	15790	1st	Mon/Wend/Fry 21/09 to 23/10	17:30/19:00	Maths (3rd floor)
Fernando J. López García	15781			Oct23 16h- 19h	

IDENTIFICATION FORM

Course Data

Course number	P1251110
Subject	Chemical Synthesis
Title	Chemistry at the interface with Biology and Materials Science (ChemBio&Mat) P1251V01
Course Level	Master
Credits	3.0
Module	IV (Reactivity and Synthesis)
Academic Year	2019-2020

Titulation

Title	Center	Course	Semester
ChemBio&Mat	FACULTAD de QUÍMICA/CiQUS	1	First

Subject

Title	Course Title	Course type
ChemBio&Mat	Chemical Synthesis	Compulsory

Coordination

Name	Department	Contact
F. Javier Sardina	Organic Chemistry	javier.sardina@usc.es/15715

SUMMARY

The synthesis of new molecules and materials is the most fundamental tool to achieve any significant progress in the Chemical Sciences, whether basic or applied. New molecules and materials are needed to create new functions and properties in fields ranging from Biology and Medicine to Electronics and Photonics. Understanding and learning to use the strategies, tactics and basic tools for devising synthesis of new molecules and materials, or improved synthesis of existing interesting molecules and materials, are the central objectives of this course.

In their first part of the course, we shall survey the basic and classical concepts involved in synthesis planning, such as retrosynthetic analysis, focused on the preparation of a single organic compound (Target Oriented Synthesis), as well as more recently developed methodologies to achieve the synthesis of a focused library of organic compounds (Diversity Oriented Synthesis). We shall also deal with more specific synthetic themes, such as the asymmetric synthesis of chiral molecules.

The second part of the course will deal with the intricacies and tools required for the synthesis of organometallic compounds and of molecular frameworks (MOFs and COFs).

PREREQUISITES

Relation with other topics of the Master

No enrollment restrictions have been specified with other subjects of the curriculum.

Other requirements

No enrollment restrictions have been specified with other subjects of the curriculum. Broad knowledge of general organic and inorganic chemistry is required, especially in its synthetic and structural aspects.

COMPETENCES

Basic

- **CB6:** Possess and understand the knowledge that provides a basis or an opportunity for being creative and unique in the development and/or implementation of ideas, often in a research context.
- **CB7:** Students should know how to use the knowledge acquired and their problem-solving capacity in new or little known environments within wider (or multidisciplinary) contexts related to their field of study.
- **CB8:** That students are able to integrate knowledge and face the complexity of making judgments based on information that, being incomplete or limited, includes reflections on social and ethical responsibilities linked to the application of their knowledge and judgments
- **CB9:** Students should know how to communicate their findings and the knowledge and underlying reasons underpinning them to specialised and non-specialised audiences in a clear and unambiguous way.
- **CB10:** Students should have the learning skills that allow them to carry on studying in such a way that should be mainly self-directed or autonomous.

General

- **CG2:** Know how to apply the scientific method and acquire skills for developing the necessary protocols for the design and critical assessment of chemical experiments.
- **CG3:** Be able to discuss and communicate ideas, in both oral and written form, to specialised and non-specialised audiences (congresses, conferences, etc.) in a clear and reasoned way.
- **CG5:** Have the skills that allow students to develop an autonomous method for studying and learning.
- **CG6:** To have the ability for leadership, creativity, initiative and entrepreneurial spirit.
- **CG7:** To be able to work as part of multidisciplinary teams and collaborate with other professionals, both nationally and internationally.
- **CG8:** To be able to use scientific literature and develop the judgement needed for its interpretation and use.

- **CG10:** To be able to develop the different stages involved in a research (from conceiving an idea and doing a bibliographical search to the approach of the objectives, the design of the experiment, the analysis of the results and the deduction of the corresponding conclusions).
- **CG11:** To be able to adapt efficiently to future doctoral studies in multidisciplinary

Transversal

- **CT2:** Draft scientific and technical reports and defend them publicly.
- **CT3:** To work autonomously and efficiently in the daily practice of research or professional activity.
- **CT4:** Apply the concepts, principles, theories and models related to Biological Chemistry and Molecular Materials to new or little-known environments within multidisciplinary contexts.
- **CT5:** Appreciate the value of good quality and continuous improvement by acting rigorously, responsibly and ethically.
- **CT6:** To be able to adapt to changes, being able to apply with initiative new and advanced technologies and other relevant developments.
- **CT7:** Show critical and self-critical reasoning when seeking scientific rigour and quality. Handle IT tools and information and communication technology (ICT), as well as on-line access to databases.

Specific

- **CE20:** To understand the necessity and importance of chemical synthesis.
- **CE21:** To know the most relevant chemical synthesis methods, including the fundamentals of stereoselective processes in chemistry, and be able to design synthetic routes of complex molecules.

OBJECTIVES OF TRAINING

- To provide a solid, balanced and current training in chemical synthesis and in the theoretical tools that facilitate its success.
- Simultaneous and complementary learning of the most common synthetic strategies and tactics to provide students with a comprehensive and current view of this fundamental area of chemistry.
- To provide an overview of the methods of synthesis of individual molecules, libraries of organic molecules, organometallic complexes and inorganic compounds.
- To analyze the available methodologies for performing asymmetric synthesis.
- To deepen the synthetic methodology used in the preparation of complex organic, inorganic and organometallic compounds.
- To develop skills that allow the future professional application of the knowledge provided.

COURSE CONTENTS

1. Overview of the course

- Synthesis of organic substances:
 - Target-Oriented synthesis (TOS)
 - Diversity-Oriented synthesis (DOS)
- Synthesis of organometallic complexes
- Synthesis of materials (MOF's and COF's)

2. Basic tools for the synthesis of organic compounds

- Structure(s)
- Reactions
- Retrosynthetic analysis

3. Strategy

- Target-Oriented synthesis
 - Transform-based strategies
 - Structure-based and topological strategies
 - Functional group-based strategies
 - Stereochemical strategies
 - Computer-Assisted Synthetic Planning: Human vs. Machine or Human + Machine?
- Diversity-Oriented synthesis
 - Multicomponent reactions
 - Cycloaddition reactions
 - Tandem reactions
 - Functional group pairing strategies
 - Privileged structures
 - Ring-closing metathesis

4. Asymmetric synthesis

- Chiral pool
- Chiral auxiliaries
- Chiral catalysis

5. Synthesis of organometallic complexes

- Necessity for the synthesis of organometallic complexes: preparation of metal catalysts and study of reaction mechanisms

- Metal-X complexes
 - Hydrocarbyl (alkyl, aryl, vinyl) complexes
 - π -allyl complexes
 - Metal-hydride complexes
 - Metal-porphyrin, amido and alkoxo complexes
 - Metal-boryl complexes
- Metal-carbene complexes
 - Types
 - Reactivity: metathesis
- Metal imido and metal-oxo complexes: synthesis and applications (e.g. dioxygen and dinitrogen activation in biological systems; metalloenzymes)

6. Synthesis of MOF's and COF's

- Definition and concept of MOF's and COF's
- Synthetic strategies:
 - Metal geometry
 - Linkers
 - Design and control over pore size and functionality
- Applications

COURSE BIBLIOGRAPHY

1. Basic

- R. E. Gawley, J. Aubé, Principles of Asymmetric Synthesis, 2nd Ed., Elsevier: Oxford, 2012.
- Asymmetric Synthesis, The Essentials, M. Christmann and S. Bräse, Eds. Wiley-VCH: Weinheim, 2007.
- J. Clayden, N. Greeves, S. Warren, Organic Chemistry, 2nd Ed., Oxford University Press: Oxford, 2012.
- S. G. Warren, P. Wyatt, Organic Synthesis: The Disconnection Approach, 2nd. Ed., Wiley, 2009.
- P. Wyatt, S. Warren, Organic Synthesis: Strategy and Control, Wiley, 2007.
- E. J. Corey, X.-M. Cheng, The Logic of Chemical Synthesis, Wiley, 1989.
- A. Trabocchi, Ed., Diversity-Oriented Synthesis, Basics and Applications in Organic Synthesis, Drug Discovery and Chemical Biology, Wiley 2013.
- Hartwig, J. F. *Organotransition Metal Chemistry: From Bonding to Catalysis*, 1st Ed.; University Science Books. Sausalito, USA 2010.

2. Complementary

- *Enantioselective Organocatalysis: Reactions and Experimental Procedures*, P. I. Dalko, Ed., Wiley-VCH: Weinheim, 2007.
- *Stereoselective Organocatalysis: Bond Formation Methodologies and Activation Modes*, R. Rios Torres, Ed., John Wiley and Sons: New Jersey, 2013.
- *Organic Synthesis Workbook*, J. A. Gewert, J. Görlitzer, S. Götze, J. Looft, P. Menningen, T. Nöbel, H. Schirock, C. Wulff, Wiley- VCH: Weinheim, 2000.
- *Organic Synthesis Workbook II*, C. Bittner, A. S. Busemann, U. Griesbach, F. Hauernert, W.-R. Krahnert, A. Modi, J. Olschimke, P. L. Steck, Wiley-VCH: Weinheim, 2001.

STUDENT WORKLOAD

The training activities will be distributed according to the following table.

	Activity	hours	% presential
Presential classes	Lectures and conferences	14	100%
	Seminars and classroom exercises	4	100%
	Tutorials	1	100%
	Practical classes	0	100%
	Oral presentations	2	100%
	Final exam	3	100%
Non Presential	Preparation and study of problems	10	0%
	Elaboration of individual work	36	0%
	Literature searching and so on	5	0%
	TOTAL	75	

TEACHING METHODOLOGY

The Virtual Campus will be used for delivering the necessary material to the students, according to the professor criterion. This material will include: the course program, exercises and problems to be solved, copies of the classroom presentations, etc.

Along the course, the student should participate in various formative activities, with the aim of acquiring the established knowledge and skills.

Master classes: Explanation of theoretical contents supplemented by audiovisual aids. The active participation of the students will be intended, through the formulation of appropriate questions that they should try to answer.

Seminars: There will be two classroom hours before the partial exams dedicated to review concepts and/or clarify doubts.

Use of fast and anonymous response methods in class (clickers) to know the degree of follow-up of the subject.

Presentation of individual works on some topics related to the subject, including the debate with his classmates and teachers.

Group and individual tutoring.

ASSESSMENT SYSTEM

With the aim of encouraging the constant student work to favor the learning, a continuous evaluation will be applied. This methodology will inform the professor about the content's assimilation by the student as well as their ability to apply them to problem solving. The evaluation will be individual.

Along the course, on professor criterion, the students will have to solve some exercises and hand them in at the scheduled date. Performing short tests in classroom is also foreseen. (30%)

In order to evaluate the knowledge related to the master classes and the problem-solving ability of the students, one exam and/or individual oral presentation will be performed. (70%)

The students who did not pass the continuous evaluation will have the opportunity to perform a second-chance exam. To pass the course, it will be mandatory obtaining 5 points out of 10.

For the case of scenarios 2 or 3, see the observations section.

COMMENTS

CONTINGENCY PLAN

Scenario 2: Distance

Teaching methodology:

The teaching of the exhibition can be carried out in its totality by telematic means, or combined with the face-to-face mode, in those teaching spaces where distance is possible. In the interactive teaching of seminars, physical and telematic attendance may be combined, up to a maximum of 50% of the hours of the subject in telematic mode, when distance requires it.

Tutorials will be preferably telematic.

Evaluation system:

The evaluation of this subject will be done through continuous assessment and a final exam.

The submissions for continuous evaluation may be in person or virtually.

The final tests will preferably be telematic in nature.

The continuous evaluation will have a weight of 25% in the qualification of the subject. The final exam will cover all the contents of the subject and will have a weight of 75%.

The student's grade will not be lower than that of the final exam or that obtained by weighting with the continuous assessment.

Scenario 3: Closing down the facility

Teaching methodology:

All teaching (lectures, seminars and tutorials) will be completely virtual, using the Moodle and MS Teams platforms.

Evaluation system:

The evaluation of this subject will be done through continuous assessment and a final exam.

The submissions for continuous evaluation will be exclusively virtual.

The final tests will be exclusively of a telematic nature.

The continuous evaluation will have a weight of 25% in the qualification of the subject. The final exam will cover all the contents of the subject and will have a weight of 75%.

The student's grade will not be lower than that of the final exam or that obtained by weighting with the continuous assessment.

In the case of fraudulent exercises or tests, the provisions of the "Regulations for the assessment of students' academic performance and the revision of qualifications" shall apply.

FACULTY DATA

Faculty	Contact	Semester	Day	Time	Class
F. Javier Sardina López	15715	1 st and	Thue/Thurs	17:30-19:00	Maths (3 rd floor)
Martín Fañanás Mastral	15787	2 nd	12/11 to 28/01 1,3,5 Feb	Feb 5, 16:00/19:00	

IDENTIFICATION FORM

Course Data

Course number	P1251205
Subject	Determination with Reaction Mechanisms
Title	Chemistry at the interface with Biology and Materials Science (ChemBio&Mat) P1251V01
Course Level	Master
Credits	3.0
Module	IV (Reactivity and Synthesis)
Academic Year	2019-2020

Titulation

Title	Center	Course	Semester
ChemBio&Mat	FACULTAD de QUÍMICA/CiQUS	1	Second

Subject

Title	Course Title	Course type
ChemBio&Mat	Determination with Reaction Mechanisms	Optative

Coordination

Name	Department	Contact
Jesús Ángel Varela Carrete	Organic Chemistry	jesus.varela@usc.es

SUMMARY

The aim of this course is the study of reactions from the point of view of their mechanism and the relationship between structure and reactivity. For this purpose, the determination of the products of the reaction is just the starting point of any mechanistic investigation, being necessary to know everything which happens between reactants and products. This include not only the formation of intermediates and transition structures, the mapping out of reaction trajectories and the free energy changes that occur along the reaction path, but also our attempts at understanding why a reaction “choose” a particular mechanism.

PREREQUISITES

Relation with other topics of the Master

No enrollment restrictions have been specified with other subjects of the curriculum. The topics of this course are very related with the other subjects of the module IV (reactivity and synthesis): catalysis, chemical synthesis and computational chemistry.

Other requirements

No enrollment restrictions have been specified with other subjects of the curriculum. Broad knowledge of general organic and inorganic chemistry is required, especially in its synthetic and structural aspects.

COMPETENCES

Basic

- **CB6:** Possess and understand the knowledge that provides a basis or an opportunity for being creative and unique in the development and/or implementation of ideas, often in a research context.
- **CB7:** Students should know how to use the knowledge acquired and their problem-solving capacity in new or little known environments within wider (or multidisciplinary) contexts related to their field of study.

General

- **CG1:** Know how to use the knowledge acquired for practical problem solving in the field of research and innovation, in the multidisciplinary context of biological chemistry and molecular materials.
- **CG2:** Know how to apply the scientific method and acquire skills for developing the necessary protocols for the design and critical assessment of chemical experiments.
- **CG3:** Be able to discuss and communicate ideas, in both oral and written form, to specialised and non-specialised audiences (congresses, conferences, etc.) in a clear and reasoned way.
- **CG5:** Have the skills that allow students to develop an autonomous method for studying and learning.
- **CG8:** Be able to use scientific literature and develop the judgement needed for its interpretation and use.

Transversal

- **CT2:** Draft scientific and technical reports and defend them publicly.
- **CT5:** Appreciate the value of good quality and continuous improvement by acting rigorously, responsibly and ethically.
- **CT7:** Show critical and self-critical reasoning when seeking scientific rigour and quality. Handle IT tools and information and communication technology (ICT), as well as on-line access to databases.

Specific

- **CE2:** Be capable of comparing experimental data and theoretical assumptions in a critical manner.
- **CE17:** Be able to establish relationships between structure and reactivity

OBJECTIVES OF TRAINING

- Know the main reaction mechanisms, the effects of the different experimental variables, as well as the methods used for their study.
- Ability to understand and evaluate mechanistic investigations described in the chemical bibliography.
- Ability to design experiments that allow to elucidate the mechanism of a determined chemical reaction.

COURSE CONTENTS

1. Basic kinetic concepts and their application to the study of reaction mechanisms

Introduction to the basic kinetic concepts, reaction orders, experimental methods for investigating kinetics.

2. The use of isotopes in the determination of reaction mechanisms

Non kinetic uses. Kinetic isotopic effects. Solvent kinetic effect.

3. Free energy linear relationships

Electronic properties of the substituents. Steric properties of the substituents. Solvents properties. Nucleophilicity and electrophilicity.

4. Introduction to the computational study of reaction mechanisms.

Computational methods. Potential energy surfaces (PES).

5. Study of the mechanisms of chemical reactions through the bibliographic analysis of mechanistic investigations and the resolution of exercises.

Case studies using the acquired knowledge.

COURSE BIBLIOGRAPHY

1. Basic

- E. V. Anslyn, D. A. Dougherty, Modern Physical Organic Chemistry, University Science: Sausalito, 2006

2. Complementary

- H. Maskill Ed., *The Investigation of Organic Reactions and Their Mechanisms*, Blackwell Publishing, Oxford, 2006.
- T. H. Lowry, K. S. Richardson, *Mechanism and Theory in Organic Chemistry*, 3a edición. Harper and Row, New York, 1987.

STUDENT WORKLOAD

The training activities will be distributed according to the following calendar.

	Activity	hours	% presential
Presential classes	Theoretical classe	6	100%
	Seminars and classroom exercises	10	100%
	Tutorials	1	100%
	Computer practical classes	2	100%
	Oral presentations	2	100%
	Final exam	3	100%
Non Presential	Preparation and study of problems	10	0%
	Elaboration of individual work	36	0%
	Literature searching and so on	5	0%
	TOTAL	75	

TEACHING METHODOLOGY

The Virtual Campus will be used for delivering the necessary material to the students, according to the professor criterion. This material will include: the course program, exercises and problems to be solved, copies of the classroom presentations, etc.

Along the course, the student should participate in various formative activities, with the aim of acquiring the established knowledge and skills.

Master classes: Explanation of theoretical contents supplemented by audiovisual aids. The active participation of the students will be intended, through the formulation of appropriate questions that they should try to answer.

Seminars: There will be two classroom hours before the partial exams dedicated to review concepts and/or clarify doubts.

Use of fast and anonymous response methods in class (clickers) to know the degree of follow-up of the subject.

Presentation of individual works on some topics related to the subject, including the debate with his classmates and teachers.

Group and individual tutoring.

ASSESSMENT SYSTEM

With the aim of encouraging the constant student work to favor the learning, a continuous evaluation will be applied. This methodology will inform the professor about the content's assimilation by the student as well as their ability to apply them to problem solving. The evaluation will be individual.

Along the course, on professor criterion, the students will have to solve some exercises and hand them in at the scheduled date. Performing short tests in classroom is also foreseen. (50%)

In order to evaluate the knowledge related to the master classes and the problem-solving ability of the students, one exam and/or individual oral presentation will be performed. (50%)

The students who did not pass the continuous evaluation will have the opportunity to perform a second-chance exam. To pass the course, it will be mandatory obtaining 5 points out of 10.

In cases of fraudulent performance of exercises or tests, the provisions of the regulations for evaluating student academic performance and reviewing qualifications will apply.

According to the document "Guidelines for the development of safe in classroom teaching, academic year 2020-2021", two new possible scenarios are envisioned for the assessment system just in case that the indicated scenario of adapted normality cannot be carried out. The new scenarios are included in the comment section under the title of the Contingency Plan.

COMMENTS

Revise basic biochemistry and physics concepts

CONTINGENCY PLAN

According to the document "Guidelines for the development of safe face-to-face teaching, academic year 2020-2021", two possible new scenarios are envisioned for the teaching methodology and the assessment system just in case that the adapted normality scenario cannot be carried out:

Scenario 2: social distancing (with partial restrictions on physical presence).

- The in classroom lectures will be on line and the seminars and practical laboratory and computer sessions will be in classroom. However, the distance measures imposed may mean that it is necessary to reduce the size of the practice groups and, therefore, the number of contact hours (up to a maximum of 50% of the practical hours of the subject) that must be complemented with non-contact activities.
- The tutorials will preferably be virtual.
- The final tests will preferably be telematic.

Scenario 3: closure of the facilities (impossibility of teaching in classroom).

- Teaching will be completely virtual, with synchronous or asynchronous mechanisms.
- The tutorials will be exclusively virtual.
- The final tests will be exclusively telematic.

For virtual teaching, Moodle platform will be used for the final test and continuous assessment and MS Teams for interactive classes, seminars and tutorials.

FACULTY DATA

Faculty	Contact	Semester	Day	Time	Class
José Ramón Leis Fidalgo	joseramon.leis@usc.es	2nd	25,27 Jan,	16:00/17:30	Maths (3 rd floor) Chem
Jesús Ángel Varela Carrete	jesus.varela@usc.es		2,4,8,10,12,18 22,24,26 Feb 1,3 Mar	Mar3, 16:00/19:00h	

IDENTIFICATION FORM

Course Data

Course number	P1251106
Subject	Computational chemistry
Title	Chemistry at the interface with Biology and Materials Science (ChemBio&Mat) P1251V01
Course Level	Master
Credits	3.0
Module	IV (Reactivity and Synthesis)
Academic Year	2019-2020

Titulation

Title	Center	Course	Semester
ChemBio&Mat	FACULTAD de QUÍMICA/CiQUS	1	Second

Subject

Title	Course Title	Course type
ChemBio&Mat	Computational Chemistry	Optative

Coordination

Name	Department	Contact
Rebeca García Fandiño	Organic Chemistry rebeca.garcia.fandino@usc.es/15708	

SUMMARY

The objective of this subject is to understand the basic concepts of computational chemistry. It is intended that the student knows and understands the different methodologies that can be used to solve a problem using computational chemistry. The theoretical bases of these methodologies will be studied, with special emphasis on a considerable number of applications that will allow the student to know the most used programs and methods to perform computational calculations of molecular properties and chemical reactivity, currently essential to contrast and predict results in a rigorous and faster and cheaper than the experimental. Given the transversal role of these computational methodologies, the student will be shown an integral and multidisciplinary view of computational chemistry within the area, in the context of other branches of science. Knowing the applications of this branch of chemistry, the student will understand the synergy between experimental methods and theoretical and computational chemistry.

PREREQUISITES

Relation with other topics of the Master

No enrollment restrictions have been specified with other subjects of the curriculum.

Other requirements

Although it is not mandatory, basic knowledge of Linux and / or programming is recommended. However, all the necessary knowledge for the correct comprehension of the contents of the subject will be imparted to the students.

COMPETENCES

Basic

- **CB7:** Students should know how to use the knowledge acquired and their problem-solving capacity in new or little known environments within wider (or multidisciplinary) contexts related to their field of study.
- **CB9:** Students should know how to communicate their findings and the knowledge and underlying reasons underpinning them to specialised and non-specialised audiences in a clear and unambiguous way.
- **CB10:** Students should have the learning skills that allow them to carry on studying in such a way that should be mainly self-directed or autonomous.

General

- **CG1:** Know how to use the knowledge acquired for practical problem solving in the field of research and innovation, in the multidisciplinary context of biological chemistry and molecular materials.
- **CG3:** Be able to discuss and communicate ideas, in both oral and written form, to specialised and non-specialised audiences (congresses, conferences, etc.) in a clear and reasoned way.
- **CG5:** Have the skills that allow students to develop an autonomous method for studying and learning.
- **CG7:** Be capable of working in multidisciplinary teams and collaborating with other specialists, both nationally and internationally

Transversal

- **CT1:** Develop teamwork skills: cooperation, leadership and good listening skills. Adapt to multidisciplinary teams.
- **CT2:** Draft scientific and technical reports and defend them publicly.

- **CT4:** Apply the concepts, principles, theories and models related to Biological Chemistry and Molecular Materials to new or little-known environments within multidisciplinary contexts.

Specific

- **CE2:** Be capable of comparing experimental data and theoretical assumptions in a critical manner.
- **CE6:** Know the physicochemical bases of biological processes.
- **CE8:** Gain technical skill for carrying out the structural characterization of molecules, biomolecules, supramolecules and nanoparticles and interpreting the experimental data obtained.

OBJECTIVES OF TRAINING

- Understanding the basis of computational chemistry.
- Knowing and understanding the different methodologies that can be used to solve a problem using computational chemistry.
- Obtaining a comprehensive and multidisciplinary vision of the area, in the context of other branches of science.
- Understanding the existing synergy between experimental methods and theoretical and computational chemistry.
- Knowing the applications of computational chemistry

COURSE CONTENTS

1. Introduction to Computational Chemistry. Quantum methods and classical methods. Basic tools.

Introduction to Computational Chemistry. Quantum methods and classical methods: advantages and limitations. Basic computational tools: Linux, Bash and Python languages. Molecular visualizers and constructors.

2. Quantum mechanics. General concepts and application to the study of reaction mechanisms and the prediction of molecular properties

Methods of the electronic structure: semi-empirical, DFT and ab initio methods. Potential energy surface (SEP): Stationary points and geometric optimization. Obtaining molecular properties from the electronic structure: dipole moments, electrostatic potential, atomic charges, polarizability and hyperpolarizability. Partition functions and calculation of thermodynamic functions such as enthalpy, entropy and Gibbs free energy. Estimation of the velocity constant of a chemical reaction: calculating kinetic constants using the transition state theory.

3. Molecular Mechanics and Molecular Dynamics. Theoretical bases and applications in organic chemistry and biological chemistry.

Theoretical basis of classical methods and presentation of the computational methodologies most used today in this field: Molecular Mechanics, Docking, Virtual Screening and Molecular Dynamics. Molecular Dynamics: fundamental basis and applications. Carrying out Molecular Dynamics simulations using the GROMACS package: setting-up, execution and analysis.

4. Docking and QM / MM: General concepts. Applications to enzymatic catalysis

Locating the active center of an enzyme: Fundamentals of the Docking technique (rigid and flexible). Carrying out docking using Autodock Vina package. Fundamental bases of hybrid QM / MM methods. Applications to the study of reaction mechanisms in biological and supramolecular systems.

COURSE BIBLIOGRAPHY

1. Lesson 1

Material deposited in the virtual classroom.

Introduction to Computational Chemistry:

- Molecular Modeling. Principles and Applications (Ed Pearson Education, 2001), Andrew R. Leach
- Introduction to Computational Chemistry (Ed Wiley), Frank Jensen.

Introduction to Linux and Bash:

- <https://computernewage.com/2018/09/16/scripting-linux-introduction/>
- <https://www.howtoforge.com/tutorial/linux-shell-scripting-lessons/>
- <https://linuxconfig.org/bash-scripting-tutorial-for-beginners>

Introduction to Python:

- <https://www.python.org/about/gettingstarted/>
- <https://www.learnpython.org/en/>

Molecular Viewers :

- <http://cheminf.cmbi.ru.nl/molde/>
- <http://www.cambridgesoft.com/support/ProductHomePage.aspx?KBCatID=112>
- <http://www.ks.uiuc.edu/Training/Tutorials/vmd-index.html>
- <http://pymol.sourceforge.net/newman/user/toc.html>
- <https://avogadro.cc/>

2. Lesson 2

Material deposited in the virtual classroom.

- IN Levine, Quantum Chemistry, 5th Ed., Pearson Education (2001).
- CJ Cramer, Essentials of Computational Chemistry, John Wiley & Sons (2002).
- F. Jensen, Introduction to Computational Chemistry, 2nd Edition, John Wiley & Sons (1999).

- PW Atkins, RS Friedman, Molecular Quantum Mechanics, 3rd Ed., Oxford Univ. Press (1997).
- PW Atkins, RS Friedman, Solutions Manual for Molecular Quantum. Oxford Univ. Press (1997).
- A. Szabo, NS Ostlund, Modern Quantum Chemistry. Introduction to Advanced Electronic Structure Theory, Dover Pub., Inc. (1996).
- T. Helgaker, P. Joergensen, J. Olsen, 'Molecular Electronic-Structure Theory', John Wiley & Sons (2000).
- J. Simons, J. Nichols, Quantum Mechanics in Chemistry, Oxford Univ. Press (1997).
- JB Foresman, Æleen Frisch, Exploring Chemistry with Electronic Structure Methods, 2nd Ed., Gaussian, Inc. (1995-96).

3. Lesson 3

Material deposited in the virtual classroom.

- Molecular Modeling. Principles and Applications (Ed Pearson Education, 2001), Andrew R. Leach
- Introduction to Computational Chemistry (Ed Wiley), Frank Jensen.

MOLECULAR DYNAMICS:

http://www.gromacs.org/Documentation/Terminology/Molecular_Dynamics_Simulations

<http://www.mdtutorials.com/gmx/>

<http://www.gromacs.org/Documentation/Tutorials>

<http://cgmartini.nl/index.php/tutorials>

4. Lesson 4

Material deposited in the virtual classroom.

- Molecular Modeling. Principles and Applications (Ed Pearson Education, 2001), Andrew R. Leach
- Introduction to Computational Chemistry (Ed Wiley), Frank Jensen.

DOCKING:

<http://autodock.scripps.edu/faqs-help/tutorial>

<http://vina.scripps.edu/manual.html>

QM / MM:

<http://www.gromacs.org/Documentation/How-tos/QMMM>

<https://gaussian.com/oniom/>

STUDENT WORKLOAD

The training activities will be distributed according to the following table.

	Activity	hours	% presential
Presential classes	Lectures and conferences	10	100%
	Seminars and classroom exercises	2	100%
	Tutorials	1	100%
	Practical classes	8	100%
	Oral presentations	2	100%
	Final exam	3	100%
Non Presential	Preparation and study of problems	15	0%
	Elaboration of individual work	34	0%
	TOTAL	75	

TEACHING METHODOLOGY

The Virtual Campus will be used for delivering the necessary material to the students, according to the professor criterion. This material will include: the course program, exercises and problems to be solved, copies of the classroom presentations, etc.

Along the course, the student should participate in various formative activities, with the aim of acquiring the established knowledge and skills.

A) Theoretical-practical sessions: This subject is divided into nine sessions of 2 hours each. Each session combines expository and practical classes, as shown in the scheme of the previous section. This methodological scheme intends to replace the lectures where the student barely intervenes, by theoretical-practical sessions that encourage self-learning of the student, relating the assimilation of theoretical concepts to the resolution of problems and practical situations that could be found in their possible professional future. During these sessions, the teachers will combine explanations of theoretical concepts, the approach and resolution of practical exercises with instructions directly related to the practice that the student will carry out within the same session. The teachers will have the support of audiovisual and computer media. A computer will be available to students, although it is recommended that they bring their own laptops, where they can install the programs used in the practices, and thus be used during non-presential work. During each session, the student must carry out a practical part independently. For this, they will have a Reference Manual, which will include an introduction to computer work and, in particular, its application to computational calculations, as well as a script for each of the practices to be performed, which will consist of a brief presentation of the theoretical foundations of the practice and the indication of the calculations to be made and the results to be presented. The student will do the practices individually and will present the results to be evaluated at the end of the sessions (2 hours of oral expositions of the students supported by audiovisual material). Attendance at these nine sessions (Session 1-9) is mandatory. The absences must be documentary justified, accepting reasons of examination and health, as well as those cases contemplated in the current university regulations.

B) Seminars and practical blackboard classes: The aim of these sessions is to resolve doubts about the theory, practices and exercises proposed in Bulletins 1-3, with the active participation of the student: delivery of exercises to the teacher, resolution of exercises in the classroom, etc. Attendance at these classes is mandatory.

C) Tutorials scheduled by teachers and coordinated by the Center. The aim of these sessions is to resolve any doubts that students may have regarding any content of the subject. Attendance to this class is not mandatory.

ASSESSMENT SYSTEM

1. Attendance

Attendance at the 9 theoretical-practical sessions is mandatory. The absences must be documentary justified, accepting reasons of examination and health, as well as those cases contemplated in the current university regulations.

2. The evaluation will consist of two parts (% final grade):

2.1. Continuous evaluation (50%), consisting of:

- i. Tests delivered to the teacher (15%)
- ii. Computer practices (20%)
- iii. Oral exposure (15%)

2.2. Final exam (50%)

The final exam will consist of a theoretical part (test questions, duration: 30 minutes) and a practical part of computing (in which exercises similar to those carried out during the practices will be considered, duration 2.5 hours).

The qualification of the student will not be inferior to the one of the final examination nor to the obtained one pondering it with the one of continuous evaluation. In any case, to pass the subject, it will be an essential requirement to have the qualification of APTO in computer practices. Repeating students will have the same attendance regime for classes as those who take the subject for the first time.

COMMENTS

CONTINGENCY PLAN in case of a possible change of scenario

- 1) Objectives: no changes
- 2) Content: no changes
- 3) Bibliographic material: no changes
- 4) Competences: no changes
- 5) Methodology:

Scenario 1: Adapted normality.

The expository and interactive teaching will be fundamentally of face-to-face character, although of exceptional and justified form the virtual teaching will be able to be combined with the face-to-face up to a

maximum of 10% of the h of the subject and in the case of practices carried out with telematic means 25%. In the event that part of the teaching is virtual, the Moodle and MS Teams platforms will be used, synchronously and asynchronously.

Tutorials can be carried out partially virtually (synchronously)

Scenario 2: distancing.

The expository teaching will be non-contact and the seminars and practices of laboratory and computer room face-to-face. However, the distance measures imposed may mean that it is necessary to reduce the size of the practice groups and thus the number of contact hours (up to a maximum of 50% of the practical hours of the subject) that will be complemented with non-contact activities. For virtual teaching, the Moodle and MS Teams platforms will be used, carrying out the same activities as in scenario 1 but virtually synchronously and asynchronously.

Tutorials will be virtual.

Scenario 3: Closure of facilities.

Teaching will be completely virtual. For virtual teaching, the Moodle and MS Teams platforms will be used, carrying out the same activities as in scenario 1 but virtually synchronously and asynchronously.

Tutorials will be exclusively virtual.

6) Evaluation system

Scenario 1: Adapted normality.

The final tests will be face-to-face.

Scenario 2: distancing

The final tests will be telematic. Students may be called for an interview to comment on or explain part or all of the test.

Scenario 3: Closure of facilities.

The final tests will be telematic. Students may be called for an interview to comment on or explain part or all of the test.

7) Study time and individual work: no changes.

FACULTY DATA

Faculty	Contact	Semester	Day	Time	Class
Rebeca García Fandiño	15708	2nd	26,28 Jan; 1,3,5,9,	19:00/21:00	Maths (3 rd floor)
Antonio Fernández Ramos			11,17,23,25 Feb; 2,4,9,15 Mar	Mar15, 16:00/19:00h	

IDENTIFICATION FORM

Course Data

Course number	P1251112
Subject	<i>Introductory Research Project</i>
Title	Chemistry at the interface with Biology and Materials Science (ChemBio&Mat) P1251V01
Course Level	Master
Credits	15.0
Module	V (Research)
Academic Year	2019-2020

Titulation

Title	Center	Course	Semester
ChemBio&Mat	FACULTAD de QUÍMICA/CiQUS	1	Second

Subject

Title	Course Title	Course type
ChemBio&Mat	Introductory Research Project	Compulsory

Coordination

Name	Department	Contact
Juan R. Granja	Organic Chemistry	juanr.granja@usc.es/15746

SUMMARY

The objective of this subject is to put the student in the context of an experimental work destined to gain work experience prior to the realization of the research project of the final master's project. The student can carry out this project in a research laboratory of the center, in other research laboratories, both national and international, or in key companies. In this context, is is offered an internship that enables you to put theory into practice and use the work experience to complete and further shape your study program at a different context of the CiQUS. It provides a unique opportunity to competent and motivated students to work on relevant tasks and projects at international or industrial level.

PREREQUISITES

Relation with other topics of the Master

No enrollment restrictions have been specified with other subjects of the curriculum.

Other requirements

No enrollment restrictions have been specified with other subjects of the curriculum.

COMPETENCES

Basic

- **CB6:** Possess and understand the knowledge that provides a basis or an opportunity for being creative and unique in the development and/or implementation of ideas, often in a research context.
- **CB7:** Students should know how to use the knowledge acquired and their problem-solving capacity in new or little known environments within wider (or multidisciplinary) contexts related to their field of study.
- **CB9:** Students should know how to communicate their findings and the knowledge and underlying reasons underpinning them to specialised and non-specialised audiences in a clear and unambiguous way.
- **CB10:** Students should have the learning skills that allow them to carry on studying in such a way that should be mainly self-directed or autonomous.

General

- **CG1:** Know how to use the knowledge acquired for practical problem solving in the field of research and innovation, in the multidisciplinary context of biological chemistry and molecular materials.
- **CG2:** Know how to apply the scientific method and acquire skills for developing the necessary protocols for the design and critical assessment of chemical experiments.
- **CG3:** Be able to discuss and communicate ideas, in both oral and written form, to specialised and non-specialised audiences (congresses, conferences, etc.) in a clear and reasoned way.
- **CG6:** Have leadership, creativity, initiative and entrepreneurship abilities.
- **CG7:** Be capable of working in multidisciplinary teams and collaborating with other specialists, both nationally and internationally.
- **CG8:** Be able to use scientific literature and develop the judgement needed for its interpretation and use.
- **CG9:** Be capable of handling chemical substances safely and work in a chemical laboratory without risks.
- **CG10:** Be able to develop the different research stages (from the conception of an idea and the literature search through to target setting, experiment design, analysis of the results and drawing conclusions).

Transversal

- **CT1:** Develop teamwork skills: cooperation, leadership and good listening skills. Adapt to multidisciplinary teams.

- **CT2:** Draft scientific and technical reports and defend them publicly.
- **CT3:** Perform day-to-day research or professional activity in an independent and efficient manner.
- **CT5:** Appreciate the value of good quality and continuous improvement by acting rigorously, responsibly and ethically.
- **CT7:** Show critical and self-critical reasoning when seeking scientific rigour and quality. Handle IT tools and information and communication technology (ICT), as well as on-line access to databases.

Specific

- **CE3:** Know the rules on risk prevention in the laboratory and within the chemistry-related industry.
- **CE9:** Use advanced instrumentation related to research on biological chemistry and molecular materials.
- **CE20:** Know how to plan and carry out new laboratory experiments in an autonomous and independent manner.

OBJETIVES OF TRAINING

- Knowledge of the methodology to be followed for the development of a research project: literature search, design, planning and development of experiments, data analysis, proposals for improvement and conclusions of the work.
- Learn the handling of specialized laboratory instruments and materials for the synthesis, characterization, purification and / or analysis of chemical products, nanomaterials, biomolecules or cell samples.
- Learn to treat the experimental data obtained and relate them to the appropriate physical, chemical and biological theories, using primary bibliographic sources.
- Recognition of the risks associated with the development of an experimental project, and the appropriate security measures.

For the realization of this work the student will select experimental (computer) works proposed by the postgraduate commission, previous offer of the CiQUS researches together with the subject.

COURSE CONTENTS

COURSE BIBLIOGRAPHY

1. Basic

2. Complementary

STUDENT WORKLOAD

The training activities will be distributed according to the following calendar.

	Activity	hours	% presential
Presential classes	Tutorials of orientation for the planning and monitoring of the project	4	100%
	Experimental work on the techniques of synthesis, analysis and study of the properties that are used today in both university research laboratories and in the chemical and / or biotechnology industry	280	100%
	Analysis and data evaluation	30	100%
	Presentation and public defense of the work	1	100%
Non Presential	Use of literature searches and database	10	0%
	Preparation of inform and thesis defense	50	0%
	TOTAL	375	

TEACHING METHODOLOGY

Taking into account a student's dedication of 25 hours of total work per ECTS credit, a face-to-face work of approximately 375 hours will be carried out. Along the course, the student should participate in various formative activities, with the aim of acquiring the established knowledge and skills.

- Individual experimental (or computational) work under supervision, with adequate infrastructure and necessary means to achieve the proposed objectives.
- Tutorials for work planning, supervision of experimental work and analysis of results.
- Use of specialized software, databases and web resources. Online teaching support (Virtual Campus).
- Preparation of a brief report / research report.
- Presentation and defense of the work done.

ASSESSMENT SYSTEM

General considerations

- Experimental work done.
- Written report detailing the most relevant results of the work performed and the skills acquired.
- Oral exhibition and defense of the work done and the skills acquired.

In cases of fraudulent performance of exercises or tests, the provisions of the *“Regulations for evaluating student academic performance and reviewing grades”* will apply.

The evaluation system will be exactly the same regardless of the type of teaching used (in classroom or

virtual), with the only difference that the evaluation activities will be carried out, as established by the competent authorities, either in person in the classroom or remotely through the telematic means available at the USC. (*Scenario 1*: Final in classroom exam. *Scenario 2 and 3*: Final remote exam).

COMMENTS

CONTINGENCY PLAN

Contingency plan for remote teaching activities:

They would be carried out synchronously / asynchronously and always according to the schedule established by the center, through the different telematic means available at the USC, preferably the Virtual Campus and Ms Teams.

Due to the nature and content of this subject, as well as the methodology used, the main difference between face-to-face teaching and remote teaching is (*Scenario 1*: in classroom teaching. *Scenario 2*: Expository classes and tutorials will be in classroom between 0% -50% of the classes, while the seminars will be in classroom between 50% -100% of the lectures. *Scenario 3*: 100% remote classes).

To carry out tutorials, as well as to maintain direct communication both between the students themselves and between them and the teacher, they can be done through the Virtual Campus forum, through Ms. Teams or by email.

FACULTY DATA

Faculty	Contact	Semester	Day	Time	Class
Juan R. Granja	16746	1 st and 2 nd			

IDENTIFICATION FORM

Course Data

Course number	P1251113
Subject	<i>Master dissertation</i>
Title	Chemistry at the interface with Biology and Materials Science (ChemBio&Mat) P1251V01
Course Level	Master
Credits	30.0
Module	V (Research)
Academic Year	2019-2020

Titulation

Title	Center	Course	Semester
ChemBio&Mat	FACULTAD de QUÍMICA/CiQUS	2	First

Subject

Title	Course Title	Course type
ChemBio&Mat	Master Dissertation	Compulsory

Coordination

Name	Department	Contact
Juan R. Granja	Organic Chemistry	juanr.granja@usc.es/15746

SUMMARY

The MA dissertation is the culmination of the Master programme. It is a piece of independent writing carried out by Master students under faculty supervision on a topic chosen by the student in coordination with his tutor. It is undertaken with the guidance of a faculty supervisor and involves an extended period of research which is finally reflected in a written document.

Masters Dissertation requires students to engage with their subject area in a more critical manner than they will have done at the undergraduate level. Students are expected to have a solid knowledge on their topic of interest, demonstrate a general grasp of the relevant literature and the various disciplinary contributions, as well as an understanding of the concepts and methods used to address the research questions.

PREREQUISITES

Relation with other topics of the Master

No enrollment restrictions have been specified with other subjects of the curriculum.

Other requirements

No enrollment restrictions have been specified with other subjects of the curriculum.

COMPETENCES

Basic

- **CB6:** Possess and understand the knowledge that provides a basis or an opportunity for being creative and unique in the development and/or implementation of ideas, often in a research context.
- **CB7:** Students should know how to use the knowledge acquired and their problem-solving capacity in new or little-known environments within wider (or multidisciplinary) contexts related to their field of study.
- **CB9:** Students should know how to communicate their findings and the knowledge and underlying reasons underpinning them to specialised and non-specialised audiences in a clear and unambiguous way.
- **CB10:** Students should have the learning skills that allow them to carry on studying in such a way that should be mainly self-directed or autonomous.

General

- **CG1:** Know how to use the knowledge acquired for practical problem solving in the field of research and innovation, in the multidisciplinary context of biological chemistry and molecular materials.
- **CG2:** Know how to apply the scientific method and acquire skills for developing the necessary protocols for the design and critical assessment of chemical experiments.
- **CG3:** Be able to discuss and communicate ideas, in both oral and written form, to specialised and non-specialised audiences (congresses, conferences, etc.) in a clear and reasoned way.
- **CG6:** Have leadership, creativity, initiative and entrepreneurship abilities.
- **CG7:** Be capable of working in multidisciplinary teams and collaborating with other specialists, both nationally and internationally.
- **CG8:** Be able to use scientific literature and develop the judgement needed for its interpretation and use.
- **CG9:** Be capable of handling chemical substances safely and work in a chemical laboratory without risks.
- **CG10:** Be able to develop the different research stages (from the conception of an idea and the literature search through to target setting, experiment design, analysis of the results and drawing conclusions).

Transversal

- **CT1:** Develop teamwork skills: cooperation, leadership and good listening skills. Adapt to multidisciplinary teams.
- **CT2:** Draft scientific and technical reports and defend them publicly.
- **CT3:** Perform day-to-day research or professional activity in an independent and efficient manner.
- **CT5:** Appreciate the value of good quality and continuous improvement by acting rigorously, responsibly and ethically.
- **CT7:** Show critical and self-critical reasoning when seeking scientific rigour and quality. Handle IT tools and information and communication technology (ICT), as well as on-line access to databases.

Specific

- **CE2:** Be capable of comparing experimental data and theoretical assumptions in a critical manner.
- **CE3:** Know the rules on risk prevention in the laboratory and within the chemistry-related industry.
- **CE5:** Know how to analyse and use the data obtained autonomously in complex laboratory experiments by relating them to the suitable chemical, physical or biological techniques.
- **CE9:** Use advanced instrumentation related to research on biological chemistry and molecular materials.
- **CE19:** Know how to carry out, submit and defend individually, and once all curriculum credits are obtained, a comprehensive research project on Biological Chemistry and Molecular Materials which synthesizes the skills learnt in the Masters course.
- **CE20:** Know how to plan and carry out new laboratory experiments in an autonomous and independent manner.

OBJETIVES OF TRAINING

- Knowledge of the steps and the methodology to develop a research project: the bibliographic search, the design, the planning and the development of the experiments, the data analysis, the proposals for improvement and conclusions of the work.
- Use of databases and specialized bibliography to analyze, critically, the background, originality, interest and viability of a research project.
- Ability to integrate the previously acquired knowledge, and to apply it to the planning, development and analysis of the results of the research work.
- Acquisition of experience in the experimental techniques and / or computational methods necessary to carry out a research project in the field of chemical synthesis, biological chemistry or materials chemistry.
- Recognition of the risks associated with the development of an experimental project and of the appropriate security measures.
- Be able to prepare a report of the work done and the results obtained in a research work, in the appropriate format for a scientific document.

- Ability to present and defend, before a specialized audience, the development, results and conclusions of a research project.

The experimental work is carried out by the student individually under the supervision of a CiQUS tutor. Its purpose is for the student to apply the knowledge acquired throughout the Bachelor's and Master's degree in the realization of a technical work that have relation with some of the contents of the degree and the activities professionals for whom you are trained.

For the realization of this work the student will select experimental (computer) works proposed by the postgraduate commission, previous offer of the CiQUS researches together with the subject. Students will submit their application for assignment of research work with an order of preference. The offer will be broad enough to guarantee the assignment to all students enrolled.

COURSE CONTENTS

1. Introduction to master thesis

Guidelines. Tutors. Work development. Memory. Final presentation.

2. Project under tutor guidance

Topic selection. Literature searching. Proposal of a working plan. Chronogram.

3. Project development

Experimental work. Progress report and periodical tutor's meetings. Achievements.

4. Finishing thesis

Writing thesis. Oral presentation and defense of experimental work

COURSE BIBLIOGRAPHY

1. Basic

2. Complementary

STUDENT WORKLOAD

The training activities will be distributed according to the following calendar.

	Activity	hours	% presential
Presential classes	Tutorials of orientation for the planning and monitoring of the project	15	100%
	Experimental work (or computational) associated to the development of the project	580	100%
	Analysis and data evaluation	50	100%
	Oral presentation in seminars of the research progress	3	100%
	Presentation and public defense of the work	2	100%
Non Presential	Use of literature searches and database	15	0%
	Preparation of reports and informs	60	0%
	Preparation of seminar oral presentation	5	0%
	Preparation of thesis defense	20	0%
	TOTAL	750	

TEACHING METHODOLOGY

Taking into account a student's dedication of 25 hours of total work per ECTS credit, a face-to-face work of approximately 750 hours will be carried out. Along the course, the student should participate in various formative activities, with the aim of acquiring the established knowledge and skills.

Introductory class: the coordinator explains the generalities about the development and objectives of the master dissertation and preparation of the final report.

Meetings with the assigned tutor: In the initial meeting the approach will be outlined of the project, the scientific literature and the chronogram for the development of the work. In the follow-up meetings will be evaluated of progress of the work, difficulties encountered, and objectives achieved.

Work development. The methodological procedure will be outlined in the initial research proposals.

Preparation of the final report. A written document and an oral presentation and defense of the experimental work carried out.

ASSESSMENT SYSTEM

The evaluation of the Master's Thesis will be carried out by a committee appointed for this purpose, which will be made up of three professors who teach in the Master.

The student must present a report that will include:

- A brief introduction on background
- The objectives and the work plan
- The results with a critical and reasoned discussion of them
- The conclusions
- The bibliography consulted

The memory will have a maximum of fifty pages in A4 size written to a space in Arial font of twelve dots per inch.

The student will also make a public presentation of the experimental work, presentations will not be longer than fifteen minutes.

The committee will evaluate the oral presentation of the work carried out, the written report and its public defense.

The final grade awarded by the Court will be obtained taking into account:

- Tutor's report (50%)
- The elaborated memory (30%)
- The oral presentation, its defense and the knowledge demonstrated by the student (20%)

The ratings will be based on the absolute score over 10 points and in accordance with the scale established in RD 1125/2003.

COMMENTS

CONTINGENCY PLAN

METHODOLOGY

Contingency plan for remote teaching activities:

They would be carried out synchronously / asynchronously and always according to the schedule established by the center, through the different telematic means available at the USC, preferably the Virtual Campus and Ms Teams.

Due to the nature and content of this subject, as well as the methodology used, the main difference between face-to-face teaching and remote teaching is (Scenario 1: in classroom teaching. Scenario 2: Expository classes and tutorials will be in-person between 0% -50% of the classes, while the seminars will be in-classroom between 50% -100% of the classes. Scenario 3: 100% telematic).

To carry out tutorials, as well as to maintain direct communication both between the students themselves and between them and the teacher, they can be done through the Virtual Campus forum, through Ms. Teams or by email.

EVALUATION SYSTEM

In cases of fraudulent performance of exercises or tests, the provisions of the *“Regulations for evaluating student academic performance and reviewing grades”* will apply.

The evaluation system will be exactly the same regardless of the type of teaching used (in classroom or telematic), with the only difference that the evaluation activities will be carried out, as established by the competent authorities, either in person in the classroom or remotely through the telematic means available at the USC. (Scenario 1: Final in classroom. Scenario 2 and 3: Final telematic exam).

FACULTY DATA

Faculty	Contact	Semester	Day	Time	Class
		3rd			

IDENTIFICATION FORM

Course Data

Course number	P1251111
Subject	<i>Tutored Training Activities</i>
Title	Chemistry at the interface with Biology and Materials Science (ChemBio&Mat) P1251V01
Course Level	Master
Credits	3.0
Module	V (Research)
Academic Year	2019-2020

Titulation

Title	Center	Course	Semester
ChemBio&Mat	FACULTAD de QUÍMICA/CiQUS	1	1st and 2nd

Subject

Title	Course Title	Course type
ChemBio&Mat	Tutored Training Activities	Compulsory

Coordination

Name	Department	Contact
Juan R. Granja	Organic Chemistry	juanr.granja@usc.es/15746

SUMMARY

The main objective of this subject is to provide tools to acquire a general view of the state of the art in the scientific fields of the master. In addition, it is also aimed to get a general view of relevant and current scientific aspects. A variety of academic activities, seminars, lectures, courses and other activities will be provided by the centers related to master with this goal.

PREREQUISITES

Relation with other topics of the Master

No enrollment restrictions have been specified with other subjects of the curriculum.

Other requirements

No enrollment restrictions have been specified with other subjects of the curriculum.

COMPETENCES

Basic

- **CB6:** Possess and understand the knowledge that provides a basis or an opportunity for being creative and unique in the development and/or implementation of ideas, often in a research context.
- **CB7:** Students should know how to use the knowledge acquired and their problem-solving capacity in new or little known environments within wider (or multidisciplinary) contexts related to their field of study.
- **CB8:** Students should be able to integrate knowledge and deal with the complexity of making judgements from information which – being incomplete or limited – includes reflections on the social and ethical responsibilities linked to the use of their knowledge or judgements.
- **CB9:** Students should know how to communicate their findings and the knowledge and underlying reasons underpinning them to specialised and non-specialised audiences in a clear and unambiguous way.
- **CB10:** Students should have the learning skills that allow them to carry on studying in such a way that should be mainly self-directed or autonomous.

General

- **CG3:** Be able to discuss and communicate ideas, in both oral and written form, to specialised and non-specialised audiences (congresses, conferences, etc.) in a clear and reasoned way.
- **CG4:** Be able to understand the social and ethical responsibilities linked to the use of knowledge or judgements in research, development and innovation in the field of biological chemistry and molecular materials.
- **CG8:** Be able to use scientific literature and develop the judgement needed for its interpretation and use.
- **CG10:** Be able to develop the different research stages (from the conception of an idea and the literature search through to target setting, experiment design, analysis of the results and drawing conclusions).

Transversal

- **CT3:** Perform day-to-day research or professional activity in an independent and efficient manner.
- **CT5:** Appreciate the value of good quality and continuous improvement by acting rigorously, responsibly and ethically.

Specific

- **CE1:** Know the impact of chemistry, biological chemistry and molecular materials on the industry, environment, health, agrofood and renewable energies.
- **CE2:** Be capable of comparing experimental data and theoretical assumptions in a critical manner.
- **CE4:** Know and understand the chemical tools and analytical techniques used for biological chemistry and molecular materials.
- **CE15:** Students should be familiarized with nanotechnology methods and usefulness for studying processes of medical and biological interest.

OBJETIVES OF TRAINING

- The main objective of this subject is to provide tools to acquire a general view of the state of the art in the scientific fields of the degree.
- To get a general vision of relevant and current scientific aspects through the participation in conferences, lectures, research seminars organized by the centers related to master.
- Strengthen the knowledge acquired in the other modules by triggering the attendance at different scientific/educational events [national and international schools in which CiQUS members participate (national school of materials, Moreno Mañas school, etc.)].
- Proficiency in the techniques of writing, presentation and exposition of scientific works.
- Acquisition of skills related to employability and entrepreneurship.
- Acquisition of other transversal competences, under the supervision of a tutor.

COURSE CONTENTS

- The contents of the activities offered could be different in each academic year.
- The contents to which each student would access will be different depending on the specific offer and the recommendations of the tutor.
- In any case, these contents will include: current state of research in biological chemistry / nanoscience / materials science (through prestigious guest lecturers), scientific communication and debate (research seminars); skills in employability and entrepreneurship, etc.

COURSE BIBLIOGRAPHY

1. Basic

2. Complementary

STUDENT WORKLOAD

The training activities will be distributed according to the following calendar.

	Activity	hours	% presential
Presential classes	Conferences given by prestigious international professors/researchers, on the themes of the Master	10	100%
	Group and CiQUS research seminars	10	100%
	Workshops on employability and entrepreneurship	Up to 10	100%
	Attendance at courses, workshops, national schools, etc.	Up to 15	100%
	Other training activities recommended by the tutor	Up to 10	100%
	Tutoring with subject coordinator and scientific tutor	3	100%
Non Presential	Preparation of tests and directed work	25	0%
	Study and personal work of the student	5	0%
	Bibliographic search and use of databases	5	0%
	TOTAL	75	

TEACHING METHODOLOGY

- Organization of programs of conferences, seminars and workshops (coordinator of the Master / CiQUS staff).
- Personalized advice on the possible activities to be carried out (scientific tutor and / or course coordinator).
- Supervision of the assistance and use of the activities carried out, through the virtual and on-site tutorials (Virtual Campus) (scientific tutor and / or course coordinator).
- Preparation of a brief report highlighting the most relevant activities carried out (student).

ASSESSMENT SYSTEM

The assessment process will not only serve to know if the student has acquired the programmed competences but also to overview the teaching methodology.

- Accredited assistance to conferences and organized workshops.
- Assistance and active participation in research seminars.
- Participation in national and international schools, courses and workshops on topics related to biological chemistry and molecular materials.
- Written memory, personal debate and / or public presentation of the activities carried out and the competences acquired.

The acquisition of competences will be evaluated through the different systems: Evaluation weights:

Minimum weighting (MiW)- Maximum weight (MaW)

Memory and/or presentation activities: 20%-30%

Oral presentations: 10%-20%

Training activities carried out: 25%-40%

Transversal competences evaluation: 0%-20%

Tutor report: 30%-50%

COMMENTS

CONTINGENCY PLAN

According to the document "Guidelines for the development of safe classroom teaching, academic year 2020-2021", two possible new scenarios are contemplated for the teaching methodology and the evaluation system in case it is not possible to develop the adapted normality scenario :

Scenario 2: distancing (with partial restrictions on physical presence).

- The expository teaching will be non-face-to-face and the seminars and practical laboratory and computer classroom. However, the distance measures imposed may mean that it is necessary to reduce the size of the practice groups and, therefore, the number of contact hours (up to a maximum of 50% of the practical hours of the subject) that must be complemented with non-contact activities.
- The tutorials will preferably be virtual.
- The final tests will preferably be telematic.

Scenario 3: closure of the facilities (impossibility of teaching face-to-face).

- Teaching will be completely virtual, with synchronous or asynchronous mechanisms.
- The tutorials will be exclusively virtual.
- The final tests will be exclusively telematic.

For virtual teaching, Moodle platforms will be used for the final test and continuous assessment and MS Teams for expository classes, seminars and tutorials.

FACULTY DATA

Faculty	Contact	Semester	Day	Time	Class
Juan R. Granja	15746	1 st and 2 nd			

TEACHING STAFF 2020/2021



Juan R. Granja Guillán
Full Professor – CiQUS PI



Prof. Juan R. Granja received the PhD in chemistry from the University of Santiago de Compostela in 1988, under the guidance of Profs. Antonio Mouriño and Luis Castedo, working on the synthesis of the main metabolites of vitamin D₂. After postdoctoral studies in the group of Prof. Barry M. Trost at the Chemistry Department of Stanford University working on the synthesis of macrolides using Pd chemistry, he returned to the University of Santiago de Compostela as Assistant Professor (Oct-1991). In 1995 he was promoted at the University of Santiago de Compostela to associate professor (Professor Titular) and in 2006 to Full Professor after a national habilitation in 2005 in Barcelona.

He was visiting professor at The Scripps Research Institute in La Jolla in different periods since 1992. He has established a long and productive scientific collaboration with Prof. M. Reza Ghadiri to develop self-assembling peptides, and self-replicating systems. In 2017 he was visiting professor at University of Cambridge to study self-assembling process and microfluidics.

One of his research programs is seeking for the synthesis of functional nanotubes by self-assembling process of cyclic peptides. Specially, he is interested on peptide nanotubes based on cyclic peptides that contains cyclic gamma-amino acids. The goal is to create tubular shaped structure with tailor-made properties and use their internal and external characteristics to create new tools for material sciences and biology. At this respect we are especially interested to create this type of structures with pre-designed properties to interfere with the phospholipid membranes to change their biological properties.



José Luis Mascareñas
Full Professor – CiQUS PI



José Luis Mascareñas completed his PhD at the University of Santiago in 1988. He was a postdoctoral fellow at Stanford University (USA) under the supervision of Prof. Paul Wender (1989-1990); and became permanent professor in 1993, and full professor in 2005, at the University of Santiago.

He has been visiting scholar in Harvard University (USA) in the summers of 1992 and 1995, and visiting scientist in the University of Cambridge (UK, 2009) and the MIT (USA, 2013). In 2009 he received the Organic Chemistry award of the Spanish Royal Society of Chemistry and in 2015 he received the Gold Medal (maximum recognition) of the same society. In 2013 he received and **ERC Advanced Grant** of the EU for his project METBIOCAT.

He has published more than 170 papers and he has given over 120 invited and plenary lectures. He has supervised 18 postdoctoral associates (10 currently in the group), 31 doctoral theses (11 more ongoing), more than 55 masters and undergrad students. 5 former PhD students of the group gained a Ramón y Cajal position, 3 were awarded by the RSEQ awards for young leaders.

His current research splits between a synthetic program aimed at discovering novel methods based on metal catalysis, and a chemical biology program focused to the development of synthetic tools for biological intervention.



José Manuel Martínez Costas
Associate Professor – CiQUS PI



Jose M. Martinez Costas holds a degree in Biology from the University of Santiago de Compostela (USC).

He did his doctoral thesis at the Department of Biochemistry and Molecular Biology, University of Santiago under the supervision of Professor Javier Benavente.

In January 1994 began a postdoctoral fellow at Oxford (UK) in the laboratory of Dr. Polly Roy, where he worked with Bluetongue Virus (BTV). In September 1996 he was awarded a “Contrato de Reincorporación de Doctores y Tecnólogos del Ministerio de Educación” to return to the University of Santiago. Since 2003 he is Associate Professor at USC.



Dolores Pérez Meirás
Full Professor – CiQUS PI



Dolores Pérez completed her graduate studies at the University of Santiago de Compostela, under professors E. Guitián and L. Castedo, working in the total synthesis of antitumour alkaloids. After obtaining the PhD in 1991, she was awarded with a MEC-Fullbright fellowship to conduct postdoctoral training at the University of California at Berkeley (1992-1993) in the group of Prof. K. Peter C. Vollhardt, where she became interested in the field of organometallic chemistry applied to organic synthesis. She broadened her training in this field in 1996, as visiting scientists in the group of Prof. Stephen L. Buchwald at MIT.

In 1995 she joined the faculty of the University of Santiago de Compostela as Assistant Professor. In 2000 she was promoted to Associate Professor of Organic Chemistry and in 2019 to Full Professor at the USC. Her group pioneered the discovery of metal-catalyzed reactions involving short-lived aryne intermediates, a work which resulted highly influential for the renaissance of aryne chemistry in recent years.

Her current research interests are focused in the discovery of new metal-catalyzed reactions of synthetic interest, the further development of aryne chemistry and, in particular, its application to the synthesis of complex polycyclic aromatic systems and nanographenes. In 2010 D. Pérez was appointed as Commissioner Director of the Center for Research in Biological Chemistry and Molecular Materials (CIQUS), where she is currently Deputy Director (since 2014).



Pablo del Pino

Ramón y Cajal Researcher – CiQUS PI



Pablo del Pino graduated in Physics from the University of Sevilla (2002), and obtained his PhD (Dr. rer. nat., 2007) from the Technische Universität München (TUM), where he carried out his PhD work in Molecular Biophysics under the guidance of Prof. Fritz G. Parak. He has held postdoc positions in the group of Prof. Wolfgang J. Parak (Center of Nanoscience at Ludwig-Maximilian Universität LMU München, 2007-2009; AG Biophotonik at Philipp-Universität Marburg, 2012 y 2016) and the group of Dr. Jesús M. de la Fuente (Instituto de Nanociencia de Aragón INA, 2009-2012).

After his postdoctoral stage, he has been ARAID (INA, 2013) researcher and has been in charge (together with Prof. W. J. Parak) of the Bioengineered Particles laboratory (CIC biomaGUNE, 2013-2015). Currently he holds a “Ramon y Cajal” contract (call 2014) associated to the Condensed Matter Physics Department (USC) and CIQUS, where he leads the group BioNanoTools.

Our research is focused on the development of materials for applications in biology and medicine. We design, synthesize and customize nano- and micro-materials with applications in therapy, imaging and biosensing. We are working at the interface of materials science, biology and medicine with the goal of producing next generation “smart” materials, having enhanced multifunctional capabilities.



Francisco Rivadulla

Associate Professor – CiQUS PI



Francisco Rivadulla (A Pobra do Caramiñal, 1973) graduated in Chemistry at the University of Santiago de Compostela, USC, in 1996. In 2001 he obtained the PhD at the Physical chemistry Department of the same university (“Magnetotransport and Electron Spin Resonance in Magnetoresistive Manganites”).

He performed a two years postdoctoral stay (2001-2003) as a Fulbright Fellow at the University of Texas at Austin, in the laboratory of Prof. John B. Goodenough. During this time, he worked in the problem of metal-insulator transitions induced by electronic correlations in solids (Mott-Hubbard transitions), developing the idea of an intrinsic coupling between the electronic and lattice degrees of freedom in magnetic insulators that approach the itinerant electron limit.

In 2004 he joined the University of Santiago de Compostela as a Ramón y Cajal fellow, and since 2009 he is Associate Professor. Since 2010 he is the group leader of the Condensed Matter Chemistry Lab (CmCLab), at CIQUS. The main interest of his group is the development of new materials for thermoelectric energy conversion, as well as the basic aspects (electronic and transport properties, magnetic structure, etc.) of strongly correlated electron systems.

Dr. Francisco Rivadulla published around 75 papers (not including conference papers), which have been cited 2500 times, resulting in an h-index of 27 (ISI Web of Science, November 2015).

In June 2010 he was awarded an **ERC-Starting Grant**, to develop the project “Design of new thermoelectric devices based on 2D and field modulated nanostructures”, during the following five years. In 2017 he started the **ERC-Proof of Concept** project "ANTS": A new technology of microthermal sensing for application in microcalorimetry.



Miguel Vázquez López
Associate Professor – CiQUS PI



Miguel Vázquez López graduated in Chemistry in 1996 at the Universidad de Santiago de Compostela (USC). He completed his PhD in 2001 at the same university, with a dissertation about metallocsupramolecular helicates. He was postdoctoral fellow of the Xunta de Galicia at the Laboratory of Molecular Magnetism of the Università di Firenze (Florence, Italy) in 2001, working under the supervision of Prof. Dante Gatteschi in the study of the magnetic properties of a family of helicates. In 2002-2003 he was postdoctoral fellow of the Marie Curie EU TMR Programme at the Laboratory of Supramolecular Chemistry of the Università di Pavia (Pavia, Italy), working under the supervision of Prof. Luigi Fabbrizzi in the area of Molecular Devices and Machines.

In 2004 he joined the Department of Inorganic Chemistry of the Universidad de Vigo (Vigo, Spain) as Isidro Parga Pondal researcher, where he worked on the development of coordination polymers. He returned to the USC as Ramón y Cajal researcher in 2006. In 2009 he made a short research stay in the Laboratory of Lanthanide Supramolecular Chemistry of Prof. Jean-Claude G. Bünzli at the École Polytechnique Fédérale de Lausanne (Lausanne, Switzerland). He obtained his permanent position as Associate Professor at the Department of Inorganic Chemistry of the USC in 2010. In February 2011 he moved to the Center for Research of Biological Chemistry and Molecular Materials (CiQUS) of the USC as PI.

He is author of more than 50 scientific papers in peer-reviewed international journals, referee of several international chemistry journals (Chem. Commun., Inorg. Chem., ...), guest editor of a special issue of the journal *Molecules*, PI of several scientific projects (regional, national and european) and remote expert evaluator for some national scientific agencies and also for the Research Executive Agency of the European Commission. Between 2012-2016 he was board member of the Specialist Group of Chemical Biology (GEQB) of the Spanish Royal Society of Chemistry (RSEQ).



Ramón J. Estévez Cabanas
Full Professor – CiQUS PI



Ramón J. Estévez Cabanas (La Estrada, Pontevedra) studied Chemistry at the University of Santiago de Compostela (USC, 1975) and performed his PhD studies at the same university under the supervision of Prof. Dr. Luís Castedo and Prof. Dr. Rafael Suau (USC, 1979). He made several postdoctoral stays at Oxford University, in the group of Professor George W. J. Fleet.

In 1984 he acquired the condition of Associate Professor of Organic Chemistry and in 2003 the Full Professor condition.

His interests about the valorization of research and university entrepreneurship led him to participate in the creation of two technology-based companies that surged from the USC (Galchimia and AMSlab).

He has been vice president and president of the Carbohydrates Group of the Spanish Royal Society of Chemistry (RSEQ).

Currently, he is the Director of the Organic Chemistry Department at the USC, as well as the coordinator of the inter-university Master in Organic Chemistry and the PhD Program in Chemical Sciences & Technology (Mention for Excellence by the Ministry of Education).



Martín Fañanás-Mastral

Ramón y Cajal Researcher – CiQUS PI



Martín Fañanás Mastral (Zaragoza, 1980) graduated in Chemistry from the University of Oviedo in 2002. He performed his PhD studies at the same university under the supervision of Prof. José Barluenga and Prof. Fernando Aznar, working on the development of cascade reactions of Fischer carbene complexes and their application in organic synthesis. He received his PhD in 2007 and his doctoral thesis was awarded with the "Extraordinary Doctorate Award". He performed a predoctoral stay at the group of Prof. Steven Ley at the University of Cambridge (UK), where he worked in the total synthesis of the natural product Bengazole A.

In 2009 he joined the group of Prof. Ben L. Feringa at the University of Groningen (The Netherlands) as postdoctoral researcher. There he worked on the development of enantioselective catalytic allylic substitution reactions, cross-coupling of organolithium reagents and catalytic oxidation processes.

In 2014 he moved to the Centro Singular de Investigación en Química Biológica y Materiales Moleculares (CIQUS), at the University of Santiago de Compostela, as Ramón y Cajal researcher. In 2015 he was awarded with the "Thieme Chemistry Journal Award", in 2016 with the "Young Researchers Award" of the Spanish Royal Society of Chemistry and in 2018 with the "Lilly Young Researcher Award".

His research is based on the development of novel transition metal catalyzed reactions which allow to perform highly atom-efficient and sustainable transformations oriented towards enantioselective C-C bond formation, alkane functionalization and synthesis of biologically active phosphorous compounds.



Eduardo Fernández-Megía

Associate Professor – CiQUS PI



Eduardo Fernandez-Megia completed a PhD in Chemistry in 1995 under the supervision of Prof. F. J. Sardina at the University of Santiago de Compostela (USC). After a postdoctoral stay at the University of Cambridge (Prof. Steven V. Ley, 1997-99), he returned to USC as a Marie Curie Fellow and Associated Professor. In 2003, he became Ramon y Cajal Fellow and in 2008 was appointed Prof. Contratado Doctor. Since 2010 is Profesor Titular of Organic Chemistry and works at the Center for Research in Biological Chemistry and Molecular Materials (CIQUS) at USC.

His research focuses on the interface between organic and polymer chemistry with emphasis on the preparation of well-defined polymeric nanostructures for biomedical applications and the development of NMR tools for their characterization. With this aim his group relies on dendrimers, synthetic polymers, and polysaccharides. The efficient conjugation of these multivalent structures to ligands of biomedical interest affords novel drug delivery systems, diagnosis agents, and tools to study the complex mechanisms governing multivalent interactions. The characterization of polymeric nanostructures and complex mixtures by NMR relaxation is used to develop procedures for the accelerated recording of NMR spectra and selective suppressions.



Antonio Fernández-Ramos
Associate Professor – CiQUS PI



Antonio Fernández-Ramos received his B.A in Chemistry in 1993 and his Ph.D. in 1998 from the Universidade de Santiago de Compostela (USC), the later under the supervision of Miguel A. Ríos and Jesús Rodríguez. He started his postdoctoral training as Visiting Fellow of the Steacie Institute for Molecular Sciences (SIMS) of Ottawa from 1998 to 2000, and he has worked in collaboration with Zorka Smedarchina, Willem Siebrand and Marek Zgierski in the development of an approximate instanton method to model proton transfer reactions at low temperatures.

In 2001, he was awarded a postdoctoral grant from the Fundação para a Ciência e a Tecnologia of Portugal to work in the Universidade de Coimbra with Antonio Varandas. At the end of 2001 he is awarded with a Ramon y Cajal grant to work in the Grupo de Química Teórica y Computacional de la USC. In 2005 he gets the I3 positive evaluation from the Ministerio de Ciencia y Tecnología, and in 2006 becomes Profesor Contratado Doctor of the USC. The same year he gets the Habilitation and at the end of 2007 becomes Lecturer in the USC.

During the last ten years he has been working in collaboration with Zorka Smedarchina and Willem Siebrand and has developed an approximate instanton method. In collaboration with Donald Truhlar from the University of Minnesota, he has developed several tunneling approximations within variational transition state theory. He has authored about 60 scientific articles and 4 book chapters and has supervised one Ph.D. Thesis. In 2003 he was awarded with the Spanish Royal Society Chemistry Award to young scientists.

His research interests are focused in the development and application of methods for the study of chemical reaction dynamics. He carries out his research in the Centro Singular de Investigación en Química Biolóxica e Materiales Moleculares (CiQUS).



Félix Freire Iribarne
Associate Professor – CiQUS PI



Félix Freire (Marín, 1977) received his B.S. (2000), M.S. (2002) from the University of Santiago de Compostela. He got his Ph.D. (2005) from the same University working under the supervision of Prof. Ricardo Riguera and Emilio Quiñoá, working on the study of the absolute configuration of diols and triols by using ^1H NMR. During his Ph.D. he spent 4 months at Prof. Jesús Jiménez Barbero (CIB-CSIC, Madrid) to study the peptide folding by NMR.

In 2005 he performed a first postdoctoral stage in Prof. Jesús Jiménez Barbero and Dr. Juan Luis Asensio group (IQOG-CSIC (Lora Tamayo), Madrid) to work on peptide folding and protein/protein interactions by using NMR. In 2006, he moved to USA to work under the supervision of Prof. Samuel H. Gellman in Foldamers (MEC-Fulbright). His research was focused on the design, synthesis and structural studies of parallel β -sheets that fold in water. In 2009 he moved back to the USC to work in the helical polymers field as a Juan de la Cierva researcher. In 2010 he got the prestigious Ramón y Cajal research contract, to continuously working in the chiral polymer field. In 2012 he was awarded with the “SUSCHEM award” in the category of POSTDOC. Since 2016 he is Associate Professor at the USC.

His research is based on determining the relationship between monomer and the helical structure adopted by its corresponding polymer, the study of different chiral amplification mechanisms, and the formation of chiral nanostructures.



María Giménez López
Ramón y Cajal Researcher – CiQUS PI



Dr. Maria Gimenez is Principal Investigator at CiQUS and Honorary Associate Professor at the University of Nottingham. In 2006 she received her PhD from the University of Valencia working under the supervision of Prof. Eugenio Coronado on multifunctional materials of interest in molecular magnetism. She then joined the Supramolecular Chemistry and Chemical Nanosciences Group of Prof. Neil Champness at the University of Nottingham working as postdoctoral research fellow for almost three years. In 2009 she was awarded with a two-year Marie Curie Intra-European Fellowship in the Nanocarbon Group of Prof. Andrei Khlobystov.

In 2011, she started her independent career as Royal Society Research Fellow and in 2015 she became Assistant Professor of Materials Chemistry in Nottingham. In February 2018, she joined the CiQUS, launching her project **ERC-STG "NANOCOMP"**. The main interest of her group is the development of hybrid functional nanomaterials for spintronics and energy-related applications.

Maria studies have included a number of “firsts”, including the first observation of pressure-induced linkage isomerisation of the cyanide anion in Prussian Blue analogues; the first demonstrations of a molecular rhombus tiling; unusual nanoribbons inside carbon nanotubes; the encapsulation of single molecule magnets inside carbon nanotubes and assembly on a surface; the controlled assembly of preformed magnetic and electrocatalytic nanoparticles inside hollow nanostructures.

In 2012 she was awarded with a very prestigious prize (Emerging Investigator Award 2012) by the Spanish Royal Society of Chemistry for outstanding and novel research. In two consecutive years (2016 & 2017) she became Emerging Talent SRUK/CERU Award finalist for the impact of her studies on the development of materials chemistry using carbon nanostructures.



Concepción González Bello
Associate Professor – CiQUS PI



Concepción González-Bello, born in Vigo (Pontevedra, Spain) and graduated in Chemistry with honours at the University of Santiago de Compostela (Santiago de Compostela, Spain, 1989), obtained her PhD at the University of Santiago de Compostela (Santiago de Compostela, Spain) in 1994 under the supervision of Prof. Enrique Guitián. During her PhD studies, she did two predoctoral stays, first in the University of Gent (Gent, Belgium, 1991) with Prof. M. Vandewalle and then in the Scripps Research Institute (La Jolla, USA, 1992) with Prof. K. C. Nicolaou.

After a postdoctoral stay as an EC-fellow in the University of Cambridge (UK) with Prof. Chris Abell (1994-96), she joined the University of Santiago de Compostela as an Assistant Professor in 1996. She was promoted to Associate Professor in 2003 and obtained the Spanish habilitation to full Professor in 2011. She is a member of the International Advisory Board of the ChemMedChem (2010-) and an academic editor of PLOS ONE (2015-). She is one of the group leaders at the CiQUS.

Her main research interest is to develop updated therapies targeting infectious diseases, in particular, drugs with new mechanisms of action. She is an expert in the structure-, motion- and mechanism-based design of compounds and in computational studies to study the structural changes caused by these inhibitors. She is also interested in the resolution by X-ray crystallography of the enzyme-inhibitor complexes.



Enrique Guitián Rivera
Full Professor – CiQUS PI



Prof. Enrique Guitián received his PhD degree from the University of Santiago de Compostela (Spain) in 1981 for work in the field of natural product synthesis. After a postdoctoral work at the University of Hannover under Professor Winterfeldt he continued his career at Santiago (Associate Professor, 1985–1992; Full Professor, 1992-). His main research interests lie in the fields of aryne chemistry, especially pericyclic and transition-metal-catalyzed reactions of arynes, molecular materials and on-surface chemistry. He has published more than 100 papers and has supervised 20 doctoral thesis. His research interest has evolved from natural products synthesis to molecular materials and more recently to on-surface chemistry.



Moisés Gulías
Associate Professor – CiQUS PI



Moisés Gulías Costa graduated in chemistry at the University of Santiago de Compostela in 2001 and obtained his PhD in 2006 at the same university, under the supervision of Professor José L. Mascareñas, receiving the Extraordinary Doctorate Award of the University of Santiago de Compostela. During his PhD he made a doctoral stay at Stanford University (2004) with Prof. BM Trost.

Between 2007 and 2009 he was Marie-Curie postdoctoral fellow in the group of Professor Matthew Gaunt, (University of Cambridge). A year later (2010) he returned to the University of Santiago de Compostela as a Parga-Pondal Researcher. In 2015 he received the Thieme Chemistry Journal Award and the RSEQ Young Investigator Prize, given by the Spanish Royal Society of Chemistry (RSEQ). Since 2016 he is Associate Professor at the USC.

His work is focused in the development of new synthetic methods for the functionalization of carbon-hydrogen bonds through transition metal catalysis. In practice, it means he intends to develop a more direct, economic, simple and environmentally friendly access to drugs and biologically active compounds.



Massimo Lazzari

Associate Professor – CiQUS PI



Massimo Lazzari received his PhD in Macromolecular Chemistry in 1996 from the University of Torino (Italy). Postdoctoral Research Associate at the Prof. K. Hatada's laboratory (Osaka University, Japan, 1996-97), where he learned the secrets of anionic polymerisation.

In 1998 he joined as assistant professor the Group of Polymeric Materials at the University of Torino, working on the characterisation and degradation of complex polymer systems. After a short permanence as visiting professor at the University of Santiago de Compostela (Spain) in 2001, and then as Postdoctoral Research Associate (Marie Curie Fellowship by the European Union, 2002-03; Block copolymers for the fabrication of nanomaterials), he got a tenure track position at the Institute of Technological Investigations on research leave from the University of Torino.

He is Associate Professor at the University of Santiago de Compostela since the beginning of 2010, teaching at the Faculties of Chemistry and Physics (Bachelor and Master courses, such as Macromolecules and Colloids, Nanostructured Materials, Degradation, Stabilization and Recycling of Polymers).

His current research interests include (<http://www.fun-nanotech.org/>): fabrication of nanostructured polymeric materials; self-assembly of block copolymers in solution; hierarchical self-assembly of metal nanoparticles/block copolymers hybrid systems; polymeric systems as protecting/reducing agents in the synthesis of metal nanoparticles; polymer synthesis by controlled radical polymerization. He is co-author of about 50 papers on ISI journals and several book chapters, as well as co-editor of a book (Block Copolymers in Nanoscience, 2006 Wiley-VCH).



Fernando López

CSIC Senior Research Scientist – CiQUS PI



Fernando López García was born in 1975 in A Estrada; he studied Chemistry at the University of Santiago de Compostela where he obtained his degree in 1998. During his PhD at the same University, under the supervision of Prof. José L. Mascareñas, he carried out two predoctoral stays at the ETH-Zürich (with Prof. Erick M. Carreira) and at Yale University (with Prof. John F. Hartwig).

After receiving his PhD in 2003, he was awarded with a Marie-Curie Postdoctoral fellowship to join the group of Professor Ben L. Feringa at the University of Groningen, where his work was focused on enantioselective catalysis.

In 2006, he joined the University of Santiago de Compostela under the Ramón y Cajal programme. In 2008, he became Tenured Scientist at the Spanish National Research Council (CSIC) and joined the Instituto de Química Orgánica General (IQOG). In 2009 he received the RSEQ-SIGMA-ALDRICH Young Chemists Award of the Spanish Royal Society of Chemistry.

Presently, he has been assigned to the Centro Singular de Investigación en Química Biolóxica e Materiais Moleculares (CIQUS), at the University of Santiago de Compostela. His research is focused on the development of new transition metal-catalyzed processes with a focus on enantioselective catalysis.



Javier Montenegro

Ramón y Cajal Researcher – CiQUS PI



Javier Montenegro received his master degree (2003) and PhD (2009) from the University of Santiago de Compostela, under the direction of Prof. Susana López, working in the field of synthetic retinoids. In 2005 he was a visiting scientist in the group of Prof. Steven Ley at Cambridge University (Total Synthesis). In 2007 he was a visiting scientist at the Scripps Research Institute (La Jolla) working with Prof. Reza M. Ghadiri in prebiotic chemistry and supramolecular dynamic polymers. In 2009 he moved to the University of Geneva for postdoctoral studies with Prof. Stefan Matile in biosensing, synthetic transport systems and controlled delivery.

In 2012 he returned to Spain as a Juan de la Cierva fellow to work at the CIQUS associated with Prof. Juan R. Granja. He obtained a Ramon y Cajal contract at the Organic Chemistry Department and the CIQUS in the University of Santiago de Compostela. In 2015 he was awarded with an **ERC - Starting Grant** from the European Research Council (ERC).

His research interests are at the interphase between organic synthetic and supramolecular chemistry applied to biological systems and the discovery of new materials. Currently, he is mainly focused in the topological control of supramolecular assemblies for broad applications such as differential sensing, controlled delivery and tubular-templated composites.



Diego Peña Gil

Associate Professor – CiQUS PI



Diego Peña Gil was born in Santiago de Compostela in 1974. He graduated in Chemistry at the University of Santiago de Compostela in 1998, where he also obtained his PhD degree under the guidance of Profs. Enrique Guitián and Dolores Pérez, working in transition metal catalyzed cycloaddition reactions of arynes (2001, Special Doctorate Award).

He spent short predoctoral stays in the groups of professors Eric N Jacobsen (1999, Harvard University), Paul Knochel (2000, LMU, Munich) and Antonio M. Echavarren (2001, UAM, Madrid). During 2002 and 2003 he joined the group of Ben L. Feringa (Groningen University, The Netherlands) as a Marie Curie postdoctoral fellow working on asymmetric catalysis, with short research stays in the group of Hans de Vries (DSM, Geleen, The Netherlands).

In 2004 he returned to the University of Santiago de Compostela as Ramón y Cajal researcher, where he is Associate Professor since 2008. His main research interest is focused on the development of new synthetic methodologies, metal-based homogeneous catalysis, the chemistry of organic intermediates such as arynes, the synthesis of nanosized polycyclic aromatic compounds and nanographenes, and their study as new molecular materials.



Emilio Quiñoá Cabana
Full Professor – CiQUS PI



Emilio Quiñoá, a native of Lugo (Spain), obtained his B.S. and Ph.D. degrees in Chemistry from the University of Santiago de Compostela (USC), the latter in 1985 for work on Marine Natural Products from the Galician Coast under the supervision of Prof. Ricardo Riguera. From 1985 to 1988 he worked as a postdoctoral fellow with Professor Phillip Crews at the University of California, Santa Cruz (UCSC), where he participated in the study of bioactive metabolites from marine organisms of tropical waters. He returned to UCSC in 1989 and 1990 as Visiting Associate Professor, where he taught several Courses for Graduate Students.

After his return to the University of Santiago, he became Associate Professor in Organic Chemistry in 1989 and Full Professor in 1998. He is co-author of more than one hundred scientific publications, several textbooks for students, 5 patent applications, advisor in 15 Ph. D. Theses and has received several research awards. Also, he has been director of the Infrastructure Networks of Support to Research and Technological Development (RIAIDT) of USC.

After working on the Development of Novel NMR Methods for the Assignment of Absolute Configuration in the last decade, his current research interests are focused on the study of Stimuli-Responsive Dynamic Polymers and their Applications in Nanotechnology. H-index: 33



Ricardo Riguera Vega
Emeritus Professor – CiQUS PI



Prof. Ricardo Riguera received (1973) his Ph.D. in Chemistry from the University of Santiago de Compostela (Spain), under the supervision of Prof. I. Ribas, and carried out postdoctoral studies at University College London with Prof. P. Garrat (1974). In 1978, he was appointed Lecturer and in 1990 he became full Professor of Chemistry at the University of Santiago. His research is represented by around 200 papers and patents covering bioactive natural products, medicinal chemistry and NMR methods for determination of absolute configuration. In 2013 he was awarded the Félix Serratosa Medal by the Organic Chemistry Specialist Group (Royal Spanish Society of Chemistry).

He is now interested on polymeric nanostructures for biomedical applications and on stimuli responsive dynamic polymers. As academic he has authored three textbooks for students and served the University as Chairman of the Department, Dean of the Faculty and Vice-Chancellor.



Carlos Saá Rodríguez
Full Professor – CiQUS PI



Carlos Saá, born in Lugo (Spain), studied chemistry at the Universidad de Santiago de Compostela (Spain) where he received his PhD in 1985 under the supervision of Profs. L. Castedo, R. Suau and J. M. Saá for research on synthesis of isoquinoline alkaloids. Since 2004 he is Full Professor of Organic Chemistry at the Universidad de Santiago de Compostela (Spain).

He spent two-year (1987-1988) as a NATO postdoctoral research associate at the University of California, Berkeley, working with Prof. K. P. C. Vollhardt on Co(I)-catalyzed [2+2+2] cycloaddition of alkynes to nitriles: synthesis of ergot alkaloids.

His research interest centers on the discovery of new reactions using transition-metal catalysts and its applications in synthesis of valuable organic products.



Francisco Javier Sardina López
Full Professor – CiQUS PI



Prof. Javier Sardina was born in Santiago de Compostela (Spain) in 1958. He was trained as a synthetic organic chemist at the University of Santiago de Compostela (USC), where he received both his B.S. (1980) and Ph.D. (1985) degrees.

From 1986 to 1988 he was a Fulbright Scholar at the University of California, Berkeley, working in the laboratory of the late Prof. Henry Rapoport. Currently, he is a Professor of Organic Chemistry at the University of Santiago and his research interests range from asymmetric organic synthesis to the development of scientific computer software.

Professor Sardina is a co-founder and Director of the Scientific Advisory Board of MESTRELAB RESEARCH S. L., a USC spin-off company. Since 2013, he is a member of the INDITEX's Social Council, collaborating in the development of R&D about product health standards ("Clear to Wear and Safe to Wear") in the production of safe products, including the auxiliary chemical industry and its suppliers.



Eddy Sotelo Pérez

Associate Professor – CiQUS PI



Eddy Sotelo graduated in Chemistry at the University of Havana (1993) and obtained his PhD in 2000 under the guidance of Professor Enrique Raviña, at the Department of Organic Chemistry of the University of Santiago de Compostela. His post-doctoral experience has been developed in multidisciplinary research projects, in collaboration with the pharmaceutical industry, (University of Vienna, University Pompeu Fabra, University of Vigo, University of Bari).

In 2006 he joined the Institute of Industrial Pharmacy of the University of Santiago de Compostela as a Parga Pondal fellow, where he founded the Combinatorial Chemistry Unit (2006) and the COMBIOMED group (2008). Since January 2011 he is associate professor of Organic Chemistry at the Faculty of Pharmacy of the University of Santiago.

His research develops at pre-clinical phases of drug discovery, in close collaboration with groups from different disciplines. In this area he focuses on the development of high throughput synthetic methodologies as tools to accelerate the generation, identification and optimization of new candidates (Lead Generation and Lead Optimization), establish structure-activity relationships (SAR), the validation of new therapeutic strategies and the development of bivalent fluorescent pharmacological probes.



Jesús A. Varela Carrete

Associate Professor – CiQUS PI



Jesús A. Varela Carrete was born in 1971 in Lugo, Spain, and studied chemistry at the Universidad de Santiago de Compostela, Spain. He completed his M. Sc. in 1994 and his Ph. D. thesis in 1999 (excellent award) both under the supervision of Prof. Dr. Carlos Saá for research on synthesis of oligopyridines via cobalt chemistry. He spent a predoctoral research training period in Harvard University under supervision of Prof. Dr. Matthew Shair working on polyol synthesis by C-H insertion of metal-carbenes.

From 1999 to 2001, he spent a postdoctoral period as an Alexander Von Humboldt and Marie Curie Fellow with Prof. Dr. Paul Knochel at Ludwig Maximilians Universität in Munich (Germany), working on remote C-H activation via hydroboration. He joined the faculty at the Universidad de Santiago de Compostela as Ramón y Cajal researcher, and since 2008 as Profesor Titular.

His research interest centers on the elaboration and application of new catalytic methods in organic chemistry in order to facilitate new and better synthetic ways to organic molecules, specifically, in the synthesis of natural and synthetic bioactive products and in new organic materials.



M. Eugenio Vázquez Sentís
Associate Professor – CiQUS PI



M. Eugenio Vázquez (1973) graduated in Chemistry from the University of Santiago de Compostela in 1996 and obtained his PhD under the supervision of Prof. José Luis Mascareñas, working on synthetic DNA-binding peptides. In 2001 he received the "Human Frontier Science Program" (HFSP) long-term fellowship and joined Prof. Barbara Imperiali at MIT, where he worked for three years on the development of caged compounds and fluorescent probes as tools for studying complex biological processes.

He returned to Santiago as a "Ramón y Cajal" researcher in 2004, and received the "Career Development Award" from the HFSP. He obtained his permanent position at the Organic Chemistry Department in 2010. In 2008 he received the Sigma-Aldrich Young Researchers Award of the Spanish Royal Society of Chemistry, and in 2010 he received the Lilly young researcher award.

Our research is characterized by a multidisciplinary problem-solving approach that includes organic synthesis, spectroscopy, biochemistry and computational chemistry, applied to the development of chemical tools for biological research, such as luminescent probes to monitor kinase activity, and biomolecular interactions, caged compounds for spatial and temporal control of the biological response, and DNA binding agents, including supramolecular metallopeptides targeting non-canonical DNA



Rebeca García Fandiño
Ramón y Cajal Researcher



Dr. Rebeca Garcia-Fandiño, "Ramón y Cajal" researcher at CIQUS-USC, member of the Granja-Montenegro's group. Research career: graduated in Chemistry from USC (2001); PhD student in the group of Prof. L. Castedo and J. R. Granja (2001-2006); postdoctoral researcher in the group of Prof. M. Orozco (IRBB-Universidad de Barcelona, 2006-2009), and Prof. M. S. P. Sansom (Oxford-UK, 2009-2010); "Juan de la Cierva" researcher at CIQUS-USC (2010-2014); Ministerio da Ciência, Tecnologia e Ensino Superior de Portugal (FCT) Starting Grant researcher at Universidade de Ciências-Porto (Portugal, 2016-2018). Principal Investigator in different national and international projects: Investigadores Emerxentes 2012, MINECO-Retos 2015 (Jóvenes Investigadores), MINECO-Retos 2018, FCT-Projeto Exploratorio 2015 (Portugal), FCT National project (Portugal). Participation in the Management Committee of European COST Action (CM1306-H2020). More than 30 published articles in high impact journals, several book chapters and author of an internationally extended patent, a registered public database transferred to industry, and a registered software to visualize molecules in Augmented and Virtual Reality. Main founder of MD.USE Innovations SL, a University start-up that develops commercial scientific software & apps for molecule visualization & simulation based on state-of-the art technologies.



Miguel González Blanco
Ramón y Cajal Researcher



He obtained his PhD degree at Universidade de Santiago de Compostela, working on recombinogenic human minitallite sequeces in Dr. Gómez Márquez's lab. After short research stays at Instituto de Investigaciones Biomédicas "Alberto Sols" (Madrid) and Memorial Sloan-Kettering Cancer Center (New York), in 2006 he moved to Dr. Stephen C. West lab at Clare Hall Laboratories, London Research Institute (now part of The Crick Institute) as a postdoctoral fellow. There, he contributed to the characterization of yeast and human Holliday junction resolvases Yen1/GEN1 and the unveiling of the cell cycle-dependent regulatory mechanisms that control these and other structure-specific endonucleases. In 2014 he came back to Spain with a Ramón y Cajal contract and established the DNA Repair & Genome Integrity laboratory at the Center for Research in Molecular Medicine and Chronic Diseases (CiMUS), Universidade de Santiago de Compostela. The lab became part of the Health Research Institute of Santiago (IDIS) in 2017. His group focuses on understanding how cells coordinate essential DNA transactions, like replication, chromosomal segregation and DNA damage repair, in order to safeguard genome integrity.



Ramón Leis Fidalgo
Full Professor



Prof. Leis graduated from the Faculty of Chemistry of University of Santiago de Compostela in 1980 and received a Ph.D. degree in Chemistry in 1984. He has been a member of the USC Faculty since 1985, first as an assistant professor and, two years later, as an Associate Professor. He has worked as a post-doctoral research fellow at the University of Durham (UK) (1986) and University College London (UK) (1987) and as a visiting professor at the University College Wales, UK (1989), and at the ITODYS Institute de Topologie et Dynamique de la Reaction Chimique depending from CNRS and Universite de Paris VII (July 1997). In 2012 he was visiting scientist in the Department of Biomedical Engineering of Boston University.

J. R. Leis, is widely known for his contributions to Reaction Mechanism of Organic compounds, in particular he focused in nitroso group transfer and reactivity. Since 1993 his group has produced an important and internationally recognized work on the effect of the media on chemical reactivity with special focus on the role of microheterogeneous and biomimetic media such as colloidal solutions, micelles, microemulsions, vesicles, bilayers, etc.

Along with his teaching and research activities, J.R. Leis had important managing and High Direction activities, both at his University and in the Government of the Autonomous Region of Galicia. He was Vice-Rector of Research, Innovation and Post Graduate Studies of USC (1998-2002), Dean of the Faculty of Chemistry of USC (2003-2005), General Director of Universities of Galicia (2005-2009) and President of Galician Committee for Research Policies (2003-2006). From 2014 to 2019 Prof. Leis was Director of the International PhD School of the University of Santiago



Arturo López Quintela
Full Professor



Full Professor of Physical Chemistry at the University of Santiago de Compostela (USC, Spain). Postdoc in Germany at MPI für Biophysikalische Chemie, Göttingen and University of Bielefeld. Visiting Professor at MPI für Metallforschung, Stuttgart, Germany; Centre for Magnetic Recording Research, UCLA, USA; Yokohama Natl. University, Japan and Research Centre for Materials Science, Nagoya, Japan. Solvay Award in Chemistry and Burdinola Award in the Field of New Nanotechnologies in Chemistry. Co-founder and Principal Scientific Advisor of the company NANOGAP (www.nanogap.es), a spin-off from the USC founded in 2006 and dedicated to the production of nanomaterials and sub-nm metal (0) clusters. In 2019 co-founder of Nanogap Therapeutics (www.nanogaptherapeutics.com) to explore clusters as a new type of treatment to address major problems in oncology. Since 2005 Co-editor of the Journal of Colloid and Interface Science (Elsevier, Impact factor 6.4). He has published more than 300 publications (h-index 53), is co-author of 26 international patents (most of them under exploitation). His current research interests are: synthesis and properties of nanomaterials and “ligand-free” metal clusters by soft chemical techniques; synthesis of anisotropic nanomaterials and nanocomposites; catalytic, electrocatalytic, photocatalytic and therapeutic properties of “ligand-free” clusters.



Beatriz Pelaz
Ramón y Cajal Researcher



Dr. Beatriz Pelaz, co-director of the BNT Lab, research associate and member of the gfCP Lab. Research career: graduated in Chemistry from University of Valladolid (2005) and Biochemistry from University of Zaragoza (2011); master degree in experimental organometallic chemistry of the University of Valladolid (2006); PhD student in the group of Jesús M. de la Fuente at INA (2007-2012); European PhD degree from University of Zaragoza (2012); member of the group of Prof. Wolfgang J. Parak in the Philipps-University of Marburg (Germany), first as a postdoctoral researcher and since 2013, as a Humboldt Fellow. I was awarded with a Ramon y Cajal contract (ranked 3th in the Chemistry panel, 2017 call).



Víctor Sánchez Pedregal

Associate Professor



Graduate in Chemistry at the University of Oviedo (1992, Special Graduate Award). Ph.D. from the same university, under the supervision of prof. Vicente Gotor and Francisca Rebolledo (1997), working on the application of biocatalysis to organic chemistry. After working a few years for the industry (1998-2002), I moved to the Max Planck Institute (MPI-BPC Göttingen, 2002) with a Marie Curie Fellowship, to work on the NMR-based structural determination of proteins and RNA (NMR, Nuclear Magnetic Resonance).

In 2005, I joined the University of Santiago de Compostela (USC) holding a Fellowship from the program *Ramón y Cajal*. In 2010 I was appointed *Profesor Titular (Associate Professor)* at the USC. My current research focuses on the application of NMR to address structural questions at the interface between chemistry and biology, comprising the analysis of small molecules (e.g. with residual dipolar couplings, RDC) as well as the study of ligand/receptor interactions with large biomolecules.



Carlos Vázquez Vázquez

Associate Professor



He obtained his PhD degree in 1998 at Universidade de Santiago (USC) working on magnetic nanoparticles in the lab of Prof. M. Arturo López Quintela. He did post-doctoral stays at Université du Maine (Le Mans, France), Research Center for Materials Science (Nagoya University, Japan) and Max-Planck Institute of Colloids and Interfaces (Potsdam, Germany). He is Associate Professor of Physical Chemistry of the USC (Spain) and has large experience in the synthesis and characterization of different nanomaterials by wet chemical routes. He is co-founder of NANOGAP SUB-NM POWDER S.A. and Scientific Advisor from 2011. His research interest fields are synthesis and properties of nanomaterials; experimental study of nanostructured systems: films and particles; transport and magnetic properties in metal oxides and nanocomposites; self-assembly in colloidal dispersions; synthesis and properties of sub-nanometric atomic quantum clusters and anisotropic growth of nanomaterials (nanorods, nanofibers).



Ester Polo

Juan de la Cierva "Incorporación" Researcher



Dr. Ester Polo, research associate and member of gfCP Lab. Research career: degree in Biochemistry (2006) and M.Sc. in Molecular and Cellular Biology (2008) from the University of Zaragoza; PhD from Zaragoza University (INA, Spain, 2013); postdoctoral researcher at the CBNI (Center for BioNano Interactions, University College Dublin) directed by Prof. Kenneth Dawson; fellow of the CiQUS international postdoctoral program (2017-2018). I was awarded with a Juan de la Cierva -Incorporación contract (Chemistry panel, 2016 call).



Julián Bergueiro

Juan de la Cierva “Incorporación” Researcher



Dr. Julián Bergueiro Álvarez received his BS in Chemistry from the University of Santiago de Compostela (Spain) in 2007. In 2008 he obtained the MS in Organic Chemistry and in 2013 he received his PhD from USC for his work in sterecontrolled synthesis of retinoids employing transition metal catalyzed reactions in the key steps. During the last year of his PhD he joined the group of Prof. R. Riguera and Prof. E. Quiñoá to work on the synthesis and characterization of stimuli response helical polymers and poly(phenylacetylene)s@gold nanoparticles nanocomposites. In October 2013, he joined Prof. M. Calderón group to carry out his postdoctoral research at Freie Universität Berlin. In 2016 he stayed at Aida lab in Tokyo University. Recently he joined Granja/Montenegro labs at CIQUS (University of Santiago de Compostela) within the Spanish Ministry of Science returning program Juan de la Cierva.

His current research is focused on thermoresponsive helical polymers, polymer-gold nanoparticle supramolecular assemblies, and thermoresponsive nanogels as novel drug delivery nanocarriers.

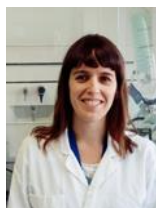


Marc Font Molins

Juan de la Cierva “Incorporación” Researcher



Marc Font studied Chemistry at the University of Girona, where he was awarded his MChem in 2011. In 2015 he earned his PhD in Chemistry from the University of Girona for studies focused on the elucidation of the mechanisms of the coinage metal-catalysed cross-coupling reactions under the guidance of Dr. Xavi Ribas and Dr. Miquel Costas. His PhD studies included a research period with Prof. John F. Hartwig at the University of California at Berkeley. Following this, he joined the group of Prof. Igor Larrosa at the University of Manchester pursuing postdoctoral studies on the development of novel methods for C–H functionalisation. He is currently a postdoctoral fellow at the University of Santiago de Compostela working in Prof. José Luis Mascareñas and Dr. Moisés Gulías laboratories.



Fátima García Melo

Juan de la Cierva “Incorporación” Researcher



Fátima studied Chemistry at Universidad Complutense de Madrid. She obtained her PhD degree in 2013 at the same University under the supervision of Prof. Luis Sánchez working on self-assembly and supramolecular polymers, focusing on chirality transfer processes. During her PhD she was a visitor at Eindhoven University of Technology (2011 and 2012, E. W. Meijer’s group). In 2016-2018 she was a postdoctoral researcher at the group of Dr. Maarten Smulders (Wageningen University, The Netherlands) working of functional materials responsive to multiple stimuli. Since 2016 she joined the group of Prof. Enrique Guitián, Prof. Dolores Pérez and Dr. Diego Peña at CiQUS to work on the synthesis of polyaromatic hydrocarbons and on-surface chemistry.

**Ignacio Insua López**

Juan de la Cierva "Formación" Researcher



Nacho received his PhD from the University of Birmingham in 2017 (Dr. Francisco Fernández-Trillo). He then joined the University of Melbourne as a Postdoc (Prof. Greg Qiao, 2017-18). His research focuses on the application of polymers and peptides, through self-assembly and nanotechnology, as biomedical tools. He enjoys playing the bass and chess. He joined Javier Montenegro group as a Juan de la Cierva postdoctoral researcher. He is currently a Marie Curie postdoctoral fellow.

**Christian Vidal**

Juan de la Cierva "Formación" Researcher



Cristian Vidal Vides studied PhD at the University of Oviedo under the supervision of Joaquín García Álvarez, a "Ramón y Cajal" fellow, and Prof. Victorio Cadierno. Then, he joined our group as a Postdoctoral Researcher, working under the supervision of Prof. José L. Mascareñas (CiQUS, University of Santiago de Compostela). Nowadays he is a Postdoctoral fellow under the "Juan de la Cierva" program.

**Manuel Amorín**

Associate Professor



Dr. Manuel Amorín studied his Degree in Chemistry at the University of Santiago de Compostela (2000), where he also obtained his PhD degree under the supervision of Professor Juan R. Granja, on supramolecular chemistry, more specifically in the field of peptide nanotubes (2005, Special Doctorate Award). During that time, he spent short pre-doctoral stays in the group of Professor M. R. Ghadiri (Scripps Research Institute, USA) and in the group of Professor H. Bayley (University of Oxford, United Kingdom). - In the period 2006 - 2008, thanks to a MEC / Fulbright Scholarship, he complemented his training with a postdoctoral stay in the group of Prof. M. R. Ghadiri. Where he worked in the design and synthesis of new systems of DNA sequencing with nanopore proteins and in antimicrobial systems based on peptide nanotubes. In 2009, he returned to the University of Santiago de Compostela as Ramón y Cajal researcher. He is currently Prof. Contratado Doctor (Associate Professor, 2015) in the Department of Organic Chemistry. His research lines are focused on the structural design and applications of new peptide nanotubes that incorporate alpha-, gamma- and delta-amino acids, which allow the internal and external modification of these supramolecular systems. This provides, to these structures, a wide variety of properties for their application in the biological and in the materials fields.



María Tomás
CiQUS Research Associate



María Tomás Gamasa studied Chemistry at University of Oviedo where she obtained his degree in 2006. She carried out her PhD studies as FPU fellow at the same University under the supervision of Prof. J. Barluenga Mur. As result, her thesis was awarded with the Extraordinary Award of University of Oviedo. She was also recognized with the Award SUSCHEM” 2010 (PREDOC) from the Spanish Royal Society of Chemistry”. During her PhD she also carried out two predoctoral stays at Bristol University (England) under the supervision of Prof. V. K. Aggarwal and at Université de Montréal (Canada) under the supervision of Prof. A. Charette.

After receiving her PhD, she was awarded with a Spanish fellowship to join the group of Prof. T. Carell, at the University of Munich. Between 2012 and 2014 she was awarded with an Alexander von Humboldt grant. In 2015 she joined the University of Santiago de Compostela as “Juan de la Cierva” fellow, under the supervision of Prof. J. L. Mascareñas.

Her research is focused on the development of metal-catalyzed transformations in biological habitats, including living cells, and their implementation for bio-sensing and targeted therapy.

Teaching Timetable

ACADEMIC COURSE 2020/2021: Teaching timetable

Experimental courses

SUBJECTS ACRONYMS: **Catal** – Catalysis; **MagRes** – Magnetic Resonance; **EspecTech** – Espectroscopic and Espectrometric Techniques; **MolMat** – Molecular Materials; **Microsc** – Microscopy.

SEPTEMBER 2020

Monday		Tuesday		Wednesday		Thursday		Friday		Sat	Sun
1		2		3		4		5		6	7
7		8		9		10		11		12	13
14		15		16		17		18		19	20
21	16h-17:30h MolMat	22	16h-17:30h MagRes	23	16h-17:30h MolMat	24	16h-17:30h MagRes	25	16h-17:30h MolMat	26	27
	17:30h-19h Catal		17:30h-19h Microsc		17:30h-19h Catal		17:30h-19h Microsc		17:30h-19h Catal		
	19h-20:30 EspecTech		9:30h-12h safety course at CiQUS		19h-20:30h EspecTech						
28	16h-17:30h MolMat	29	16h-17:30h MagRes	30	16h-17:30h MolMat						
	17:30h-19h Catal		17:30h-19h Microsc		17:30h-19h Catal						
	19h-20:30 EspecTech		10h-13h Initiation to NMR		19h-20:30h EspecTech						

PLACE: Chemistry Faculty (maths room, third floor)

SUBJECTS ACRONYMS: **Catal** – Catalysis; **MagRes** – Magnetic Resonance; **EspecTech** – Spectroscopic and Espectrometric Techniques; **MatMol** – Molecular Materials; **Microsc** – Microscopy; **ColIntChar** – Coloidal and Interface Characterization.

OCTOBER 2020

Monday		Tuesday		Wednesday		Thursday		Friday		Sat	Sun
						1	16h-17:30h MagRes 17:30h-19h Microsc	2	16h-17:30h MolMat 17:30h-19:30h Catal	3	4
5	16h-17:30h MolMat 17:30h-19h Catal 19h-20:30h EspecTech	6	16h-17:30h MagRes 17:30h-19h ColIntChar	7	16h-17:30h MolMat 17:30h-19:30h Catal	8	16h-17:30h MagRes 17:30h-19h ColIntChar	16	16h-17:30h MolMat 17:30h-19:30h Catal	10	11
12	FESTIVITY	13	16h-17:30h MagRes 17:30h-19h ColIntChar	14	16h-17:30h MolMat 17:30h-19h Catal	15	16h-17:30h MagRes 17:30h-19h ColIntChar	16	16h-17:30h MolMat 17:30h-19h Catal	17	18
19	11h-12h Prof. Dirk Guldi "Energy - Demand and Supply" 16h-17:30h MolMat 17:30h-19h Catal 19h-20:30h EspecTech	20	11h-12h Prof. Dirk Guldi "Basic Principles of Electron Transfer" 16h-17:30h Microsc 17:30h-19h ColIntChar	21	11h-12h Prof. Dirk Guldi "Natural Photosynthesis" 16h-17:30h MolMat 17:30h-19h Catal	22	11h-12h Prof. Dirk Guldi "Artificial Photosynthesis" 16h-17:30h Microsc 17:30h-19h ColIntChar	23	11h-12h Prof. Dirk Guldi "Photovoltaics" 16h-19h Catal	24	25
26	16h-19h MatMol	27	16h-17:30h Microsc 17:30h-19h ColIntChar	28		29	16h-17:30h Microsc 17:30h-19h ColIntChar	30		31	

PLACE: Chemistry Faculty (maths room, third floor)

SUBJECTS ACRONYMS: **BioCelChem** – Biological and Cellular Chemistry; **NanoEstMat** – Nanostructured Materials; **ChemSyn** – Chemical Synthesis; **QSupramol** – Supramolecular Chemistry; **MagRes** – Magnetic Resonance.

NOVEMBER 2019

Monday	Tuesday	Wednesday	Thursday	Friday	Sat	Sun
						1
2	3	4	5	6	7	8
		16h-19h MatMol (Exam)				
9	10	11	12	13	14	15
	16h-19h Catal (Exam)		16h-17:30h SupramolChem	FESTIVITY		
			17:30h-19h ChemSyn			
16	17	18	19	20	21	22
16h-17:30 NanoEstMat	16h-17:30h SupramolChem	16h-17:30 NanoEstMat	16h-17:30h SupramolChem	16h-17:30 NanoEstMat	16h-17:30 NanoEstMat	16h-17:30 NanoEstMat
17:30h-19h BioCelChem	17:30h-19h ChemSyn	17:30h-19h BioCelChem	17:30h-19h ChemSyn	17:30h-19h BioCelChem	17:30h-19h BioCelChem	17:30h-19h BioCelChem
		19-20:30h QSupramol				
23	24	25	26	27	28	29
16h-17:30 NanoEstMat	16h-17:30h SupramolChem	16h-17:30 NanoEstMat	16h-17:30h SupramolChem	16h-17:30 NanoEstMat	16h-17:30 NanoEstMat	16h-17:30 NanoEstMat
17:30h-19h BioCelChem	17:30h-19h ChemSyn	17:30h-19h BioCelChem	17:30h-19h ChemSyn	17:30h-19h BioCelChem	17:30h-19h BioCelChem	17:30h-19h BioCelChem
		19-20:30h SupramolChem				
30						
16h-17:30 NanoEstMat						
17:30h-19h BioCelChem						

PLACE: Chemistry Faculty (maths room, third floor)

SUBJECTS ACRONYMS: **BioCelChem** – Biological and Cellular Chemistry; **NanoEstMat** – Nanostructured Materials; **ChemSyn** – Chemical Synthesis; **SupramolChem** – Supramolecular Chemistry.

DECEMBER 2019

Monday		Tuesday		Wednesday		Thursday		Friday		Sat	Sun
		1	16h-17:30h SupramolChem 17:30h-19h ChemSyn	2	16h-17:30 NanoEstMat 17:30h-19h BioCelChem 19-20:30h SupramolChem	3	16h-17:30h SupramolChem 17:30h-19h ChemSyn	4	16h-17:30 NanoEstMat 17:30h-19h BioCelChem	5	6
7		8	FESTIVITY	9	16h-17:30 NanoEstMat 17:30h-19h BioCelChem 19-20:30h SupramolChem	10	16h-17:30h SupramolChem 17:30h-19h ChemSyn	11	16h-17:30 NanoEstMat 17:30h-19h BioCelChem	12	13
14	16h-17:30 NanoEstMat 17:30h-19h BioCelChem	15	16h-17:30h SupramolChem 17:30h-19h ChemSyn	16	16h-17:30h NanoEstMat	17	16h-19h SupramolChem	18	17:30h-19h BioCelChem	19	20
21		CHRISTMAS BREAK (22-31)									

PLACE: Chemistry Faculty (maths room, third floor)

SUBJECTS ACRONYMS: **ExpTechMBM** – Experimental Techniques in Molecular Biology and Biomedicine; **ChemSyn** – Chemical Synthesis; **MolMag** – Molecular Magnetism; **DetReacMec** – Determination of Reaction Mechanism; **NanoBioTech** – Nanobiotechnology; **CompChem** – Computational Chemistry.

JANUARY 2020

L	M	MI	J	V	S	D
CHRISTMAS BREAK				8	9	10
11	12	13	14	15	16	17
		16h-19h SupramolChem (Exam)				
18	19	20	21	22	23	24
		16h-19h BioCelChem (Exam)		16h-19h NanoEstMat (Exam)		
25	26	27	28	29	30	31
16h-17:30h DetReacMec	16h-17:30h ChemSyn	16h-17:30h DetReacMec	16h-17:30h ChemSyn	FESTIVITY		
17:30h-19h MolMag	17:30h-19h NanoBioTech	17:30h-19h MolMag	17:30h-19h NanoBioTech			
19h-20:30h ExpTechMBM	19h-21h CompChem	19h-20:30h ExpTechMBM	19h-21h CompChem			

PLACE: Chemistry Faculty (maths room, third floor)

SUBJECTS ACRONYMS: **ExpTechMBM** – Experimental Techniques in Molecular Biology and Biomedicine; **ChemSyn** – Chemical Synthesis; **MolMag** – Molecular Magnetism; **DetReacMec** – Determination of Reaction Mechanism; **NanoBioTech** – Nanobiotechnology; **CompChem** – Computational Chemistry; **BioPhys** – Biophysic.

FEBRUARY 2020

L		M		MI		J		V		S	D
1	16h-17:30h ChemSyn	2	16h-17:30h DetReacMec	3	16h-17:30h ChemSyn	4	16h-17:30h DetReacMec	5	16h-19h ChemSyn	6	7
	17:30h-19h NanoBioTech		17:30h-19h MolMag		17:30h-19h NanoBioTech		17:30h-19h MagMol				
	19h-21h CompChem		19h-20:30h ExpTechMBM		19h-21h CompChem		19h-20:30h ExpTechMBM				
8	16h-17:30h DetReacMec	9	16h-17:30h BioPhys	10	16h-17:30h DetReacMec	11	16h-17:30h BioPhys	12	16h-17:30h DetReacMec	13	14
	17:30h-19h MolMag		17:30-19h NanoBioTech		17:30h-19h MolMag		17:30h-19h NanoBioTech		17:30h-19h MolMag		
	19h-20:30h TécBioMol		19h-21h CompChem		19h-20:30h ExpTechMBM		19h-21h CompChem		19h-20:30h ExpTechMBM		
15	FESTIVITY	16	FESTIVITY	17	16h-17:30h BioPhys	18	16h-17:30h DetReacMec	19	FESTIVITY	20	21
					17:30h-19h NanoBioTech		17:30h-19h MolMag				
					19h-21h CompChem		19h-20:30 ExpTechMBM				
22	16h-17:30h DetReacMec	23	16h-17:30h BioPhys	24	16h-17:30h DetReacMec	25	16h-17:30h BioPhys	26	16h-17:30h DetReacMec	27	28
	17:30h-19h MolMag		17:30-19h NanoBioTech		17:30h-19h MolMag		17:30h-19h NanoBioTech		17:30h-19h MolMag		
	19h-20:30h ExpTechMBM		19h-21h CompChem		19h-20:30h ExpTechMBM		19h-21h CompChem		19h-21h CompChem		

PLACE: Chemistry Faculty (maths room, third floor)

SUBJECTS ACRONYMS: **ExpTechMBM** – Experimental Techniques in Molecular Biology and Biomedicine; **ChemSyn** – Chemical Synthesis; **MolMag** – Molecular Magnetism; **DetReacMec** – Determination of Reaction Mechanism; **NanoBioTech** – Nanobiotechnology; **CompChem** – Computational Chemistry; **BioPhys** – Biophysic.

MARCH 2020

L		M		MI		J		V		S	D
1	16h-17:30h DetReacMec	2	16h-17:30h BioPhys	3	16h-19h DetReacMec	4	16h-17:30h BioPhys	5	16h-19h MolMag	6	7
	17:30h-19h MolMag		17:30h-19h NanoBioTech				17:30h-19h NanoBioTech				
	19h-20:30h BioPhys		19h-21h CompChem				19h-21h CompChem				
8	16h-19h BioPhys	9	16h-19h NanoBioTech	10		11		12	16h-19h ExpTechMBM (Exam)	13	14
			19h-21h CompChem								
15	16h-19h CompChem (Exam)	16		17	16h-19h DetReacMec (Exam)	18		19	16h-19h MolMag (Exam)	20	21
22	16h-19h ChemSynt (Exam)	24		24	16h-19h NanoBioTech (Exam)	25		26	16h-19h BioPhys (Exam)	27	28
29	EASTER BREAK	30	EASTER BREAK	31	EASTER BREAK						

APRIL 2020

L		M		MI		J		V		S	D
						1	EASTER BREAK	2	EASTER BREAK	3	4
6		7		8		9		10		11	12
13		14		15		16		17		18	19