# Dottorato di Ricerca in Scienze Chimiche - Università degli Studi di Firenze

## PROPOSTA DIDATTICA 2018

# SSD: CHIM/01

**TITOLO DEL CORSO:** NOTES ON INSTRUMENTAL METHODS IN BIOPOLYMERS ANALYSIS

**DOCENTE:** Dr. PASQUALE PALLADINO (Dept. Chemistry "Ugo Schiff", University of Florence)

**ABSTRACT:** The topics will be presented in form of lecture and discussion (two teaching hours per week). Students will be introduced to the definition and examples of biopolymers. They will be introduced to the physico-chemical-biological properties of biopolymers, especially in relation to their potential use, in comparison with the synthetic polymers. Students will be provided with description of instrumental methods in biopolymers analysis. In addition, the course covers the basic principles of data analysis and manuscript organization for a scientific journal.

**Periodo di Svolgimento:** February 2018

**Numero minimo di studenti per l'attivazione:** 5

**Prova di accertamento:** review and discussion of a scientific paper on a topic covered by the course.

# SSD: CHIM/02

**TITOLO DEL CORSO:** CONFOCAL MICROSCOPY-RELATED TECHNIQUES: THEORY AND APPLICATIONS

**DOCENTE:** Dr. COSTANZA MONTIS (Dept. Chemistry "Ugo Schiff", University of Florence)

**ABSTRACT:** The aim of the course is to provide an overview on Confocal Microscopy and on Confocal Microscopy-related techniques, both introducing the basic principles of each technique and highlighting the possible applications on different research topics. First, the topic of optical resolution and super-resolution will be introduced and the basics of confocal microscopy will be reviewed. Imaging and 3D reconstruction methodologies will be then considered with particular focus on the obtainment of quantitative information from 2D images through image analysis. Some of the main confocal microscopy-related techniques as spatially resolved fluorescence emission, spatially resolved Foerster Resonance Energy Transfer (FRET), Fluorescence Lifetime Imaging (FLIM) and FRET-FLIM will be then examined both from theoretical and applicative point of view. Finally, diffusion-related techniques will be considered: Fluorescence Recovery After Photobleaching (FRAP), Particle Tracking, Fluorescence Correlation Spectroscopy (FCS) and Fluorescence Cross-Correlation Spectroscopy (FCCS).

**Periodo di Svolgimento:** February 2018

**Numero minimo di studenti per l'attivazione:** 1

**Prova di accertamento:** review and discussion of a scientific paper on a topic covered by the course.

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# SSD: CHIM/03

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**TITOLO DEL CORSO:** Orbital Interactions in Chemistry

**DOCENTE:** Prof. FEDERICO TOTTI (Dept. Chemistry "Ugo Schiff", University of Florence)

**ABSTRACT:** The course will cover the construction of molecular orbital interactions through a perturbative theoretical approach. In this framework, the operative applications will cover both organic and inorganic species. The aim of the course is to make the student able to sketch the electronic structure of the species under study in order to understand and predict their reactivity and electronic properties

**Periodo di Svolgimento:** February 2018: 1 – 4 – 15 – 18 (sempre alle ore 11)

**Numero minimo di studenti per l'attivazione:** 2

**Prova di accertamento:** Final discussion about the potential applications of the topics covered by the course to the research activities of the PhD student.

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**TITOLO DEL CORSO:** SOL-GEL CHEMISTRY: SYNTHESIS, CHARACTERIZATION AND APPLICATIONS OF INORGANIC POROUS MATERIALS

**DOCENTE:** Dr. NOEMI LINARES (Molecular Nanotechnology Lab, Department of Inorganic Chemistry, University of Alicante)

**REFERENTE:** Dr. Carmen Moreno-Marrodan (ICCOM – CNR Florence)

**ABSTRACT:** The course will deal with the synthesis of different inorganic materials using sol-gel chemistry. A brief introduction of the sol-gel chemistry approach will be provided, together with a detailed explanation of the type of inorganic materials that can be synthesized, the most important methods employed in their characterization and also the wide range of applications that they cover nowadays. Sol-gel chemistry is typically used in combination with molecular and supramolecular templates, especially surfactants, to produce a wide variety of porous metal oxides. Both soft templates, such as surfactant and polymers and hard templates such as carbon and metal oxides and carbonates which can be burned-off or easily dissolved at a certain pH, have being extensively used to introduce controlled mesoporosity in a wide variety of solids. This is a simple and versatile strategy able to produce very complex and interconnected porous structures. Regarding the porous texture of these solids, they can be studied by a combination of different techniques such as, physical adsorption, mercury porosimetry, X-Ray diffraction or electronic microscopy, with each

technique allowing the study of the porosity in a particular range. Finally, special attention will be paid to important applications of porous inorganic materials which in the last years have become countless. Currently, they are frequently employed in catalysis, weather as catalysts or supports, adsorption, pollutant remediation, sensors, drug delivery systems, photocatalysis, batteries, solar and fuel cells.

**Periodo di Svolgimento:** 9-13 April 2018

**Numero minimo di studenti per l'attivazione:** 5

**Prova di accertamento:** Test

# SSD: CHIM/04

**TITOLO DEL CORSO:** PLASTIC WASTE MANAGEMENT

**DOCENTE:** Dr. LUCA ROSI (Dept. Chemistry “Ugo Schiff”, University of Florence)

**ABSTRACT:** The objective of this course is to present the pyrolysis (thermal treatments) as a recycling process of plastic waste management and their valorization. Pyrolysis is able to convert these waste materials into a gas, a liquid and a solid that can have a second life realizing the last step of a circular economy. The solid may be employed as filler to obtain composites or a solid fuel while the liquid may be the source of chemicals or as liquid fuel. Some processes of catalytic upgrading of oils from pyrolisis for their use as fuels are presented.

**Periodo di Svolgimento:** 15 May - 7 September 2018

**Numero minimo di studenti per l'attivazione:** 1

**Prova di accertamento:** review and discussion of a scientific paper on a topic covered by the course.

# SSD: CHIM/06

**TITOLO DEL CORSO:** PEPTIDOMIMETICS IN ORGANIC AND MEDICINAL CHEMISTRY

**DOCENTE:** Prof. Andrea Trabocchi (Dept. Chemistry “Ugo Schiff”, University of Florence)

**ABSTRACT:** A peptidomimetic is a small protein-like chain designed to mimic a peptide with adjusted molecular properties such as enhanced stability or biological activity. It is a very powerful approach for the generation of small-molecule-based drugs as enzyme inhibitors or receptor ligands. These lessons on Peptidomimetics in Organic and Medicinal Chemistry will focus on synthetic strategies underlying the building of bioactive compounds of a peptidomimetic nature. Topics covered include the chemistry of unnatural amino acids, peptide- and scaffold-based peptidomimetics, amino acid-side chain isosteres, backbone isosteres, dipeptide isosteres, beta-turn peptidomimetics, proline-mimetics as turn inducers, cyclic scaffolds, amino acid surrogates,

and scaffolds for combinatorial chemistry of peptidomimetics. Case studies in the hit-to-lead process illustrate the successful application of peptidomimetics in drug discovery.

**Periodo di Svolgimento:** 1-15 February 2018

**Numero minimo di studenti per l'attivazione:** 5

**Prova di accertamento:** review and discussion of a scientific paper on a topic covered by the course.

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**T TITOLO DEL CORSO:** ADVANCED MASS SPECTROMETRY: PRACTICAL ASPECTS AND APPLICATIONS

**DOCENTE:** ZBIGNIEW SZEWCZUK (Faculty of Chemistry, University of Wroclaw )

**REFERENTE:** Prof. Anna Maria Papini (Dept. Chemistry "Ugo Schiff", University of Florence))

**ABSTRACT:** 1. Mass Spectrometry: Principles and Applications, (3-4 hours). Introduction, ion sources, mass analyzers, tandem mass spectrometry (MS/MS), liquid chromatography–mass spectrometry (LC-MS)
2. Interpretation of Mass Spectra: Qualitative Analysis: (3 hours). High resolution mass spectrometry, fragmentation analysis (EI, CID, ECD, and ETD), isotopic exchange, ion mobility,
3. Interpretation of Mass Spectra: Quantitative Analysis (2-3 hours) Non-derivatization and derivatization methods, stable isotope dilution (SID), Isobaric labeling (iTRAQ), multiple-reaction monitoring (MRM) mass spectrometry
Students will use the fundamentals of the above topics to solve some scientific problems, including:

- Development of analytical strategies.
- Molecular identification of unknown natural compounds by exact mass analysis and by use of tandem mass spectrometry (from recorded spectra)
- Design and evaluation of analytical techniques, including LC-MS, MS/MS, for quantification and qualification analyses of biomolecules in food, cosmetics, etc.

**Periodo di Svolgimento:** 4-11 March 2018

**Numero minimo di studenti per l'attivazione:** 5

**Prova di accertamento:** Analysis of Mass Spectra from different molecule typologies and analysis of the literature on the applications of the most recent techniques in the field of food, cosmetics, etc.

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**TITOLO DEL CORSO:** DRUG DISCOVERY: THE EXPERIENCE OF A CHEMISTRY LABORATORY IN A PARTNER RESEARCH ORGANIZATION IN ITALY

**DOCENTE:** Dr. ELISABETTA BIANCHI (Head of Peptide Chemistry at IRBM SCIENCE PARK)

**REFERENTE:** Prof. Anna Maria Papini (Dept. Chemistry "Ugo Schiff", University of Florence))

**ABSTRACT:** Historical Development of Drugs and Pharmacy, description of the drug discovery process, identification of pharmacological targets, drug target interactions, hit compounds identification and primary assays, screening funnel, secondary assay and biomarkers, concepts in medicinal chemistry and lead compound series, structure activity studies, peptide therapeutics as innovative drugs, drug metabolism and pharmacokinetics.

**Periodo di Svolgimento:** June 2018

**Numero minimo di studenti per l'attivazione:** 5

**Prova di accertamento:** review and discussion of a scientific paper on a topic covered by the course.

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**TITOLO DEL CORSO:** TRANSFER FROM A LABORATORY SYNTHETIC METHOD TO AN INDUSTRIAL METHOD FOR THE SYNTHESIS OF ACTIVE PHARMACEUTICAL INGREDIENTS (API)

**DOCENTE:** Dr. GIORGIO BERTOLINI, Dr. ALESSANDRO AGOSTI, Dr. PAOLANGELO CEREA (OLON S.p.a.)

**REFERENTE:** Prof. Alberto Brandi ( Dept. Chemistry "Ugo Schiff", University of Florence))

**ABSTRACT:** The production of Active Pharmaceutical Ingredients (API) plays a very important role in the industry in Italy since there are many companies involved in this business segment that export most of their production abroad.
This type of industry is characterized by extremely complex chemical processes using many classes of chemical reactions and technologies that usually are not thought to be applicable in large scale. Among them we can mention the use of organometallic reagents (e.g. Butyl Lithium etc) and/or very low temperature reactions (e.g. -78°C).
To scale-up these chemical processes in an efficient and safe mode it is required a deep knowledge of the organic chemistry, even the mechanism of the reaction, behind the reactions used in the process.
In addition several activities are required to transform a Lab method to a real chemical process. It is compulsory to integrate the organic chemistry with additional knowledge of physical chemistry, statistics and industrial economics.
Part of this course is the presentation and discussion of different approaches and methodologies normally used in the phases of design, optimization and scale-up of a chemical processes and that can be classified in four classes:

- General aspects to be considered and evacuate in the design phase of design of a new synthetic approach for the synthesis of complex molecules (In addition to the usual evaluation on the nature of starting materials, reagents, product and yields)
- Mythologies for the assessment of the efficiency of a chemical process (efficiency metrics) (eg. Atom economy, Environmental Impact Factor, Reaction Mass Intensity etc)
- Process safety to be used for both reduce the risk associated to a chemical process and as a tool to increase the knowledge on the mechanism of the reactions e for the optimization of the process

- Statistical approaches starting from the development/optimization phase of the process and for the results evaluation (eg. yield or quality attributes), in both scale-up and production phases as an important tool for the “continuous improvement” of the process.

**Periodo di Svolgimento:** 26 March -6 April 2018

**Numero minimo di studenti per l'attivazione:** 5

**Prova di accertamento:** Final Test

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# SSD: CHIM/12

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**TITOLO DEL CORSO:** FUNDAMENTALS OF RHEOLOGY

**DOCENTE:** Dr. EMILIANO CARRETTI (Dept. Chemistry “Ugo Schiff”, University of Florence)

**ABSTRACT:** The main target of this course is to give to the auditorium some general skills in the field of rheology. The first part of the course will be focused on the fundamental topics of rotational rheology: definition of shear stress, shear strain, shear rate and viscosity. Description of shear and extensional flow modes. Analysis of the rheology of non-Newtonian fluids and of the most important parameters of the flow curve: Zero-shear and infinite-shear viscosity and shear-thinning behavior. The second part will be concentrated on the understanding the structural effects: yield stress, thixotropy and viscoelasticity of structured fluids. Description of the main viscoelastic parameters: complex, elastic and viscous modulus, phase angle and tan. Viscoelasticity and deformation: timescale effects: the Deborah number. Introduction to non linear viscoelasticity (LAOS).

**Periodo di Svolgimento:** February 2018

**Numero minimo di studenti per l'attivazione:** 1

**Prova di accertamento:** review and discussion of a scientific paper on a topic covered by the course.

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**TITOLO DEL CORSO:** FOCAL PLANE ARRAY (FPA) IMAGING FTIR: PRINCIPLES AND APPLICATIONS

**DOCENTE:** Dr. DAVID CHELAZZI (Dept. Chemistry “Ugo Schiff”, University of Florence)

**ABSTRACT:** Coupling microscopy with Fourier Transform Infrared Spectroscopy (micro-FTIR) enables the non-invasive and non-destructive detection of molecular functional groups. The use of Focal Plane Array (FPA) detectors allows the simultaneous acquisition of spatially resolved IR spectra on an array of n x n pixels, each pixel corresponding to an independent spectrum. This technique can thus be used for the identification of low amounts of analytes that are heterogeneously distributed on relatively large areas (e.g. from millimeters to centimeters), with high spatial resolution (few microns), using arrays of 64x64 and 128x128 pixels. The possibility of working in

transmittance, reflectance and ATR (Attenuated Total Reflectance) mode, makes the technique highly versatile: possible applications cover a wide range of fields, from biomedicine (analysis of tissues) and pharmaceutical research, to environmental chemistry (detection/identification of microplastics), and conservation of cultural heritage (assessment of the degradation and cleaning of artifacts).
The course will focus both on fundamental principles and practical aspects, including some demonstration of the technique on a selection of samples.

**Periodo di Svolgimento:** July 2018

**Numero minimo di studenti per l'attivazione:** 2

**Prova di accertamento:** review and discussion of a scientific paper on a topic covered by the course.

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# SSD: FIS/07

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**TITOLO DEL CORSO:** ACCELERATOR-BASED TECHNIQUES FOR THE ENVIRONMENT

**DOCENTE:** Dr. SILVIA NAVA (LABEC laboratory, INFN,Florence)

**ABSTRACT:** The class will be focused on the use of accelerator-based nuclear techniques, like Ion Beam Analysis (IBA) and Accelerator Mass Spectrometry (AMS), for environmental applications.
In IBA analyses environmental samples are used as a target for a beam of accelerated ions (produced by small accelerators) and the interaction products (X-rays, gamma-rays, charged particles) are analysed to deduce the sample elemental composition. AMS analyses are used for the measurement of rare isotopes, like for example 14C.
These techniques will be described, together with the experimental set-ups and activities of the LABEC-INFN laboratory of Florence. Particular attention will be given to the application of these techniques for the study of atmospheric aerosols (or particulate matter, PM), also including: sampling methods, analysis by other complementary techniques and data elaboration by multivariate statistical analysis (receptor models for source apportionment). The composition of PM is quite complex and its measurement is important for the assessment of air quality, the identification of the PM sources and the study of the aerosol effects on climate (radiative forcing). Studies in both polluted and remote areas, like polar regions, will be presented.
A visit at the LABEC laboratory will be included.

**Periodo di Svolgimento:** February – May 2018

**Numero minimo di studenti per l'attivazione:** 3

**Prova di accertamento:** review and discussion of a scientific paper on a topic covered by the course.

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**TITOLO DEL CORSO:** INTRODUCTION TO RADIOCARBON DATING AND ACCELERATOR MASS SPECTROMETRY

**DOCENTE:** Dr. MARIAELENA FEDI (LABEC laboratory, INFN,Florence)

**ABSTRACT:** The class will be focused on the basics of the radiocarbon dating method and of Accelerator Mass Spectrometry (AMS), which is the most appropriate experimental method to measure radiocarbon concentration in samples collected from archaeological and cultural contexts. In particular, the possible choices of the most suitable materials will be discussed, paying attention on the possible presence of contaminations and on the following chemical strategies and procedures that can remove those contaminations.

**Periodo di Svolgimento:** May – June 2018

**Numero minimo di studenti per l'attivazione:** 4

**Prova di accertamento:** review and discussion of a scientific paper on a topic covered by the course.

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**TITOLO DEL CORSO:** X-SPECTROMETRIES AND OTHER NUCLEAR TECHNIQUES FOR MATERIAL ELEMENTAL ANALYSIS

**DOCENTE:** Prof. PIERO MANDO' (Dept. Physics and Astronomy, University of Florence)

**ABSTRACT:** In the class, the basic principles of the Ion Beam Analysis (IBA) techniques (which use a particle accelerator) will be presented. The main techniques are Particle-Induced X-ray Emission (PIXE), Particle-Induced Gamma-ray Emission (PIGE), particle Backscattering spectrometry. Specifically, PIXE will be compared with the similar X-Ray Fluorescence (XRF) technique. In XRF the same effect as in PIXE (the emission of the characteristic X-rays which allows the identification of the elements) is induced by bombarding the material to be analyzed with a primary electromagnetic beam instead of particles. XRF does not require ion beams produced by an accelerator, therefore can be made portable, but has some analytical limitations with respect to PIXE.

**Periodo di Svolgimento:** February – May 2018

**Numero minimo di studenti per l'attivazione:** 3

**Prova di accertamento:** review and discussion of a scientific paper on a topic covered by the course.