UNIVERSITY OF NAPOLI "*FEDERICO II*"
Polytechnic and Basic Sciences School
Department of Chemical Sciences
Ph. D. Course in Chemical Sciences

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- Chemical Sciences PhD course catalog -

Title	Teacher(s)
Advanced Mass Spectrometry	Prof. A. Amoresano
Applications of optical and Raman microscopy	Dr. M. Rossi, Prof. A. Vergara
Biomolecular Chirality and the Origin of Life	Prof. D. D'Alonzo
Bioplastics	Dr. C.V.L. Giosafatto
Characterization of porous solids and powders: principles and practice	Dr. R. Turco
Chemical methodologies for cultural heritage	Prof. L. Birolo, Prof. A. Vergara
Data Acquisition Systems for Chemical Laboratories	Prof. V. Russo
Didactics of chemistry	Prof. Oreste Tarallo
Electronic structure methods for solid state materials	Prof. A.B. Muñoz-Garcia
Flow Chemistry: towards a modern chemical Industry	Prof. V. Russo
Food Chemistry: preservation, processing and nutritional issues	Prof. A. Napolitano
Forensic Chemistry	Prof. M. Trifuoggi
Interpretative spectroscopy of natural organic substances	Prof. A. Cimmino, Prof. M. Masi
Microscopy Techniques for Materials Science	Prof. R. Di Girolamo
Mitigation of the Environmental Impact of Chemical Processes for Energy Production	Prof. F. Montagnaro
Molecular engineering of proteins and metalloproteins	Dr. M. Chino
Monte Carlo methods for chemical reactions simulation	Prof. R. Tesser
Nanostructures and nanotechnologies	Prof. C. De Rosa
Natural phenolic compounds: structure, reactivity and applications	Prof. L. Panzella
Persistent organic pollutants (POPs)	Dr. A. Andolfi
Physical chemistry of the Nanosystems	Prof. L. Paduano
Physico-chemical approaches to formulation science	Prof. I. Russo Krauss
Production of Native and Mutant Recombinant Proteins	Prof. A. Duilio
Recent advances in biomolecular NMR	Prof. D. Picone
Selective Organometallic Catalysis: systems and advanced techniques	Prof. P. Budzelaar
Smart Drug Delivery Systems	Prof. A. Guaragna

Coordinator: prof. Angelina Lombardi
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Structure and Dynamics of Materials and Macromolecules by Elastic and Inelastic Scattering Techniques	Prof. F. Auriemma
Synthesis, structure and applications of natural and modified oligonucleotides	Prof. D. Montesarchio, Dr. D. Musumeci
Synthetic Glycochemistry	Prof. E. Bedini, Prof. A. Iadonisi
X-ray crystallography of biological macromolecules: advanced methods and applications	Prof. A. Merlino, Prof. F. Sica

Important note: normally, each listed course will be "activated" in a given year only if at least two PhD students, even of different classes or different PhD Programs, choose to attend it. If only one student is interested, then the course can be often transformed into a "supervised reading" option.

The period of the year in which each course is scheduled is listed at xxx for a detailed timetable please contact the teacher.

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Advanced Mass Spectrometry	
Teacher	**Prof. Angela Amoresano** (angela.amoresano@unina.it)
Credits	2
Planned hours	16
Planned schedule	*Interested students have to contact* Prof. Amoresano to *arrange the detailed timetable*
Objectives	The course aims to provide the skills on advenced mass spectrometry techniques. The potentialities and weaknesses of the various mass spectral techniques are illustrated by numerous examples
Description	Basics: Isotopic profile, Resolution and Mass Accuracy. Ionization Methods: Electronic Ionization (EI); Electrospray; MALDI. Mass Analysers: Quadrupole; Time of Flight (TOF); Ion Trap; Linear Ion Trap; Orbitrap. Linked Systems: GC-MS and LC-MS/MS analyses; Select Ion Monitoring (SIM); Ion Mobility Mass Spectrometry. Tandem Mass Spectrometry: Collision Induced Dissociation (CID); Tandem in Space; Tandem in Time; Product Ion Scan. Tandem MS Scan Mode: Precursor Ion Scan (PIS); Neutral Loss Scan (NLS); Select Reaction Monitoring (SRM); Multiple Reaction Monitoring (MRM). Quantitative Tandem Mass Spectrometry analyses. Application of LC-MS/MS Analyses: Forensic Sciences; Diagnostic in Cultural Heritage; Environmental Analyses; Neonatal Diagnostic; Drugs determination
Final evaluation	Oral discussion

Applications of optical and Raman microscopy	
Teachers	**Dr. Manuela Rossi** (manuela.rossi@unina.it) **Prof. Alessandro Vergara** (avergara@unina.it)
Credits (planned)	2
Planned hours	16
Planned schedules	*Interested students have to contact* Prof. Vergara or Dr. Rossi to *arrange the detailed timetable*
Objectives	The course aims to provide the theoretical and applied aspects of optical microscopy (boh stereo and polirazation microscopy) and Raman microscopy (in its variants non-stimulated and stimulated) also compared to IR microspectroscopy.
Description	*Part A. Optical Microscopy.* The short course presents techniques concerning the microscopic observation of materials, using stereomicroscopes (three dimensional observations) and polarizing microscope (two dimensional observations). Topics related to optical, textural, morphological and physical properties of inorganic material will be primarily addressed. The interaction phenomena of light and matter in optically isotropic and anisotropic materials will be presented and applied to the materials study with petrographic microscope, specifying the equipment correct alignment for properties observation as index of refraction, pleochroism, cleavage, interference color, extinction angle, optical indicatrix and particular features as twinning and chemical zoning. These remarks are focused both to recognition of the material under study and to characterize the crystal physics. The other part of the course will focus on material morphological and textural features with three-dimensional observations. The various morphologies typically applied to the study of inorganic material as aggregates and single crystals will be presented. Regarding composite materials, textural features (essential to understanding growth relationships between the various components) will be presented. The setting of the microscope on the basis of the type of material under investigation (observation in transmitted or reflected light) will be discussed. *Part B. Raman Microscopy.* A brief introduction on the theory of Raman spectroscopy (resonance Raman, CARS and SERS), followed by some examples of application of Raman imaging.
Final evaluation	Presentation of an application of Raman and/or optical microscopy to be defined with the teacher.

Biomolecular Chirality and the Origin of Life	
Teacher	**Prof. Daniele D'Alonzo** (dandalonzo@unina.it)
Credits	2
Planned hours	16
Planned schedules	*Interested students have to contact* Prof. D'Alonzo to *arrange the detailed timetable*
Objectives	Acquisition of knowledge on the most important theories regarding the origin and amplification of biomolecular chirality and homochirality.
Description	One of the most fundamental and intriguing aspects of life is the homochirality of biomolecules. Single-handedness of aminoacids and sugars plays a crucial role in molecular recognition and replication processes, and this property seems to represent a prerequisite for the origin of life. Since the early days of stereochemistry, the origin of chirality in biological systems has been a challenge to chemists, physicists and biologists, and numerous theories and experiments have been reported to address the puzzle of how single chirality of biological molecules arose from an optically inactive primordial soup. In this course, an in-depth investigation into the origin of chirality in the early Earth will be provided. The course will be divided into three sections. The first section will focus on molecular chirality, with a special attention to homochirality, and on physical chirality, covering concepts such as symmetry breaking and parity violation. In the second section, we will analyze the main theories based on the physical and chemical processes that may have contributed to symmetry breaking, including those potentially originating from extra-terrestrial sources. Finally, in the third section, the most significant processes enabling the amplification of chirality will be discussed, with a focus on the formation of the earliest biomolecules crucial for the emergence and evolution of life on Earth.
Final evaluation	Interview

Bioplastics	
Teacher	**Dr. C. Valeria L. Giosafatto** (giosafat@unina.it)
Credits	2
Planned hours	16
Planned schedules	*Interested students have to contact* Dr. Giosafatto to *arrange the detailed timetable*
Objectives	The course aims at illustrating the power of bioplastics, as an attractive eco-friendly alternative to petroleum-derived plastics, whose disposal is highly pollutant for ground, water as well as marine life. In addition, the plastics burning releases poisonous chemicals in the air.
Description	• Plastic revolution and plastic pollution. • Bio-based, biodegradable, compostable, edible and digestible materials. • Different origin, possible ways of production, physico-chemical/biological characterization and industrial applications of the bioplastics. • Use of different methods (casting, dipping, spraying) for the preparation of polysaccharide- and protein-based bioplastics. • Bioplastic main properties characterization Bioplastics produced from biodegradable molecules seem an attractive eco-friendly alternative since they can be easily degraded by the enzymes present in different microorganisms occurring in the environment. The technical attitude, such as mechanical and barrier properties of the bioplastics are crucial for their industrial application. The methods for preparation of the bioplastics are different depending on their specific use since they can be applied in the agriculture and food as well in biomedical and pharmaceutical sectors. For an industrial application it is of a paramount importance to characterize the bioplastics according to their structure and biodegradability. Different case-studies based on the production of hydrocolloid-based bioplastics made of proteins and carbohydrates will be shown. In particular, the matrix of protein-based bioplastics can be modified by means of the enzyme microbial transglutaminase, an enzyme able to catalyse the isopeptide bonds between glutamines and lysines into proteins. Such enzyme has been exploited in the last 15 years to enhance the technological features of hydrocolloid-based bioplastics. The use of different nanoparticles ill be also taken into account as potential method to improve the features of the novel bioplastics. The study of their morphological, gas barrier and mechanical properties (elongation at break, tensile strength, Young's modulus and sealing strength, is, thus, essential for making them promising environmentally friendly candidates able to replace the petroleum-derived plastics.
Final evaluation	Interview

Characterization of porous solids and powders: principles and practice	
Teacher	Dr.ssa Rosa Turco (rosa.turco@unina.it)
Credits (planned)	2
Planned hours	16
Planned schedules	Interested students must contact dr. Rosa Turco to arrange the detailed timetable
Objectives	The course aims at providing an overview of principles associated with the characterization of solids about their surface area, pore size, pore volume. It covers methods mainly based on gas adsorption both physic and chemisorption. In the course, the theoretical and experimental basics of these techniques are presented in detail together with the analysis of applications in the solution of actual case studies. <u>The course will appeal to PhD students who need accurate and comprehensive pore and surface area characterization of their materials, and those who have the need to quickly learn the rudiments of the measurements</u>. It is divided into two parts: the first part is devoted to theoretical concepts, while the second is practice with the actual application of them.
Description	The topics will be: **<u>Theoretical</u>** Gas Adsorption Adsorption Isotherms Surface Area Analysis Mesopore Analysis Micropore Analysis Chemisorption: Site Specific Gas Adsorption **<u>Experimental</u>** Physical Adsorption Measurement Dynamic Flow Method Chemisorption techniques The course includes a practice on an adsorption analyzer
Final evaluation	Interview

Chemical methodologies for cultural heritage	
Teachers	**Prof. Leila Birolo** (birolo@unina.it) **Prof. Alessandro Vergara** (avergara@unina.it)
Credits (planned)	2
Planned hours	16
Planned schedules	*Interested students have to contact* Prof. Birolo or Prof. Vergara to *arrange the detailed timetable*
Description	Theoretical and experimental aspects of the analytical methodologies applied to cultural heritage. Introduction to the chemistry of material constituents of works of art: Proteins, lipids, carbohydrates, natural resins, natural materials, synthetic polymers, dyes and pigments Chemical tests on paintings, books, natural and synthetic materials, textiles, potteries, glasses, metals. Spectroscopic and microscopic methodologies applied to archaeological remains and works of art. Mass spectrometry and proteomic methodologies. Please, further details on Chemistry of Cultural Heritage at UNINA is available at the website http://www.cbc.unina.it/index.php/it/
Final evaluation	Inteview

Electronic structure methods for solid state materials	
Teacher	**Prof. Ana Belen Muñoz García** (anabelen.munozgarcia@unina.it)
Credits	2
Planned hours	16
Planned schedules	*Interested students have to contact* Prof. Ana B. Muñoz García *to arrange the detailed timetable*
Objectives	The course is proposed for PhD Students in Chemical Sciences with interest in solid-state materials. The main objective is to gain knowledge on the different methodologies available for calculating electronic structure of periodic systems, paying attention to the differences between solids and molecules and to the approximations that are suited/unsuited for each kind of solid. Flaws and limits of state-of-the-art methods will be discussed. Two practical sessions of 2 hours each will be devoted to the actual application of the concepts discussed during lectures
Description	This course will cover state-of-the-art methods for predicting materials properties from first- principles. The topics will be: (1) Solid state materials: structure, properties and functions; (2) Basics of electronic structure theory and density functional theory; (3) Numerical methods to describe electronic variables: pseudo-potentials and basis sets (4) Super-cell methods to study materials bulk and surface properties. Transition state searching: transport and reactivity (5) Failures and corrections of current methods (6) Lattice vibrations and phonons The course includes two practical sessions
Final evaluation	Interview

Data Acquisition Systems for Chemical Laboratories	
Teacher	**Prof. Vincenzo Russo** (v.russo@unina.it)
Credits (planned)	2
Planned hours	16
Planned schedule	*Interested students have to contact* Prof. Vincenzo Russo to *arrange the detailed timetable*
Objectives	The course will provide an overview of the most recent and advanced efforts made in the field of data acquisition for chemical laboratories.
Description	An introduction to sensors and actuators will be provided, to help the researcher choosing the best options to collect experimental data, regulating process variables (e.g temperature, pressure, fluid-flows), allowing to work in safe conditions. A state-of-the-art software will be introduced (LabVIEW) and adopted to realistic Data AcQuisition (DAQ) systems. The students will get the elements to design hands-on devices for lab-scale purposes.
Final evaluation	At the end of the course there will be an oral exam.

Didactics of chemistry	
Teacher	**Prof. Oreste Tarallo** (oreste.tarallo@unina.it)
Credits (planned)	2
Planned hours	16
Planned schedules	*Interested students have to contact* prof. Tarallo to *arrange the detailed timetable*
Objectives	The aim of the course is to offer an overview of the latest and most effective didactic technologies developed in Science Education for teaching chemistry and related subjects.
Description	Beginning with an overview of the issues related to the teaching of Science and Chemistry, the course introduces impactful methods and tools for effective communication with students, emphasizing hands-on activities to directly involve participants. Key topics covered in the course include: -Fundamentals of Chemistry Education. -The learning process, learning models, and their implications for teaching chemistry. -Effective teaching models: Johnstone's triangular model; Mahaffy's tetrahedral model; Sjöström's tetrahedral model and the social dimension of chemistry; Talanquer's model. -Students' alternative conceptions and misconceptions. -Concept inventories, open-ended response tests, and alternative methods to multiple-choice tests; Ordered multiple-choice. -Teaching methodologies and best practices in chemistry education. -Laboratory teaching in chemistry learning, including methods, applicability to different contexts, and analysis and discussion of practical examples. -Active strategies for teaching chemistry: Problem-Based Learning (PBL), Project-Based Learning (PjBL), Inquiry-Based Science Education (IBSE), Cooperative learning, Peer education, Flipped classroom, Team teaching. -Teaching and learning chemistry processes through digital tools and technologies. The teaching methodology involves lectures, discussions, classroom laboratory activities, group work, and team teaching. Additionally, recent literature articles will be discussed during the classes.
Final evaluation	Inteview

Flow Chemistry: towards a modern Chemical Industry	
Teacher	**Prof. Vincenzo Russo** (v.russo@unina.it)
Credits (planned)	2
Planned hours	16
Planned schedule	*Interested students have to contact* Dr. Russo *to arrange the detailed timetable*
Objectives	The course will provide an overview of the most recent and advanced efforts made in the field of flow chemistry in both fine chemicals and pharmaceutical industry.
Description	An introduction to the concept of flow chemistry will be provided, to help the researcher choosing the best options to conduct experiments in flow, in the case of fine chemicals production. Miniaturized systems as microreactors and millireactors will be shown in deep details, focusing the attention on their potentialities to solve technological problems often found when facing with either highly exothermic or endothermic reactions. The state-of-the-art of the modern applications of flow chemistry to chemical processes will be introduced, focusing the attention on photochemistry, partial oxidation, hydrogenation reactions. The students will get the elements to scale-up an operation to a continuous process.
Final evaluation	At the end of the course there will be an oral exam.

Food chemistry: preservation, processing and nutritional issues	
Teacher	**Prof. Alessandra Napolitano** (alesnapo@unina.it)
Credits	2
Planned hours	16 (8 lectures)
Planned schedule	*Interested students have to contact* Prof. A. Napolitano *to arrange the detailed timetable.*
Objectives	The course is directed to PhD students in the field of chemistry, industrial chemistry, biotechnology, biology. It is intended to provide awareness of issue related to safety and preservation of food with respect to both natural transformations and manifacturing processes. Elements of nutritional relevance, raising increasing interest are also presented to make the attendants able to pursue further investigation and continuous updating.
Description	**Food components**: brief overview (1 lecture) **Food organoleptic characteristics:** Color: main pigments; Taste: the five main tastes; Odor : classification of odorants; methods for evaluation (1 lecture) **Food storage and preservation:** Exposure to oxygen, light, contaminants; Prolonging shelf life; Smart packaging; **Food additives:** main classes and applications (2 lectures) **Food processing and their nutritional consequences :** Hydrogenation processes (alditols, PUFA); Thermal processing (milk); oxidation of phenol components in vegetable processing; Transesterification and triglycerides modification; Hazard from food cooking: Imidazoquinoline from meat , Aminoacids transformation, Acrylamide etc (2 lectures) **Nutritional aspects:** Vitamins; Functional foods; Lipid supplements; Proteic supplements; Fortificants; Prebiotics and probiotics; Bioactives in plant derived food; antinutritional factors (1 lecture) **Focus on selected food**: cereals, tea, coffee, cocoa or others , non-conventional food (1 lecture)
Final evaluation	Seminars on arguments tackled in the course and selected by students with ample discussion and questions from the teacher (and attendants).

Forensic Chemistry	
Teacher	**Prof. Marco Trifuoggi** (marco.trifuoggi@unina.it)
Credits	2
Planned hours	16
Planned schedule	*Interested students have to contact* Prof. Trifuoggi *to arrange the detailed timetable*
Objectives	The course aims to provide the skills on analytical methods in forensic analytical chemistry. Also taken into consideration are the main problems that affect the outcome of a laboratory examination of forensic and biological samples. The potentialities and weaknesses of the various methods are illustrated by numerous examples aimed at the determination of analytes in complex biological matrices
Description	Introduction. What is a forensic analysis. Differences and analogies with traditional analyses. The problem of sampling in forensic science. Sample storage. Critical analytical "quality" parameters in forensics. Critical evaluation of results. Main analytical techniques in forensics. Complementary techniques in forensics and notions of biochemical methods. Examples and applications: psycoactive substances, fingerprints, paints, explosives residues.
Final evaluation	Oral discussion

Interpretative spectroscopy of natural organic substances	
Teachers	**Prof. Alessio Cimmino** (alessio.cimmino@unina.it) **Prof. Marco Masi** (marco.masi@unina.it)
Credits	2
Planned hours	16
Planned schedule	*Interested students have to contact* Prof. Cimmino/Masi to *arrange the detailed timetable*
Objectives	The course aims to provide knowledge on chemistry and biosynthesis of natural organic substances and on spectroscopies (IR, UV, MS and NMR) used for their structural determination. The fundamental parameters for the interpretation of ^{1}H and ^{13}C one and two-dimensional spectra and general procedures for structure elucidation of low molecular weight compounds will be acquired.
Description	The course will briefly deal with the most important classes of bioactive natural compounds such as polyketides, terpenes, steroids, phenylpropanoids and alkaloids, with potential application in different fields. Fundamentals of NMR and other spectroscopies for the structure determination of low molecular weight compounds will be illustrated. Topics covered in the course: • Bioactive natural compounds: chemical classes, biosynthesis, and purifications processes (1 lecture). • Spectroscopies (IR, UV, MS and NMR) used for structural determination of low molecular weight compounds (1 lecture). • Chemical shift, intensity and splitting of NMR signals of the ^{1}H and ^{13}C nuclei (1 lecture). • Two-dimensional NMR experiments: COSY, HSQC, HMBC and NOESY (1 lecture). • Interpretation of mono and two-dimensional spectra and strategies of structural elucidation (2 lectures). • From NMR spectra to chemical structure: examples of structural determination of selected bioactive natural compounds (2 lectures).
Final evaluation	Final interview

Microscopy Techniques for Materials Science	
Teacher	**Prof. Rocco Di Girolamo** (rocco.digirolamo@unina.it)
Credits	2
Planned hours	16
Planned schedules	*Interested students have to contact Prof. Di Girolamo to arrange the detailed timetable.*
Objectives	Learning objectives of this course involve developing an understanding principle of different microscopy techniques and applying these principles to the material science. This course will help students in selecting the most relevant microscopy or method and optimizing them for materials characterization experiments.
Description	Basics of optics. Transmitted light microscopy (brightfield, polarizing, phase contrast, darkfield). Reflected light microscopy. Differential interference contrast microscopy. Electron microscopy, including conventional transmission electron microscopy (TEM), cryo-TEM techniques, high resolution techniques, scanning transmission electron microscopy (STEM), STEM EELS, Scanning electron microscopy (SEM), SEM -EDX. Focus ion beam microscopy (FIB)) - FIB-SEM 3Dtomography. Scanning probe microscope methods (SPM) including related techniques that, using a probe that scans the specimen, image surfaces and measure surface properties on a fine scale (down to the molecular/atomic scale). SPM techniques include Scanning Tunneling Microscopy (STM), Atomic Force Microscopy (AFM), Magnetic Force Microscopy (MFM), AFM-IR, etc. For each technique, the physical and chemical fundamentals of the method, the information obtained (morphology, chemical composition, micro and macrostructure, resolution etc.) will be discussed, including data analysis, sample preparation and applications in materials science.
Final evaluation	Interview

Mitigation of the Environmental Impact of Chemical Processes for Energy Production	
Teacher	**Prof. Fabio Montagnaro** (fabio.montagnaro@unina.it)
Credits	2
Planned hours	16
Planned schedules	*Interested students have to contact* Prof. Montagnaro *to arrange the detailed timetable*
Objectives	The course is proposed for PhD Students in chemistry-, chemical engineering- and environmental sciences-related fields. The main objective is to contribute to the development of a qualitative and quantitative awareness concerning the impact of chemical processes for energy production on climate changes, and its mitigation by use of renewables, capture of gaseous pollutants, efficient design of chemical reactors, with an eye on techno-economical aspects as well.
Description	○ Climate changes and related environmental, social, economic and technical aspects. Facing climate changes by use of renewables, CO_2 capture and storage, more efficient desing of chemical reactors for energy production. ○ Solid biomasses combustion and gasification: biomasses properties and characteristics, schemes for combustion and gasification plants (fluidised beds and entrained flow reactors). ○ Combustion with in situ desulphurisation through limestone-based sorbents. ○ Methods for the mitigation of CO_2 emissions into the atmosphere: absorption with chemical reaction, oxyfuel and chemical looping combustion, calcium looping. ○ Gasification cycles integrated with CO_2 capture/storage schemes. ○ New concepts on thermochemical solar energy storage (limestone-based “solar battery”). ○ Reuse of combustion/gasification solid wastes as pollutants adsorbents or in the field of building materials from the circular economy perspective.
Final evaluation	Discussion of a scientific article assigned during the classes.

Molecular engineering of proteins and metalloproteins	
Teacher	**Dr. Marco Chino** (marco.chino@unina.it)
Credits	2
Planned hours	16
Planned schedule	*Interested students have to contact* Dr. Chino *to arrange the detailed timetable*
Objectives	The course aims to provide practical skills in the computational design of proteins and metalloproteins. In particular, through analysis and discussion of selected examples from the literature, the student will learn the most up-to-date techniques of computational protein and metalloprotein design. By reproducing current literature cases, the student will understand the main concepts that drive protein folding and, consequently, the resolution of the inverse protein folding problem. The student will develop the following skills and knowledge: (a) understand and analyze protein structures in terms of their designability; (b) master one or more computational procedure in protein design (c) propose and discuss innovative projects for the analysis and design of tailored proteins and metalloproteins.
Description	State-of-the-art design techniques are today able to build tailor-made proteins and metalloproteins for any given function, spanning from designed vaccines to bio-based materials with unprecedented features. Design of a fully de novo protein can be divided in two phases: (i) choice of a highly designable backbone, (ii) search of the most suitable sequence to drive that specific folding and/or function. Both aspects have been faced by different strategies in the literature, spanning from mathematical parameterization and atomistic score functions, to the mining of the structural databases and full-atom search of structural contexts. Each student will be involved in critical discussions about current literature, from which, he will be trained to a specific design technique. Each student will then prepare a simple project for the computational design of a protein or a metalloprotein of biotechnological, pharmacological or technological interest.
Final evaluation	Evaluation and discussion of the assigned literature and of the proposed project.

Monte Carlo methods for chemical reactions simulation	
Teacher	**Prof. Riccardo Tesser** (riccardo.tesser@unina.it)
Credits (planned)	2
Planned hours	16
Planned schedule	Interested students must contact Prof. Riccardo Tesser to arrange the detailed timetable
Objectives	The course aims at providing theoretical and practical aspects in stochastic method applied to the simulation of chemical reaction systems. Understanding the topics requires a minimum level of knowledge of Matlab language for scientific computing.
Description	Introduction to Monte Carlo method and theoretical bases. Gillespie's method for the simulation of chemical reactions. Description of the basic Matlab code. Single reaction of first and second order (irreversible and reversible). Simultaneous chemical reactions, in series, in parallel, and complex networks. Michaelis-Menten model for enzymatic catalysis. Oscillatory chemical reactions. Nonisothermal reaction system. Multiphase reactions: gas-liquid, liquid-liquid. Heterogeneous reactions: the model of Ziff-Gulari-Barshad for solid cataòyzed reaction.
Final Evaluation	Interview

Nanostructures and nanotechnologies	
Teacher	**Prof. Claudio De Rosa** (claudio.derosa@unina.it)
Credits	2
Planned hours	16
Planned schedules	*Interested students have to contact* Prof. De Rosa *to arrange the detailed timetable*
Objectives	The course aims at providing new technologies for the preparation and characterization of nanostructures and nanocomposites.
Description	Nanostructures and mesophases Formation of mesophases and nanostructures by self-assembly driver by molecular recognition and/or shape of molecules. Methods top-down and bottom-up. Formation of nanostructures in polymeric materials. Block copolymers. Self-assembly from nanophase separation, thermodynamic, phase diagram, order-disorder transition. Nanostructures in amorphous block copolymers; classic and non-conventional structures. Driving force in the formation of nanostructures by self-assembly. Preparation of block copolymers. Characterization of nanostructures. Methods for the structural characterization of nanostructures. Electron microscopy: general principles, contrast phenomena, analysis of images in the structural and morphological studies. Bright-field and dark-field imaging. Small angle X-ray diffraction. Applications of nanostructures. Nanotechnologies. Applications of block copolymers, thermoplastic elastomers and methods of fabrication of ordered nanostructures. The role of nanostructured materials in advanced technologies: polymeric materials in microelectronics. Organic electronics. Lithography in the technology of fabrication of integrated circuits. Resists. Optical, X-ray and electronic lithography. Patterning of surfaces. Lithography with patterns generated byself-assembly inblock copolymers. Nanocomposites and nanostructures. Photonic crystals. Materials for guiding and confinement of light. Photonic crystals based on block copolymers. Block copolymers for memories and sensors. Crystalline block copolymers and method for controlling orientation of nanodomains.
Final evaluation	Interview

Natural Phenolic Compounds: Structure, Reactivity and Applications	
Teacher	**Prof. Lucia Panzella** (panzella@unina.it)
Credits	2
Planned hours	16
Planned schedules	*Interested students have to contact* Prof. Panzella to *arrange the detailed timetable*
Objectives	Acquisition of knowledge related to structure-property relationships and possible manipulations of natural phenolic compounds for practical applications.
Description	1) Structural classification and occurrence of the main natural phenolic compounds. 2) Chemical reactivity of natural phenolic compounds, with particular reference to the antioxidant activity. 3) Chemical assays for assessment of the antioxidant properties of phenolic compounds. 4) Manipulation strategies to improve the antioxidant properties of natural phenolic compounds. 5) Natural phenolic polymers: classification, occurrence, antioxidant properties and methodologies for structural characterization. 6) Applications fields of natural phenolic compounds and derivatives.
Final evaluation	Written test/Interview

Persistent organic pollutants (POPs)	
Teacher	**Dr. Anna Andolfi** (anna.andolfi@unina.it)
Credits	2
Planned hours	16
Planned schedules	*Interested students have to contact* Prof. Andolfi to *arrange the detailed timetable*
Objectives	The course is proposed for PhD Students in chemistry-, chemical engineering- and environmental sciences-related fields. The main learning objectives are: • to identify POPs and their sources; • to describe the mechanisms of formation; • to understand POPs persistence in environment; • to describe the impact of POPs on the human health, as well as on the environment • to analyse a case study.
Description	Introduction to environmental problems, sustainability and green chemistry. Establish the criteria for classifying persistent organic pollutants (POPs). Relation between chemical-structure and physical and chemical properties of POPs (mobility, persistence, bioaccumulation and toxicity) Main pollutants. Organochlorine insecticides (DDT, chlorinated cyclopentadienes, hexachlorocyclohexane, mirex, taxofene). Chemical structure, synthesis, mechanism of action and environmental behavior (their transformation products), toxicity, alternatives to their use. Industrial products [polychlorinated biphenyls (PCBs)]: chemical structure, industrial production, uses, environmental behavior, toxicity, alternatives to their use. Undesirable by-products (dioxins, polychlorinated dibenzofurans). Chemical structure, main sources [synthesis of herbicides (2,4,5-T) and chlorophenols, PCBs, paper production, fires and incineration], environmental behavior, toxicity. Case studies. Limitation of their production. Polycyclic aromatic hydrocarbon (PAH). Chemical structure, formation mechanisms, behavior and reactivity in the air, metabolization, toxicity. Endocrine disruptor (Flame retardants, PFOA-PFOS, Phthalates). Definition, structure, industrial production, uses, toxicity, alternatives to their uses. Examples of pollutants of natural origin. Definition, structure and toxicity Examples of contaminated sites in Italy. **Recommended textbooks** Chimica ambientale, C. Baird, M. Cann. Zanichelli 2013 Available course notes
Final evaluation	Presentation of a topic selected by students with extensive discussion with the teacher (and attendants) covering all the contents illustrated during the course

Physical chemistry of the Nanosystems	
Teacher	**Prof. Luigi Paduano** (luigi.paduano@unina.it)
Credits	2
Planned hours	16
Planned schedules	*Interested students have to contact* Prof. Paduano to *arrange the detailed timetable*
Objectives	
Description	Thermodynamic and Statistical Aspects of Intermolecular Forces, Repulsive Steric Forces, Total Intermolecular Pair Potentials and Liquid Structure, Hydrogen-Bonding and Hydrophobic and Hydrophilic Interactions, Force between particles and surfaces. Solvation, Structural, and Hydration Forces. Adhesion and Wetting Phenomena. Thermodynamic of Self- Assembly. Colloids, micelles, bilayers, Vesicles, Liposomes, Emulsions, Microemulsions,
Final evaluation	Interview

Physico-chemical approaches to formulation science	
Teacher	**Prof. Irene Russo Krauss** (irene.russokrauss @unina.it)
Credits	2
Planned hours	16
Planned schedules	*Interested students have to contact* Prof. Russo Krauss to *arrange the detailed timetable*
Objectives	The training course aims at providing the basis of physical-chemistry of colloids to understand the behaviour of colloidal formulations, how improve their stability and how to optimize them in terms of eco-sustainability for applications in different fields.
Description	Colloidal formulations: suspensions, emulsions, microemulsions, foams, aerosols, idrogels (definition of formulations and colloidal systems, formation and stability of the different colloidal formulations, diffusion, sedimentation, creaming, coagulation, flocculation, Ostwald ripening, phase separation, phase inversion). Total intermolecular potential and stabilization of formulations (intermolecular forces, charged systems, the electrochemical double layer, electrostatic repulsive potential, van der Waals forces, DLVO theory, total intermolecular pair potential, non-DLVO forces. Examples of electrostatically, sterically and electro-sterically stabilized colloidal systems). Surfactants and association colloids (introduction to interfaces, surface and interface tension, Gibbs adsorption isotherm, adsorption and self-assembly properties of amphiphilic molecules, mixtures of surfactants, prediction of aggregate morphology, critical packing parameter) Ecosustainable formulations (biosurfactants and biopolymers in formulation science) Applications of formulations in biomedicine, food, cosmetics
Final evaluation	Interview

Production of native and mutant recombinant proteins	
Teacher	**Prof. Angela Duilio** (angela.duilio@unina.it)
Credits (planned)	2
Planned hours	16
Planned schedules	*Interested students have to contact* Prof. Duilio to *arrange the detailed timetable*
Objectives	Aquisition of the knowledges needed to design processes for the production of both native and mutant recombinant proteins.
Description	**Main topics** From gene to recombinant proteins: design and development of a recombinant expression system. Main features of host microorganisms for heterologous expression. Expression vectors: features and uses. Gene expression from strong and weak promoters. Fusion proteins. Optimization of expression conditions. Principles of protein engineering. Targeted and site-specific mutagenesis. Random mutagenesis and *in vitro* molecular evolution.
Final evaluation	Interview

Recent advances in biomolecular NMR	
Teacher	**Prof. Delia Picone** (delia.picone@unina.it)
Credits (planned)	2
Planned hours	16
Planned schedules	*Interested students have to contact* Prof. Picone to *arrange the detailed timetable*
Objectives	The students will acquire information about the potentials and limits of high resolution NMR in biomolecular studies. They will be able to read and critical discuss literature papers containing NMR experiments.
Description	Requirements and limits of multidimensional NMR to characterize biomolecule structure in solution. Fundamental homo- and heteronuclear multidimensional experiments for protein structure, dynamics and interactions. Key parameters, their extraction and use. Recent advances and application to solid state structural studies and biomolecular interactions: spin interactions at solid state, Magic Angle Spinning. High Power Decoupling. Cross-polarization. Extraction of structural information from solid state NMR experiments. Practical aspects of SS spectra acquisition on standard samples.
Final evaluation	Public discussion of a literature paper selected with the teacher. After the evaluation the student will receive an attendance certificate.

Selective Organometallic Catalysis: systems and advanced techniques	
Teacher	**Prof. Peter Budzelaar** (p.budzelaar@unina.it)
Credits	2
Planned hours	16
Planned schedules	*Interested students have to contact* Prof. Budzelaar to *arrange the detailed timetable*
Objectives	Homogeneous catalysis is becoming increasingly important in organic synthesis, in part for environmental reasons but also due to the development of less traditional catalysis. This course intends to illustrate some of the more promising developments in organometallic chemistry and homogeneous catalysis.
Description	The course will cover selected topics in modern homogeneous catalysis research: • Redox-active and chemically reactive ligands • Metallation, C-H activation and C-C bond formation • Organogold catalysis • Catalysis by "Frustrated Lewis Pairs" • Pincer type ligands Characterization methods will be discussed where appropriate. The material is based on recent research literature.
Final evaluation	Students are expected to present a recent paper (usually an Angewandte Chemie communication or similar) to the class.

Smart Drug Delivery Systems	
Teacher	**Prof. Annalisa Guaragna** (annalisa.guaragna@unina.it)
Credits (planned)	2
Planned hours	16
Planned schedules	*Interested students have to contact* Prof. Guaragna to *arrange the detailed timetable*
Objectives	The aim of the course is to give on overview of the modern smart delivery systems to selective convey a drug in the desired site of action.
Description	More than one hundred years ago, Paul Ehrlich suggested the idea of a drug acting as a "magic bullet" to selectively eradicate diseased cells without altering the surrounding healthy cells. Since then, enormous advances have been made in the field of targeted drug delivery and the course will cover its history and state of the art, giving also an overview of drug administration, distribution, metabolism and excretion criteria.
Final evaluation	Interview

Structure and Dynamics of Molecules and Macromolecules by Elastic and Inelastic Scattering Techniques	
Teacher	**Prof. Finizia Auriemma** (finizia.auriemma@unina.it)
Credits	2
Planned hours	16 14 h oral lectures, and 2 h Numerical data analysis
Planned schedules	*Interested students have to contact* Prof. Auriemma to *arrange the detailed timetable*
Objectives	The objectives of the course are of teaching the fundamental of scattering techniques for the study of the positions and motions of atoms in condensed matter; when or why to use neutrons; study of the structure and dynamics of matter at molecular level for interpretation of material properties; use of free-ware programs for data analysis.
Description	The fundamental concepts of elastic scattering at small angle and inelastic scattering of electro-magnetic radiation and neutrons for the study of nanostructured systems are illustrated. Program: Scattering vector and basic equation of elastic scattering. Autocorrelation function of particle density and Pair distribution function. Differential scattering cross-section and autocorrelation function. The scattering Invariant. Scattering of X-rays, electrons, neutron and light. Absolute Intensity and Relative Intensity 3h). Fundamental Laws of Small Angle Scattering (SAS): Babinet principle. Guinier Law, Porod Law. Forward scattering. SAS from non interacting monodisperse particles. Concentrated systems. Biphasic systems and study of interfaces. Fractal concept. Power laws and critical exponents. (3 h) Examples of nanostructured systems. Gaussian and expanded chains. Polymer Gels. Nanoporous systems (concrete and silica gels). Metallic nanoparticles. Block copolymers and nanostructures. (2 h). Inelastic scattering. Coherent and incoherent neutrons scattering and difference with coherent and incoherent X-ray scattering. The double differential cross section. The intermediate scattering function, The Van Hove Scattering function and the dynamic structure factor. (3h) Relationships of the incoherent scattering and the self-motion of individual nuclei. Enhancement of incoherent signal. Kind of information that can be deduced from quasi elastic neutron scattering: chain dynamics of polymers and impact with melt rheology and water dynamics in hydrogels. Time scale of molecular dynamics information which can be achieved by quasi elastic neutron scattering techniques (3h). Numerical exercise based on use of standard free-ware for the analysis of neutron scattering data (2h).
Final evaluation	Seminars on arguments tackled in the course and/or selected by students.

Synthesis, structure and applications of natural and modified oligonucleotides	
Teachers	**Prof. Daniela Montesarchio** (montesar@unina.it) **Dr. Domenica Musumeci** (domenica.musumeci@unina.it)
Credits	2
Planned hours	16 (8 lectures)
Planned schedules	*Interested students have to contact* Prof. Montesarchio or Prof. Musumeci *to arrange the detailed timetable*
Objectives	
Description	Chemistry and structure of nucleic acids. Main conformations of natural DNA. Chemical synthesis of oligodeoxyribo- and oligoribonucleotides. Solid phase synthesis: the phosphoramidite chemistry and the H-phosphonate method. Purification of oligonucleotides and their characterization. Synthesis of conjugated and/or modified oligonucleotides: modifications at the 5' and/or 3' ends; modifications of the internucleoside linkages; modifications of the ribose units and of the nucleobases. PNA (Peptide Nucleic Acids) and DNA/PNA chimeras. Oligonucleotides as therapeutic agents: antisense and antigene strategies. Unusual conformations of nucleic acids: triplex and quadruplex structures. Oligonucleotide-based aptamers: case studies. Anti-VEGF aptamers: Pegaptanib. Anti-thrombin aptamers: TBA (thrombin binding aptamers) and its analogues. Aptameric biosensors. Oligonucleotides and nanotechnologies.
Final evaluation	Interview

Synthetic Glycochemistry	
Teachers	**Prof. Emiliano Bedini** (ebedini@unina.it) **Prof. Alfonso Iadonisi** (iadonisi@unina.it)
Credits	2
Planned hours	16
Planned schedules	*Interested students have to contact* Prof. Iadonisi or Prof. Bedini to *arrange the detailed timetable.*
Objectives	The course aims to cover the main topics of organic carbohydrate chemistry in its synthetic aspects.
Description	The first part of the course will describe the reactions of derivatization and synthesis of mono- and oligosaccharides, with a broad focus on glycosylation. This is a key reaction for the synthesis of oligosaccharides of biological and biomedical interest. Therefore, it will be dealt with extensively, ranging from its classic aspects to the most recent and innovative ones (automated glycosylations, glycosylations in aqueous solutions, in the absence of solvent, etc.) The second part will concern the application of the concepts described above to recently developed research fields, such as the construction of multivalent glycoconjugates (glycodendrimers, glycopolymers, glyconanoparticles, etc.), the regioselective modification of complex natural products based on carbohydrates, the semi-synthesis of modified polysaccharides and their use in block co-polymers. For both parts of the course, several examples from recent literature articles will be discussed.
Final evaluation	The proficiency evaluation of the students will be determined after an oral examination.

X-ray crystallography of biological macromolecules: advanced methods and applications	
Teachers	**Prof. Antonello Merlino** (antonello.merlino@unina.it) **Prof. Filomena Sica** (filomena.sica@unina.it)
Credits	2
Planned hours	16
Planned schedules	*Interested students have to contact* Prof. Sica and Prof. Merlino *to arrange the detailed timetable*
Objectives	The aim of this course is to provide an overview of the fundamental approach and the latest developments of X-ray crystallography of biological macromolecules. Examples of studies on structure-function relationship and of studies on the elucidation of complexes with ligands will be provided.
Description	Crystallography is one of the most powerful techniques for the structural analysis at the atomic level. It has come to play an increasingly critical role in the drug discovery process and in understanding the molecular basis of many human diseases. In recent years, an increasingly important contribution to structural elucidation of bio-macromolecules and to understanding of their mechanisms of action has been obtained by electron microscopy at cryogenic conditions (Cryo-EM). This methodology allows to obtain high resolution structures of complex biomolecules and molecular machines such as chromatin, supercoiled DNA, intracellular vesicles, ion channels and single viral particles. In this course, fundamentals of X-ray diffraction and modern methodologies, including time resolved, neutron, X-ray free-electron laser and ultrahigh resolution crystallography will be illustrated, together with the theoretical bases of electron microscopy and some interesting applications. A number of interesting recent applications, including those that have allowed to delineate the mode of action of Pt-, Ru- and Au-based drugs will be presented. In this respect, crystallographic studies on the interaction between metal-based drugs, like cisplatin, carboplatin and oxaliplatin, and both DNA and proteins will be discussed. Recent structural studies that reveal the molecular bases of protein-gold compounds and protein-ruthenium compounds recognition will be also analyzed.
Final evaluation	The assessment will be done by illustration and discussion of a recent paper concerning the topics of the course.