



- Chemical Sciences PhD course catalog - 36th cycle, and till active cycles

Advanced Mass Spectrometry (Prof. Angela Amoresano)

Applications of optical and Raman microscopy
(Dr. Manuela Rossi, Prof. Alessandro Vergara)

Bioplastics (Dr. C. Valeria L. Giosafatto)

Chemical methodologies for cultural heritage
(Prof. Lelia Birolo, Prof. Alessandro Vergara)

Composite materials: design, production technologies and applications
(Prof. Ugo Caruso)

Concerning the use of some transition metal oxo-species in organic synthesis
(Prof. Vincenzo Piccialli)

Electronic structure methods for solid state materials
(Prof. Ana Belen Muñoz-Garcia)

Flow Chemistry: towards a modern Chemical Industry (Dr. Vincenzo Russo)

Food Chemistry: preservation, processing and nutritional issues
(Prof. Alessandra Napolitano)

Forensic Chemistry (Prof. Angela Amoresano, Prof. Marco Trifuoggi)

Interpretative spectroscopy of natural organic substances
(Prof. Alessio Cimmino, Prof. Antonio Evidente)

Mitigation of the Environmental Impact of Chemical Processes for Energy Production
(Prof. Fabio Montagnaro)

Molecular engineering of proteins and metalloproteins (Dr. Marco Chino)

Nanostructures and nanotechnologies (Prof. Claudio De Rosa)



Natural phenolic compounds: structure, reactivity and applications

(Prof. Lucia Panzella)

Persistent organic pollutants (POPs)

(Dr. Anna Andolfi)

Physical chemistry of the Nanosystems

(Prof. Luigi Paduano)

Production of Native and Mutant Recombinant Proteins

(Prof. Angela Duilio)

Recent advances in biomolecular NMR

(Prof. Delia Picone)

Selective Organometallic Catalysis: systems and advanced techniques

(Prof. Peter Budzelaar)

Smart Drug Delivery Systems

(Prof. Annalisa Guaragna)

Structure and Dynamics of Materials and Macromolecules by Elastic and Inelastic Scattering Techniques

(Prof. Finizia Auriemma)

Synthesis, structure and applications of natural and modified oligonucleotides

(Prof. Daniela Montesarchio, Dr. Domenica Musumeci)

Synthetic Glycochemistry

(Prof. Emiliano Bedini, Prof. Alfonso Iadonisi)

Use and misuse of chemicals

(Dr. Fabio Temussi)

X-ray crystallography of biological macromolecules: advanced methods and applications

(Prof. Antonello Merlino, Prof. Filomena 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.

Advanced Mass Spectrometry	
Teacher	Prof. Angela Amoresano (angela.amoresano@unina.it)
Credits	2
Planned hours	16
Planned schedule	June-July <i>Interested students have to contact Prof. Amoresano to arrange the detailed timetable</i>
Objectives	The course aims to provide the skills on advanced mass spectrometry techniques. The potentialities and weaknesses of the various mass spectral techniques are illustrated by numerous examples
Description	<p>Basics: Isotopic profile, Resolution and Mass Accuracy.</p> <p>Ionization Methods: Electronic Ionization (EI); Electrospray; MALDI.</p> <p>Mass Analysers: Quadrupole; Time of Flight (TOF); Ion Trap; Linear Ion Trap; Orbitrap.</p> <p>Linked Systems: GC-MS and LC-MS/MS analyses; Select Ion Monitoring (SIM); Ion Mobility Mass Spectrometry.</p> <p>Tandem Mass Spectrometry: Collision Induced Dissociation (CID); Tandem in Space; Tandem in Time; Product Ion Scan.</p> <p>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.</p> <p>Application of LC-MS/MS Analyses: Forensic Sciences; Diagnostic in Cultural Heritage; Environmental Analyses; Neonatal Diagnostic; Drugs determination</p>
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	<i>Interested students have to contact Prof. Vergara or Dr. Rossi to arrange the detailed timetable</i>
Objectives	The course aims to provide the theoretical and applied aspects of optical microscopy (both stereo and polarization microscopy) and Raman microscopy (in its variants non-stimulated and stimulated) also compared to IR microspectroscopy.
Description	<p><i>Part A. Optical Microscopy.</i> 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.</p> <p>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.</p> <p>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.</p> <p><i>Part B. Raman Microscopy.</i> A brief introduction on the theory of Raman spectroscopy (resonance Raman, CARS and SERS), followed by some examples of application of Raman imaging.</p>
Final evaluation	Presentation of an application of Raman and/or optical microscopy to be defined with the teacher.

Bioplastics	
Teacher	Dr. C. Valeria L. Giosafatto (giosafat@unina.it)
Credits	2
Planned hours	16
Planned schedules	<i>Interested students have to contact Dr. Giosafatto to arrange the detailed timetable</i>
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	<ul style="list-style-type: none"> • 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 <p>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 will be also taken into account as potential method to improve the features of the novel bioplastics.</p> <p>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.</p>
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	Half of June/half of July <i>Interested students have to contact Prof. Birolo or Prof. Vergara to arrange the detailed timetable</i>
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

Composite materials: design, production technologies and applications	
Teacher	Prof. Ugo Caruso (ugo.caruso@unina.it)
Credits	2
Planned hours	16
Planned schedules	<i>Interested students have to contact Prof. Caruso to arrange the detailed timetable</i>
Objectives	<p>The basic concepts for the design of composite materials will be illustrated in the course. The fundamental Structure-Property relationships responsible for the very high physical and mechanical characteristics will be analysed. The close connection between the composition of the material, the structural optimization project and the forming technology will also be illustrated, in a convergent and interactive process.</p> <p>The main applications in the automotive and aeronautical industry will be illustrated.</p> <p>Understanding the topics requires a minimum level of knowledge of chemistry, physics and mechanics.</p>
Description	<p>Topics covered in the course:</p> <ul style="list-style-type: none"> • Introduction: Definition of composite material; • Fillers and matrices; • Forming technologies: manual, autoclave, Resin Transfer Moulding, wrapping (FW), pultrusion, infusion; • Thermoplastic matrix composite materials; • Design and applications: micromechanics and macromechanics of the lamina; • Analysis of the structure design; • Applications of composites. <p><u>Recommended textbooks</u></p> <ul style="list-style-type: none"> ○ Ignazio Crivelli Visconti - Materiali compositi - ed. Hoepli. ○ Mario Marchetti, Domingo Cutolo - Tecnologie dei materiali compositi - ed. ESA ○ Available course notes
Final evaluation	The course will end with a discussion on the knowledge acquired in the form of a brief report on a specific sector or system among those treated, examined from the summary to the use up to the specific characteristics

Concerning the use of some transition metal oxo-species in organic synthesis

Lecturers	Prof. Vincenzo Piccialli (vinpicci@unina.it)
Credits (planned)	2
Planned hours	16
Planned schedules	July <i>Interested students have to contact Prof. Piccialli to arrange the detailed timetable</i>
Objectives	The course is aimed at offering an overview of the use of some transition metal oxo-species in organic synthesis.
Description	Some aspects of the oxidation chemistry of, among others, osmium tetroxide, ruthenium tetroxide, permanganate and methyltrioxorhenium will be discussed through the examination of the synthesis of selected natural polyethereal substances. A special emphasis will be given to the synthesis of mono- or polytetrahydrofuran subunits.
Final evaluation	The acquisition of competences will be established through an interview.

Electronic structure methods for solid state materials	
Teacher	Prof. Ana Belen Muñoz García (anabelen.munozgarcia@unina.it)
Credits	2
Planned hours	16
Planned schedules	<i>Interested students have to contact Prof. Ana B. Muñoz García to arrange the detailed timetable</i>
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

Flow Chemistry: towards a modern Chemical Industry	
Teacher	Dr. Vincenzo Russo (v.russo@unina.it)
Credits (planned)	2
Planned hours	16
Planned schedule	October-February <i>Interested students have to contact Dr. Russo to arrange the detailed timetable</i>
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	July/September <i>Interested students have to contact Prof. A. Napolitano to arrange the detailed timetable.</i>
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 manufacturing processes. Elements of nutritional relevance, raising increasing interest are also presented to make the attendants able to pursue further investigation and continuous updating.
Description	<p>Food components: brief overview (1 lecture)</p> <p>Food organoleptic characteristics: Color: main pigments; Taste: the five main tastes; Odor : classification of odorants; methods for evaluation (1 lecture)</p> <p>Food storage and preservation: Exposure to oxygen, light, contaminants; Prolonging shelf life; Smart packaging; Food additives: main classes and applications (2 lectures)</p> <p>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)</p> <p>Nutritional aspects: Vitamins; Functional foods; Lipid supplements; Proteic supplements; Fortificants; Prebiotics and probiotics; Bioactives in plant derived food; antinutritional factors (1 lecture)</p> <p>Focus on selected food: cereals, tea, coffee, cocoa or others , non-conventional food (1 lecture)</p>
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. Angela Amoresano (angela.amoresano@unina.it) Prof. Marco Trifuoggi (marco.trifuoggi@unina.it)
Credits	2
Planned hours	16
Planned schedule	February <i>Interested students have to contact Prof. Amoresano or Prof. Trifuoggi to arrange the detailed timetable</i>
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: psychoactive substances, fingerprints, paints, explosives residues.
Final evaluation	Oral discussion

Interpretative spectroscopy of natural organic substances	
Teachers	Prof. Alessio Cimmino (alessio.cimmino@unina.it) Prof. Antonio Evidente (evidente@unina.it)
Credits	2
Planned hours	16
Planned schedule	June-July <i>Interested students have to contact Prof. Cimmino/Evidente to arrange the detailed timetable</i>
Objectives	The course aims at acquiring knowledge on the most important classes of natural organic substances: on chemistry and biosynthesis. The knowledge on the structure-activity correlation, aimed at modulating their activity and specificity, will allow to plan their potential practical application in agriculture and medicine. Furthermore, the course will present the physical basis of IR, UV and NMR spectroscopies. For NMR the basis of the multi pulse experiments used in organic chemistry to define the structure of natural compounds and the fundamental parameters for the interpretation of ^1H and ^{13}C one and two-dimensional spectra will be acquired. Fundamental basis will be also acquired on mass spectroscopy.
Description	The course will briefly deal with the most important classes of natural compounds: <ul style="list-style-type: none"> - polyketides, terpenes and steroids, phenylpropanoids and alkaloids; - the chemistry, biosynthesis and structure-activity correlation; - the potential application of natural bioactive compounds in agriculture and medicine. -The resonance phenomenon; chemical shift and correlation with the structural elements; the spin-spin coupling (multiplicity); the coupling constant; ^1H and ^{13}C spectroscopy: chemical shift and correlation with the structural features; two-dimensional experiments; the most common sequences: COSY, HSQC, HMBC and NOESY; recording and interpretation of mono and two-dimensional spectra; use of NMR spectroscopy for the determination of the structure of natural compounds. Outlines of IR, UV and mass spectroscopy.
Final evaluation	Final 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	January/February/June/July/September <i>Interested students have to contact Prof. Montagnaro to arrange the detailed timetable</i>
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	<ul style="list-style-type: none"> ○ Climate changes and related environmental, social, economic and technical aspects. Facing climate changes by use of renewables, CO₂ 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 CO₂ emissions into the atmosphere: absorption with chemical reaction, oxyfuel and chemical looping combustion, calcium looping. ○ Gasification cycles integrated with CO₂ 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	<i>Interested students have to contact Dr. Chino to arrange the detailed timetable</i>
Objectives	<p>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.</p> <p>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.</p>
Description	<p>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.</p> <p>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.</p> <p>Each student will be involved in critical discussions about current literature, from which, he will be trained to a specific design technique.</p> <p>Each student will then prepare a simple project for the computational design of a protein or a metalloprotein of biotechnological, pharmacological or technological interest.</p>
Final evaluation	Evaluation and discussion of the assigned literature and of the proposed project.

Nanostructures and nanotechnologies	
Teacher	Prof. Claudio De Rosa (claudio.derosa@unina.it)
Credits	2
Planned hours	16
Planned schedules	<i>Interested students have to contact Prof. De Rosa to arrange the detailed timetable</i>
Objectives	The course aims at providing new technologies for the preparation and characterization of nanostructures and nanocomposites.
Description	<p>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 by self-assembly in block 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.</p>
Final evaluation	Interview

Natural Phenolic Compounds: Structure, Reactivity and Applications	
Teacher	Prof. Lucia Panzella (panzella@unina.it)
Credits	2
Planned hours	16
Planned schedules	January <i>Interested students have to contact Prof. Panzella to arrange the detailed timetable</i>
Objectives	Acquisition of knowledge related to structure-property relationships and possible manipulations of natural phenolic compounds for practical applications.
Description	<ol style="list-style-type: none"> 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	October/November <i>Interested students have to contact Dr. Andolfi to arrange the detailed timetable</i>
Objectives	<p>The course is proposed for PhD Students in chemistry-, chemical engineering- and environmental sciences-related fields. The main learning objectives are:</p> <ul style="list-style-type: none"> • 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	<p>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)</p> <p><u>Main pollutants.</u></p> <p>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.</p> <p>Industrial products [polychlorinated biphenyls (PCBs)]: chemical structure, industrial production, uses, environmental behavior, toxicity, alternatives to their use.</p> <p>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.</p> <p>Polycyclic aromatic hydrocarbon (PAH). Chemical structure, formation mechanisms, behavior and reactivity in the air, metabolism, toxicity.</p> <p>Endocrine disruptor (Flame retardants, PFOA-PFOS, Phthalates). Definition, structure, industrial production, uses, toxicity, alternatives to their uses.</p> <p>Examples of pollutants of natural origin. Definition, structure and toxicity</p> <p>Examples of contaminated sites in Italy.</p> <p><u>Recommended textbooks</u> Available course notes</p>
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	<i>Interested students have to contact Prof. Paduano to arrange the detailed timetable</i>
Objectives	
Description	<p>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.</p> <p>Solvation, Structural, and Hydration Forces. Adhesion and Wetting Phenomena.</p> <p>Thermodynamic of Self- Assembly.</p> <p>Colloids, micelles, bilayers, Vesicles, Liposomes, Emulsions, Microemulsions,</p>
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	July/September <i>Interested students have to contact Prof. Duilio to arrange the detailed timetable</i>
Objectives	Aquisition of the knowledges needed to design processes for the production of both native and mutant recombinant proteins.
Description	<p><u>Main topics</u></p> <p>From gene to recombinant proteins: design and development of a recombinant expression system.</p> <p>Main features of host microorganisms for heterologous expression.</p> <p>Expression vectors: features and uses.</p> <p>Gene expression from strong and weak promoters.</p> <p>Fusion proteins.</p> <p>Optimization of expression conditions.</p> <p>Principles of protein engineering.</p> <p>Targeted and site-specific mutagenesis.</p> <p>Random mutagenesis and <i>in vitro</i> molecular evolution.</p>
Final evaluation	Interview

Recent advances in biomolecular NMR	
Teacher	Prof. Delia Picone (delia.picone@unina.it)
Credits (planned)	2
Planned hours	16
Planned schedules	February/September <i>Interested students have to contact Prof. Picone to arrange the detailed timetable</i>
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	<i>Interested students have to contact Prof. Budzelaar to arrange the detailed timetable</i>
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	<p>The course will cover selected topics in modern homogeneous catalysis research:</p> <ul style="list-style-type: none"> • 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 <p>Characterization methods will be discussed where appropriate. The material is based on recent research literature.</p>
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	May <i>Interested students have to contact Prof. Guaragna to arrange the detailed timetable</i>
Objectives	The aim of the course is to give an overview of the modern smart delivery systems to selectively 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	September <i>Interested students have to contact Prof. Auriemma to arrange the detailed timetable</i>
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	<p>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.</p> <p>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.</p> <p>The scattering Invariant. Scattering of X-rays, electrons, neutron and light. Absolute Intensity and Relative Intensity (3h).</p> <p>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)</p> <p>Examples of nanostructured systems. Gaussian and expanded chains. Polymer Gels. Nanoporous systems (concrete and silica gels). Metallic nanoparticles. Block copolymers and nanostructures. (2 h).</p> <p>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)</p> <p>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).</p> <p>Numerical exercise based on use of standard free-ware for the analysis of neutron scattering data (2h).</p>
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	<i>Interested students have to contact Prof. Montesarchio or Dr. Musumeci to arrange the detailed timetable</i>
Objectives	
Description	<p>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.</p>
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	January <i>Interested students have to contact Prof. Iadonisi or Prof. Bedini to arrange the detailed timetable.</i>
Objectives	The course aims to cover the main topics of organic carbohydrate chemistry in its synthetic aspects.
Description	<p>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.)</p> <p>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.</p> <p>For both parts of the course, several examples from recent literature articles will be discussed.</p>
Final evaluation	The proficiency evaluation of the students will be determined after an oral examination.

Use and misuse of chemicals	
Teacher	Dr. Fabio Temussi (fabio.temussi@unina.it)
Credits (planned)	2
Planned hours	16
Planned schedules	September/October <i>Interested students have to contact Dr. Temussi to arrange the detailed timetable</i>
Objectives	The course will provide an overview on the EU's groundbreaking chemicals legislation.
Description	<p>An introduction to the REACH (Registration, Evaluation, Authorisation and restriction of Chemicals) regulation, whose aim is to improve the protection of human health and the environment from the risks that can be posed by chemicals.</p> <p>An introduction to the CLP (Classification, Labelling and Packaging) regulation, that ensures that the hazards presented by chemicals are clearly communicated to workers and consumers in the EU through classification and labelling of chemicals.</p> <p>Special attention will be given to the importance of accurate substance identification, the different regulatory processes, and the 'Integrated regulatory strategy'.</p>
Final evaluation	Written test/interview

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	End of September <i>Interested students have to contact Prof. Sica and Prof. Merlino to arrange the detailed timetable</i>
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.