UNIVERSITY OF L'AQUILA

Department of Physical and Chemical Sciences

2nd Cycle Degree in CHEMISTRY

Laurea Magistrale in SCIENZE CHIMICHE

Course Catalogue

Academic year starts the last week of September and ends the first week of June.
1st Semester - *Starting date:* last week of September, *end date*: 3rd week of January
2nd Semester - *Starting date:* last week of February, *end date:* 1st week of June
Exams Sessions: I) from last week of January to 3rd week of February, II) from 2nd week of June to end of July, III) from 1st to 3rd week of September

Comprehensive Scheme of the Second Cycle Degree in "CHEMISTRY"				
YEAR	CODE	COURSE	Credits (ECTS)	Semester
I	F0034	Advanced Inorganic Chemistry	9	2
	F0047	Bioorganic Chemistry	6	1
	F0049	Bioinorganic Chemistry	6	2
	F0051	Supramolecular Chemistry	6	2
	F0052	Advanced Analytical Methods	6	2
	F0986	Physical Methods in Organic Chemistry	9	2
	F0109	Advanced Organic Chemistry	9	1
	F0112	Quantum Mechanics for Material Physics	6	1
		Optional course	6	1 or 2
II	F0107	Theoretical Chemistry	6	1
	F0110	Organic Synthesis with Laboratory	6	1
	F0112	Techniques for Materials Characterization with Laboratory	9	2
		Optional Course	6	1 or 2
		Free choice Course/Courses	9	1 or 2
		Placement	6	1 or 2
		Master Thesis	30	2

Optional Courses				
YEAR	**CODE**	**COURSE**	**Credits (ECTS)**	**Semester**
Academic Year 2014/15				
I or II	F0098	Chemistry of Organometallic Compounds	6	1
	F0115	Chemistry of Natural Organic Compounds	6	2
	F0101	Chemistry of the Atmosphere	6	1
	F1140	Computer Modelling and Simulation of Biomolecules	6	1

Programme of "CHIMICA INORGANICA SUPERIORE" *"ADVANCED INORGANIC CHEMISTRY"*		
F0034, compulsory **Second Cycle Degree in "CHEMISTRY", 1st year, 1st semester**		
Number of ECTS credits: 9 (workload is 225 hours; 1 credit = 25 hours)		
Teacher: Marcello Crucianelli		
1	Course objectives and Learning outcomes	Main goals of this course are, among others: understand the quantum-mechanical basis of the electronic structure of atoms e rationalize the periodical properties of the elements; understand the evolution of the bonding theories, their success and limits in the description and rationalization of the structure of coordination complexes and in the prevision of their physico-chemical properties; classify the reactions of coordination complexes and rationalize the reactivity on the basis of the molecular geometry and oxidation number of the metallic atoms; describe the extraction methods of d- and f-block metals, their physico-chemical properties and the main classes of related compounds
2	Course content and Learning outcomes (Dublin descriptors)	Topics of the module include: Quantum-mechanical basis of the Periodic table. Electronic configuration of atoms and ions of d and f blocks. Periodical trends of atomic parameters. Focus on acidity and basicity theories. Non aqueous media. Bonding theories of coordination compounds. Molecular orbital theory applied to coordination complexes. Hydrogen chemistry. Multielectronic atoms and ions. Electronic spectra of coordination complexes. Reactions of coordination complexes. Representative compounds of transition elements. Coordination chemistry of lanthanides, thorium and uranium. On successful completion of this module, the student should: - have basic knowledge of classic thermodynamic, of quantum mechanics, of chemistry of the elements, of bonding theories for block s, p and d metals, of the molecular structure, of the main classes of organic compounds and their typical reactions, of the periodical trends and of the coordination chemistry of metal ions, - have knowledge and understanding of the main spectroscopical techniques employed on inorganic experiments, - understand and explain concepts on thermodynamic of solutions, - understand the rationale behind the progress that has produced the evolution of the main scientific theories, - demonstrate skill in understanding of the main scientific papers and ability to design their own theories to answer a number of scientific questions, - demonstrate capacity for reading and understand other texts on related topics.
3	Prerequisites and learning activities	A good knowledge and skill with the basic concepts of general chemistry, organic chemistry and physical chemistry is required
4	Teaching methods and language	Lectures, exercises and home work Language: Italian/English Ref. Text books: D. F Shriver, P. W. Atkins, C. H. Langford, *Inorganic Chemistry,* 5th edition, Ed. Oxford University Press, Oxford,2010, United Kingdom; C. E. Housecroft, A. G. Sharpe, *Inorganic Chemistry*, 4th edition, Ed. Pearson Prentice Hall, Edinburg, 2012, United Kingdom.
5	Assessment methods and criteria	Written and oral examination

Programme of"CHIMICA BIOORGANICA" "*BIORGANIC CHEMISTRY*"		
F0047, Compulsory **Second Cycle Degree in "CHEMISTY", 1st, year, 1st semester**		
Number of ECTS credits: 6 (workload is 150 hours; 1 credit = 25 hours)		
Teacher: Nicoletta Spreti		
1	Course objectives	The goal of this course is to introduce students to the theories of modern bioorganic chemistry. Much of the course focuses on understanding the chemical strategies and mechanisms behind enzyme catalysis. On successful completion of this module, the student should be able to successfully discuss new strategies to employ enzymes for organic synthesis and how the host–guest approach could be able to construct simple molecules that mimic complex biological systems.
2	Course content and Learning outcomes (Dublin descriptors)	Topics of the module include: Introduction: Catalysis, proximity effect, molecular adaptation, molecular recognition. Enzyme catalysis and kinetics: Catalytic efficiency of enzymes and mechanism of action. Enzymes in synthetic organic chemistry: Bioconversion in non-conventional media. Immobilized enzymes and methods of immobilization. Enzymes in supramolecular systems: micelles and reverse micelles, liposomes; biocatalysis in ionic liquids. Enzyme Models: Host-guest complexation chemistry. Chiral recognition and catalysis. Stereoselective transport. Enzyme models. Many examples of recent literature are presented and discussed. On successful completion of this module, the student should: - have profound knowledge of the basic concepts of bioorganic chemistry as an essential tool to the understanding of living processes in nature; - have knowledge and understanding of the main non-conventional media used for bioconversions; - understand and explain the bioorganic chemical principles and the tools of organic chemistry to mimic biological events; - understand the biomimetic approach and be aware of biomolecular processes; - demonstrate skill in comparing scientific articles and ability to design their own experiments to answer a relevant question - demonstrate capacity for reading and understand other texts on related topics.
3	Prerequisites and learning activities	The basic notions of organic chemistry and biochemistry are required.
4	Teaching methods and language	Lectures. Language: Italian Ref. Text books Lecturer notes. No text is required for the course, but it is recommended that students consult the following books: H. Dugas, *Bioorganic Chemistry: a chemical approach to enzyme action*, Springer-Verlag; J.H. Fendler, *Membrane mimetic chemistry*", Wiley Interscience.
5	Assessment methods and criteria	Oral exam.

Programme of "CHIMICA BIOINORGANICA" ***"BIOINORGANIC CHEMISTRY"***		
F0049, Compulsory **Second Cycle Degree in "CHEMISTRY", 1st year, 2nd semester**		
Number of ECTS credits: 6 (workload is 150 hours; 1 credit = 25 hours)		
Teacher: Marcello Crucianelli		
1	Course objectives	Main goals of this course are, among others: to provide a comprehensive introduction to bioinorganic chemistry of main group elements along with a focus on the role of d- and f-block elements in biology. At the end of this Unit, students should be able to: - demonstrate an understanding of how and why the coordination chemistry of metals are used in biological systems. - understand the considerable current research attention attracted by transition metals in bioinorganic chemistry. - understand the bonding features relating to structural and reactivity patterns. - critically assess current literature on bioinorganic Chemistry.
2	Course content and Learning outcomes (Dublin descriptors)	Topics of the module include: Reminders on the basic concepts of biochemistry and on the main metabolic processes - metals in biology - basic coordination chemistry and analytical methods used in bioinorganic chemistry - metal containing enzyme systems - structural role of metals - metal uptake and trafficking – biomineralization - metals in medicine and metal toxicity. On successful completion of this module, the student should be able to: - demonstrate proficiency in the basic principles of inorganic chemistry, biochemistry, and molecular biology that are necessary to approach the field of bioinorganic chemistry; - identify the appropriate analytical techniques that are useful in characterizing transition-metal complexes in biological molecules; - describe the different processes involved in the transport and storage of metal ions. - describe the role of metal ions that are involved in electron-transfer reactions in biological systems; - describe some of the historic and current medical applications of metal ions. - have knowledge and understanding the main spectroscopical techniques employed for the elucidation of bioinorganic scaffolds; - understand and explain the cycles of the main elements involved in the functioning of living organisms - understand interactions between metal ions and complexes in biomolecules - demonstrate skill in understanding of the main scientific papers and ability to design their own theories to answer a number of specific questions, - demonstrate capacity for reading and understand other texts on related topics.
3	Prerequisites and learning activities	A good knowledge and skill with the basic concepts of organic and biological chemistry is required
4	Teaching methods and language	Lectures, exercises and home work Language: Italian/English Ref. Text books: Stephen J. Lippard, Jeremy M. Berg, *Principles of bioinorganic chemistry*, University Science Books, 1994 Rosette M. Roat-Malone, "*Bioinorganic Chemistry*", 2nd edition, Wiley, 2007; Robert R. Crichton, "*Biological Inorganic Cemistry*", Elsevier, 2nd ed., 2012. Educational materials (slides) prepared by the teacher.
5	Assessment methods and criteria	Oral examination and final dissertation on a agreed topic taken from the most recent scientific literature

Programme of “CHIMICA SUPRAMOLECOLARE” “*SUPRAMOLECULAR CHEMISTRY*”		
F0051, Compulsory **Second Cycle Degree in “CHEMISTRY”, 1st year 2nd semester:**		
Number of ECTS credits: 6 (workload is 150 hours; 1 credit = 25 hours)		
Teacher: Luisa Giansanti		
1	Course objectives	The goal of this course is to introduce students to the supramolecular chemistry. Much of the course focuses on understanding how each molecular component contributes to the properties of the supramolecular assemblyheld together by non covalent bond or which possesses a significant covalent component. On successful completion of this module, the student should be able to successfully discuss host–guest chemistry (binding of cations, anions or neutral molecules), molecular devices and some examples of biochemical self-assemblies.
2	Course content and Learning outcomes (Dublin descriptors)	Topics of the module include: Introduction: Supramolecular host-guest compounds, chelate, macrocyclic and template effect, supramolecular host design. Cation-binding hosts: crown ethers, podands, cryptands, spherands, selectivity of cation complexation. Binding of anions and neutral molecules: biological anions receptors, tetrahedral receptors, neutral receptors, anticrowns, clathrate compounds and zeolites. Templates and molecular devices: Template effect in synthesis. Catenanes and rotaxanes. Photochemical and electrochemical sensors, dendrimers. Biological mimics: micelles and liposomes Many examples of recent literature and of the characterization of these systems by different techniques are presented and discussed. On successful completion of this module, the student should - have profound knowledge of the basic concepts of supramolecular chemistry as an essential tool to the understanding of self-assembling systems; - have knowledge and understanding of the main host guest compounds; - understand and explainthe nature and the factors affecting supramolecular interactions; - understand the concepts in host design; - demonstrate skill in comparing scientific articles and ability to discuss the basis of the interactions between the components of supramolecular assemblies; - demonstrate capacity for reading and understand other texts on related topics.
3	Prerequisites and learning activities	A good knowledge of organic chemistry and physical chemistry is required
4	Teaching methods and language	Lectures. Language: Italian Ref. Text books Lecturer notes. No text is required for the course, but it is recommended that students consult the following book: J.W. Steed, J.L. Atwood “*Supramolecular chemistry”* Wiley
5	Assessment methods and criteria	Oral exams

Programme of "METODOLOGIE ANALITICHE AVANZATE" "ADVANCED ANALYTICAL METHODS"		
F0052, Compulsory 2nd Cycle Degree in "CHEMISTRY", 1st year , 2nd semester		
Number of ECTS credits: 6 (workload is 150 hours; 1 credit = 25 hours)		
Teacher: Angelo Antonio D'Archivio		
1	Course objectives and Learning outcomes	The goal of this course is to provide a thorough background in the statistical and chemometric methods that are useful for the representation, analysis and interpretation of multivariate chemical data and for a rational design of chemical experiments. On successful completion of this module, the student should understand the fundamental concepts of univariate statistics and chemometrics and should be able to apply the new skills to real problems, with the aid of PC software.
2	Course content and Learning outcomes (Dublin Descriptors)	Topics of the module include: Univariate statistics: Significance tests to compare means and variances. Analysis of variance. Normality tests. Treatment of outliers. Univariate calibration. Applications of univariate statistics to analytical data. Introduction to chemometrics: Variability and information. Representation of multivariate data. Data pre-treatment. Variance-covariance and correlation matrices. Principal component analysis (PCA): Rotation matrices. Eigenvalues and variance. Loadings and scores. PCA plots. Significant principal components. PCA, information and noise. Applications to chemical data. Cluster analysis: Distance and similarity. Clustering algorithms and dendrograms. Agglomerative and divisive clustering. K-means method. Multivariate modelling: Introduction to statistical models. Validation. Classification methods. Linear and quadratic discriminant analysis. K-nearest neighbour method. SIMCA method. Multilinear regression. Variable selection by all subset models, stepwise selection and genetic algorithms. Principal component regression. Partial least square regression. Curvilinear and artificial neural network regression. Quantitative Structure Activity (Property) Relationships QSA(P)R. Optimisation and experimental design: Multivariate optimization. Simplex method. Experimental design. Response surface method. On successful completion of this module, the student should - have profound knowledge of methods of univariate statistics and chemometrics , - have knowledge and understanding of concepts of univariate statistics useful for experimental data analysis and statistical bases of chemometric approaches - understand and explain the meaning of parameters related with statistical treatment of chemical data and chemometric tools - understand the fundamental concepts of univariate and multivariate statistics and be aware of potential applications to complex chemical data - demonstrate skill in interpretation of results of statistical data treatment and ability to apply common PC chemometric software - demonstrate capacity for interpret outcomes of chemometric data treatments
3	Prerequisites and learning activities	The student must know the basic notions of univariate statistics for analytical chemistry and the fundamentals of chemical and instrumental analytical methods.
4	Teaching methods and language	Lectures and computer exercises. Language: Italian Ref. Text books Roberto Todeschini: "*Introduzione alla chemiometria*" EdiSES, Napoli. Michele Forina: "*Fondamenta per la chimica analitica*". Available upon request to the author. James N. Miller e Jane C. Miller: "*Statistics and Chemometrics for Analytical Chemistry*", Pearson-Prentice All Ed.
5	Assessment methods	Oral exam.

Programme of “METODI FISICI IN CHIMICA ORGANICA” ***“PHYSICAL METHODS IN ORGANIC CHEMISTRY“***		
F0986, Compulsory **Second Cycle Degree in “CHEMISTRY”, 1th year, 2nd semester**		
Number of ECTS credits: 9 (workload is 225 hours; 1 credit = 25 hours)		
Teachers: Francesco De Angelis – Giorgio Cerichelli		
1	Course objectives	The objective of the course relies on providing the student with motivations on the subject, knowledge and detailed understanding of the most advanced techniques in NMR 1D and 2D, EPR; low frequency NMR, and Mass Spectrometry (MS), for the structural elucidation of organic and biological molecules. As to the last technique, the following are the relevant arguments: i) Interpretation of Electron Ionisation mass spectra, ii) description of the most diffused and advanced ion analysers, iii) Electrospray (ESI) and Matrix Assisted Laser Desorption Ionisation (MALDI) MS, iv) proteomics. On successful completion of the module, the student should manage with confidence fundamental as well as practical aspects of the subjects, be able to understand and interpret the graphics and spectra relevant to the taught spectroscopies, be able to apply the correct technique for the structure determination of the analytes.
2	Course content and Learning outcomes (Dublin descriptors)	Topics include: EI-MS: interpretation of the EI spectra of simple to medium complex organic molecules; molecular ions and isotopic peaks; mass shift at high masses; principles of fragmentation of organic ions; skeletal rearrangements; mass spectra of the most important classes of organic molecules; exercises; resolving power connected with high masses. MS: ion analysers: linear and ion trap quadrupole analysers; Ion Cyclotron Resonance (ICR) MS; orbitrap; Time-of-Flight (ToF) MS for the sudy of polar and high molecular weight organic and bilogical molecules: ESI-MS; multicharged ions; tandem MS; selective ion MS (SIM, MIM, SRM). Peptides fragmentations; ion families; interpretation of ESI spectra; DESI, DART, EESI, …; MALDI MS; ion-mobility; proteomics. NMR spectroscopy: FT instruments ,1D 2D sequences; multinuclear experiments; quadrupolar nuclei. Low frequency NMR: basic kinds of instruments, applications to food analysyis; EPR: spectra analysis and applications. On successful completion of this module, the student should - have profound knowledge of the subjects fundamentals; - have knowledge and understanding of the taught techniques, and their usage for the structural elucidation of organic and biological molecules; - understand and explain fundamentals as well as use and application boundaries of the techniques of interest, by using the appropriate technical language; - understand the fundamental concepts of the taught techniques, and their connections with organic and biological chemistry and with the other structural elucidation techniques; - demonstrate skill in managing the spectra obtained by the techniques of interest, and in proposing further experiments in order to get more structural information; - demonstrate capacity to choose the right experiment to solve complex problems/structures and for reading and understanding other texts on related topics.
3	Prerequisites and learning activities	The student must know the fundamental notions of General Physics, General Chemistry, Organic Chemistry and Organic Chemistry Laboratory, basic methods for molecular structure investigations.
4	Teaching methods and language	Lectures, ppt presentations, exercises, demonstrations on the instruments; homework, reports, tests. Language: Italian; English on demand. Ref. Text books: Copies of the ppt presentations, text books. - R.M. Silverstein, “*Identificazione spettroscopica di composti organici*”. Ambrosiana editrice. - D.H. Williams, I Fleming, “*Spectroscopic Methods in Organic Chemistry*”. McGraw-Hill Co., London. A. E. Derome, “*Modern NMR techniques for chemistry research*”. Pergamon press.
5	Assessment methods and criteria	Oral exam; exercise solving.

Programme of “CHIMICA ORGANICA SUPERIORE” *“ADVANCED ORGANIC CHEMISTRY“*		
F0109, compulsory for curriculum in Chemistry **Second Cycle Degree in “CHEMISTRY”, 1th year, 1st semester**		
Number of ECTS credits: 9 (workload is 225 hours; 1 credit = 25 hours)		
Teachers: Giorgio Cerichelli – Antonio Arcadi		
1	Course objectives	Advanced course concerning structure, mechanism and correlations between structure and reactivity in organic chemistry.
2	Course content and Learning outcomes (Dublin descriptors)	Topics include: • Free Energy correlation; • Acidity functions; • Criteria to asses mechanism; • Kinetic of organic reactions • Free radical reactions; • Carbenes and Nitrenes; • Carbocations; • Pericyclic reactions : the Diels-Alder reaction, photochemical [2+2]cycloadditions, thermal [2+2] cycloadditions and 1,3-dipolar cycloadditions. On successful completion of this module, the student should - understand kinetic and thermodynamic of organic reactions and the reactivity of organic intermediates and their options for reactions; - have acquired knowledge of organic reactions mechanisms; - demonstrate capacity to predict reaction pathways and skill in designing syntheses by retrosynthesis analysis.
3	Prerequisites and learning activities	The student must know the basic notions of Organic Chemistry.
4	Teaching methods and language	Lectures . Language: Italian; English on demand Ref. Text books *“Advanced Organic Chemistry”* Carey, F. A.; Sundberg, R. J., Springer 5th ed. 2007 *“Mechanism and Theory in Organic Chemistry*” Lowry, Thomas H Richardson, Kathleen Schueller - New York Harper & Row
5	Assessment methods and criteria	Oral exam

Programme of "MECCANICA QUANTISTICA PER LA FISICA DEI MATERIALI" "QUANTUM MECHANICS FOR MATERIALS PHYSICS"		
F0111, Compulsory for curriculum in Materials Science **2nd Cycle Degree in "CHEMISTRY", 1st year , 1st semester**		
Number of ECTS credits: 6 (workload is 48 hours; 1 credit = 8 hours)		
Teacher: Gianni Profeta		
1	Course objectives and Learning outcomes	The main objective of the course is to provide an introduction of the basic principles and postulates of the quantum mechanics for a student in chemistry. The course provides, in addition, a general discussion of the implication of the quantum physics in different aspects of the chemistry. On successful completion of this course the student is able to start a more technical and deep understanding of problems in quantum mechanics, using advanced textbooks in quantum chemistry.
2	Course content and Learning outcomes (Dublin descriptors)	Topics of the course include: Limits of classical mechanics Black body radiation, Fourier transform, Planck Hypothesis, Photoelectric effect, Compton effect, electron diffraction The Wave Packet De Broglie wavelength, width of a wave-packet, Gaussian wave-packet, uncertainty principle, phase and group velocity, De Broglie relations Wave equation, Schrodinger equations, probability conservation, superposition principles. Operators Definition of linear operators, multiplication of two operators, Hermitian operators, Eigenvalues and Eigenfunctions Solution of Schrodinger equation Wavefunction expansion on a basis, Hamiltonian Operator, Eigenvalues of H Solution of the S. equation for simple unidimensional potentials Matrix formulation of the Quantum Mechanics Bra/Ket notation, Physical implication of the commutation operator, Ehrenfest theorem, Linear vector space, definition of a matrix Examples of two level systems: H2+, Ammonia, Benzene, Eigenvalues and Eigenvectors of a two-level system, Rabi's Formula Quantum Theory of the Angular Momentum Stern-Gerlach's experiment, Angular momentum and magnetic moment operators, Commutation relation for Lx, Ly, Lz, L2, Definition of Spin, Eigenstates of Lx, Ly, Lz, Pauli Matrices, Quantum treatment of Stern- Gerlach's experiment. Nuclear Magnetic Resonance Interaction of a ½ spin with a static magnetic field, classical and quantum treatment of resonance Quantum Harmonic Oscillator Classical treatment of harmonic oscillator, a and a+ operators, definition of H in terms of a and a+, energy spectrum and zero-point energy, matrix definition of H, a and a+, Hermite polynomials. On successful completion of this module, the student should - have profound knowledge of basic postulates of Quantum Physics - have knowledge and understanding of simple problems in quantum mechanics - understand and explain the meaning of possible outcomes of quantum experiments - understand the principles of main spectroscopic techniques - demonstrate capacity for reading and understand other texts on related topics.
3	Prerequisites and learning activities	The course is self-contained for both mathematical and physical aspects. However, a basics of mathematical analysis and algebra and the basics of classical mechanics and electromagnetics are required.
4	Teaching methods and language	Lectures and exercises. Language: Italian / English Reference textbooks are provided for each specific arguments
5	Assessment methods	Written and oral exam.

Programme of "CHIMICA TEORICA" ***"THEORETICAL CHEMISTRY"***		
F0107, Compulsory **2nd Cycle Degree in CHEMISTRY, 2nd year , 1st semester:**		
Number of ECTS credits: 6 (workload is 150 hours; 1 credit = 25 hours)		
Teacher: Fabio Ramondo		
1	Course objectives and Learning outcomes	The goal of this course is to learn the basic theory of quantum chemistry and to know modern theoretical methods in study of molecular structure, bonding, and reactivity. The student should be aware of advantages and disadvantages of computational ab initio methods; he should be able to use them to solve problems of interest in chemistry and molecular sciences; he should be able to use computational tools for theoretical determination. The course will be project-based, and students will be encouraged to pursue projects related to their own research if possible.
2	Course content and Learning outcomes (Dublin descriptors)	Topics of the module include: Concepts from linear algebra Review of postulates of quantum mechanics The Born-Oppenheimer approximation, potential energy surfaces, local and global minima, transition states, and Hessian indices Variational method Hartree-Fock molecular orbital theory: Slater determinants, anti-symmetry principle, deriving the Hartree-Fock equations, Hartree-Fock energy expressions for arbitrary spin-orbital configurations, spin integration, self-consistent-field (SCF) procedure Basis sets: Slater and Gaussian functions, contractions, polarization and diffuse functions, split-valence sets Geometry optimization Vibrational frequency analysis: symmetry analysis, harmonic vs. fundamental frequencies, zero-point vibrational energies, Hessian index, distinguishing minima from transition states Introduction to electron correlation Configuration interaction Many-body perturbation theory Density-functional theory After a successful course completion, the student will be able to: • have knowledge of basic techniques to solve the equations resulting from the HF model. • have ability in the use of most diffuse computational tools for quantum chemical calculations. • understand the limitations of ab initio methods in describing molecular properties, • demonstrate capacity in the choice on the level of calculation for molecular modeling; • demonstrate capacity to propose adequate basis sets for selected calculation types.
3	Prerequisites and learning activities	The student needs to know some basic notions of Physical Chemistry of atoms and molecules, some basic concepts from quantum chemistry along with notions of differential and integral calculus.
4	Teaching methods and language	Lectures and practical training. Language: Italian / English E. Lewars - *Computational Chemistry. Introduction to the Theory and Applications of Molecular and Quantum Mechanics* Kluwer, 2003. A. Szabo and N. S. Ostlund, *Modern Quantum Chemistry, Introduction to Advanced Electronic Structure Theory* Dover, 1989.
5	Assessment methods and criteria	Presentation of computational projects produced by students and oral exam.

Programme of “SINTESI ORGANICA CON LABORATORIO” “*ORGANIC SYNTHESIS WITH LABORATORY*”		
F0110, Compulsory for curriculum in Chemistry **2nd Cycle Degree in “CHEMISTRY”, 2nd year, 1st semester**		
Number of ECTS credits: 6 (workload is 150 hours; 1 credit = 25 hours)		
Teacher: Fabio Marinelli		
1	Course objectives	The goal of this course is to provide knowledge of some relevant synthetic methodologies , and of the basic techniques for the synthesis and purification of organic molecules. Practical application of NMR, MS and IR for the elucidation of the structures of compounds prepared will be illustrated. Students will be introduced to the use of databases and chemical literature
2	Course content and Learning outcomes (Dublin descriptors)	Topics of the module include: • Safety rules in chemical laboratory. Chemical literature and databases. • Protective groups in organic synthesis: hydroxyl, amine, carbonyl and carboxyl acid-protecting groups; synthetic equivalents. • C-C Bond formation using B, Si and Sn compounds: organoboranes, vinysilanes and their synthesis; reaction of organoboranes; reactions of ally and vinylsilanes; organostannanes. • Application of transition-metal complexes containing M-C sigma bonds: organocopper chemistry; cross-coupling processes: Sonogashira, Negishi, Suzuki and Stille reactions. Use of CO. Heck reaction. Buckwald- Hartwig coupling • Organocatalysis: aminocatalysis. On successful completion of this module the student should • Have a knowledge of laboratory techniques for synthesis and purification of organic compounds. • Have a knowledge and understanding of some relevant synthetic methodologies. • Applying these knowledge to the synthesis of simple target molecules . • Demonstrate ability in elucidation of the structure of compounds prepared. • Have capacities of reading and understanding research articles in the field of organic synthesis
3	Prerequisites and learning activities	The student must know Organic Chemistry at intermediate level, basic NMR/MS/IR theory, and basic laboratory techniques (TLC, chromatography, liquid-liquid extraction)
4	Teaching methods and language	Language: Italian/English Ref. Text books: Slides and notes from lessons; Hegedus, Söderberg: *Transition Metals in the Synthesis of Complex Organic Molecules*, University Science Books, 2010, Chapters 1 and 4; Carey, Sundberg: *Advanced Organic Chemistry*, Springer, 2007, Part B, Chapters 9, 16.
5	Assessment methods and criteria	Oral exam and discussion of the results of a laboratory experiment.

Programme of "TECNICHE DI ANALISI DEI MATERIALI CON LABORATORIO" *"TECHNIQUES FOR MATERIALS CHARACTERIZATION WITH LABORATORY"*		
F0112, Compulsory for curriculum in Materials Science **Second Cycle Degree in "CHEMISTRY", 2nd year, 1st semester**		
Number of ECTS credits: 9 (Workload is the global work: 225 hours)		
Teacher: Maurizio Passacantando		
1	Course objectives	This course gives an introduction to the most widely-used techniques for materials characterization.
2	Course content and Learning outcomes (Dublin descriptors)	Topics of the module include: • An introduction to what is meant by materials characterisation; • The essential elements of the physical basis for x-ray and electron diffraction; • Imaging, optical and electron-optical microscopies; • Scanning probe techniques - physical principles and generic methodologies; • Spectroscopies - techniques, with emphasis on surface and film analysis; • Tactical and practical aspects of materials characterisation; • Electrical characterizations. On successful completion of this module, the student should: - have profound knowledge of structural and electronic properties of materials. - have knowledge and understanding of experimental techniques to investigate the physical properties of materials. - understand and explain the physical properties of materials. - understand: What is the appropriate technique for studying a particular property of a material. - demonstrate skill in facing issues inherent the growth and characterization of materials. - demonstrate capacity for reading and understand other texts on related topics.
3	Prerequisites and learning activities	A background in quantum mechanics and solid state physics.
4	Teaching methods and language	Lectures, seminars and laboratory demonstrations. Lectures are given in English upon request of non-native Italian speakers. Ref. Text book: Kittel, *Introduction to Solid State Physics*. Guinier, *X-ray Diffraction in Crystals, Imperfect Crystals and Amorphous Bodies* (1994). Ertl and Küppers, *Low energy electrons and surface chemistry*, VCH (1985). Sze, *Physics of Semiconductor Devices.*
5	Assessment methods and criteria	Oral exam on topics dealt during the course.

Programme of "CHIMICA DEI BENI CULTURALI" *"CHEMISTRY OF CULTURAL HERITAGES"*		
F0099, Optional **Second Cycle Degree in "CHEMISTRY", 1st year,1st semester**		
Number of ECTS credits: 6 (workload is 150 hours; 1 credit = 25 hours)		
Teacher: Giorgio Cerichelli		
1	Course objectives	The course goal is to introduce students to the chemical/physical problems affecting conservation/restoration of art objects. The course focuses on the nature of problems arising from the very various nature of materials constituting art objects, new strategies and materials for intervention. On successful completion of this module, the student will have basic information on strategies to employ to protect/restore art objects.
2	Course content and Learning outcomes (Dublin descriptors)	Topics of the module include: Introduction: entropy and degradation; interactions of the art objects with the surrounding environment; reversibility principle. Materials mainly used and their basic chemical composition and properties: Origin and composition of various materials: stone, alloys, wood, paints, composite materials. Interactions of the art objects with the environment: aging, degradation, conservation, restoration of art objects as a function of their nature and interaction with the surrounding environment: indoor (museums, visitors, vandalism, etc.), outdoor (acid rains, corrosion, vandalism, etc.). New materials: innovative materials and techniques (invasive and not invasive) to investigate, protect, and restore art objects . Age information: new and consolidated techniques used to determine age of various materials. On successful completion of this module, the student should: - have profound knowledge of the basic concepts of chemistry of cultural goods as an essential tool to the understanding of their aging in nature; - have knowledge and understanding of the main conventional and non-conventional techniques/materials used on cultural goods; - understand and explain the main origin of degradation processes; - demonstrate skill in comparing scientific articles and ability to answer a relevant question - demonstrate capacity for reading and understanding other texts on related topics.
3	Prerequisites and learning activities	A basic knowledge of chemistry (analytical, inorganic, organic, physical) and physics is required.
4	Teaching methods and language	Lectures. Language: Italian, English on demand. Ref. Text books: Lecturer notes. Giorgio Accardo, Giuseppina Vigliano. "*STRUMENTI E MATERIALI DEL RESTAURO*" Edizioni Kappa Livio Paolillo, Italo Giudicianni. "*La Diagnostica nei Beni Culturali – Moderni Metodi di Indagine*" Loghia - Napoli Mauro Mattini, Arcangelo Moles. "*LA CHIMICA NEL RESTAURO*", Nardini Ed. Luigi Campanella ed altri. "*CHIMICA PER L'ARTE*", Zanichelli.
5	Assessment methods and criteria	Oral exam.

Programme of "CHIMICA DEI COMPOSTI ETEROCICLICI" "CHEMISTRY OF HETEROCYCLIC COMPOUNDS"		
F0114, Optional **Second Cycle Degree in "CHEMISTRY", 1st or 2nd year, 2st semester**		
Number of ECTS credits: 6 (workload 150 hours; 1 credit = 25 hours)		
Teacher: Francesco De Angelis		
1	Course objectives	The objective of the course relies on providing the student with motivations, knowledge of the subject fundamentals, definitions and nomenclature, basic and advanced competences on the chemistry of aromatic, heterocyclic compounds, their structures, physical-chemical characteristic, synthesis and reactivity. Focus is directed mainly on the general features of heteroaromatic compounds, with particular emphasis on mono- and poly-eteroaromatic, pentatomic and hexatomic systems. On successful completion of the course, the student should manage with confidence, at the theoretical level, the fundamental aspects of the subject, and also have a deeper understanding of the most important reactions for the synthesis of heterocyclic compounds as well as of their reactivity.
2	Course content and Learning outcomes (Dublin descriptors)	Topics of the course include: General aspects: Structure and nomenclature; aromaticity and reactivity in general of the heterocyclic ring; condensation and pericyclic reactions; cycloadditions; electrocyclic and sigmatropic reactions; tautomerism in the heterocyclic systems. Mono-heteropentatomic systems: furan, thiophene, pyrrole, benzoconjugates; reactions and syntheses. Mono- and poly-heterohexatomic systems: nitrogen and oxygen containing rings; reactivity at the heteroatom, at the ring and on substituents; syntheses. Di- and poly-heteropentatomic systems: nitrogen and oxygen containing rings; reactions and syntheses. Heterocyclic compounds of pharmacological interest: flavonoids, antocyanins, alcaloids, porphyrins, eumelanins. Drugs with a heterocyclic structure: β-lactam antibiotics, quinolons, quinolins, coumarins, antinflammatory pyrazolones, benzodiazepins. On successful completion of this module, the student should - have profound knowledge of the subject fundamentals; - have knowledge and understanding of the main reactions of, and synthetic pathways for the heterocyclic compounds; - understand and explain fundamentals as well reactivity and synthesis of heterocyclic compounds, using the appropriate, technical language; - understand the fundamental concepts of heterocyclic chemistry, and its connections with general organic chemistry; - demonstrate skill in managing heterocyclic structures and reactions, and ability to conceive the relevant chemistry; - demonstrate capacity for reading and understanding other texts on related topics.
3	Prerequisites and learning activities	The student must know the fundamental notions of General Chemistry, basic and advanced Organic Chemistry, basic methods for molecular structure investigations.
4	Teaching methods and language	Lectures (by writing on the board – sometimes ppt presentations on selected items), homework, reports, seminars. Language: Italian and English. Ref.Text Books: - G.A. Pagani, A. Abbotto, "*Chimica eterociclica*", Piccin Ed. - J.A. Joule, K. Mills, "*Heterocyclic Chemistry*", Wiley. - G. Broggini, G. Zecchi, "*Chimica degli eterocicli*", laScientifica.it. - M. Sainsbury, "*Heterocyclic Chemistry*" (Tutorial Chemistry Text), RSC
5	Assessment methods and criteria	Oral exam.

Programme of “FISICA DELLE NANOSTRUTTURE” “*PHYSICS OF THE NANOSTRUCTURES*”		
F0233, Optional **Second Cycle Degree in “CHEMISTRY”, 1st or 2nd year, 2nd semester**		
Number of ECTS credits: 6 (workload is 150 hours; 1 credit = 25 hours)		
Teacher: Luca Ottaviano		
1	Course objectives	The course module illustrate the fundamentals of physics of nanostructures and low dimensional systems with special emphasis on graphene and two dimensional materials, from this point of view it stands at the forefront of nanotechnology and condensed matter physics.
2	Course content and Learning outcomes (Dublin descriptors)	Topics of the module include: General physical (structural and electronic properties) of systems with reduced dimensionality, Graphene, CNT, other 2D materials, scanning probe microscopy/spectroscopy/lithography, other experimental probes for the investigation of nanostructures. On successful completion of this module, the student should: - have profound knowledge of structural and electronic properties of graphene, carbon nanotubes, and other two dimensional materials. - have knowledge and understanding of experimental techniques to investigate the physical properties of nanostructures. - understand and explain the physical properties of nanostructures - understand: Why “nano” is different. - demonstrate skill in facing novel problem at the forefront of 2D condensed matter-physics and ability to stress the differences with the “bulk” properties. - demonstrate capacity for reading and understand other texts on related topics.
3	Prerequisites and learning activities	A good background in quantum mechanics and solid state physics with specific reference to methods to determine the structural and electronic properties of the condensed matter is a preferable prerequisite of the course.
4	Teaching methods and language	Lectures, seminars of senior students, laboratory demonstrations. Language: Italian/English Ref. Text books: Lecture notes. Lectures (or summaries) are given in English upon request of non-native Italian speakers. “*Physical Properties of Carbon Nanotubes* “ Saito, Dresselhaus, & Dresselhaus
5	Assessment methods and criteria	Oral exam and seminar on a topic not dealt with in from lectures and chosen by the applicant.

Programme of “*GREEN CHEMISTRY*”:

F1132, Optional
Second Cycle Degree in “CHEMISTRY, 1st or 2nd year: 2nd semester

Number of ECTS credits: 6 (workload is 150 hours; 1 credit = 25 hours)

Teacher: Leucio Rossi

1	Course objectives	• Explore sustainability ethics and the development of green chemistry as a practical expression of the pursuit of building a sustainable civilization; • Introduce the 12 principles of green chemistry as well as the tools of green chemistry including the use of alternative feedstocks or starting materials, reagents, solvents, target molecules, and catalysts. • demonstrate how to evaluate a reaction or process and determine “greener” alternatives. • focus heavily on the application of innovative technology the development of “greener” routes to improve laboratory and industrial processes and to produce important products.
2	Course content and Learning outcomes (Dublin descriptors)	Topics of the module include: • Principles and Concepts of Green Chemistry • Waste: Production, Problems and Prevention • Newer Synthetic Methods: Catalysis and Green Chemistry; Biocatalysis; • Organic Solvents: Environmentally Benign Solutions • Emerging Greener Technologies and Alternative Energy Sources • Designing Greener Processes On successful completion of this module, the student should • Have profound knowledge of a range of fundamental and advanced concepts relating to sustainable chemistry; • Have knowledge and understanding of core and specialized concepts in green chemistry, including sustainability, life-cycle analysis, catalysis, reaction solvents, biotechnology, environmental chemistry; • Understand and explain contemporary industrial chemical syntheses and alternative synthetic approaches based upon the notion of environmental sustainability; • Understand and identify structure/function relationships with respect to chemical properties, biological activity, and product performance. Be able to rank competing synthetic methods using the twelve principles of Green Chemistry along with other technical metrics; • Demonstrate skill in apply their knowledge of sustainability to new production processes and new research projects and ability to analyze existing chemical processes, assess their sustainability and propose more sustainable amendments and/or commercially viable alternatives; • Demonstrate capacity for reading and understand other texts on related topics.
3	Prerequisites and learning activities	The student must know the basic notions of General and Organic Chemistry
4	Teaching methods and language	Lectures and exercises Language: Italian / English Ref. Text books * *Green Chemistry: an introductory text* – M. Lancaster – RSC Paperbacks (2002); * *Green Chemistry and Engineering* – D. Mukesh; K. Anil – Academic Press (2007); * *Handbook of Green Chemistry and Technology* – J. Clark; D. Macquarrie - Blackwell (2002)
5	Assessment methods and criteria	Oral exam

Programme of "CHIMICA DEI COMPOSTI ORGANOMETALLICI" ***"CHEMISTRY OF ORGANOMETALLIC COMPOUNDS"***		
F0098, Optional **Second Cycle Degree in "CHEMISTRY", 1st or 2nd year, 1st semester**		
Number of ECTS credits: = 6 (workload is 150 hours; 1 credit = 25 hours)		
Teacher: Fabio Marinelli		
1	Course objectives	The goal of this course is to provide knowledge on the structure, bonding and reactions of organometallic compounds, focusing also on their application as catalysts
2	Course content and Learning outcomes (Dublin descriptors)	Topics of the module include: • Coordination compounds. Ligand field treatment and MO model of bonding. • Ligands. Electron counting. Formal oxidation state. • Unsaturated ligands: CO, carbene, ethylene. Back-bonding. • Phosphine ligands. Electronic nature of phosphines (TEP). Hydride complexes. • Metal carbonyls. Class of carbonyls. Monsanto and Water Gas Shift processes. • Sigma-Organyl complexes. • Metal-carbene complexes. Fischer and Schrock carbenes. • Alkene complexes. Hydrogenation, hydrosilylation, hydroformylation. Reactions with nucleophiles. • M-diene and M-allene complexes. M-alkyne complexes. Reactions with nucleophiles. Ciclotrimerization. Pauson-Khand reaction • Carbocyclic poliene ligands. p-Allyls ligands. Metallocenes. M-arene complexes. Reactions. • Organometallic elementary reactions mechanism • Examples of synthetically useful processes catalyzed by Pd/Au/Cu/Rh complexes On successful completion of this module the student should • Have a knowledge of the different classes of organometallic compounds • Have a knowledge and understanding of bonding in organometallic compounds and of relevant properties (EAN, FOS) • Have a knowledge and understanding of reactions of organometallic compounds and of relevant catalytic applications • Have capacities of reading and understanding simple research articles in the field of organometallic chemistry
3	Prerequisites and learning activities	The student must know General, Inorganic and Organic Chemistry at intermediate level.
4	Teaching methods and language	Language: Italian/English Ref. Text books: Slides and notes from lessons; Crabtree, *The Organometallic Chemistry of the Transition Metals*, Wiley, 2005.
5	Assessment methods and criteria	Oral exam.

Programme of "CHIMICA DELLE SOSTANZE ORGANICHE NATURALI" ***"CHEMISTRY OF NATURAL ORGANIC COMPOUNDS"***		
F0115, optional **Second Cycle Degree in "CHEMISTRY", 1st or 2nd year, 2st semester**		
Number of ECTS credits: 6 (workload 150 hours; 1 credit = 25 hours)		
Teacher: Francesco De Angelis		
1	Course objectives	The objective of the course relies on providing the student with motivations, knowledge of the subject fundamentals, definitions and nomenclature, basic and advanced competences on the chemistry of natural organic compounds, their structures, physical-chemical characteristic, biosynthesis, use by the biological organism, application for the benefit of human beings, day life implications. Focus is directed mainly on the secondary metabolism of plants, animals including man, insects. Primary metabolism is also touched, under the molecular point of view, every time it is necessary for its implication in secondary metabolism. Some implication within the history of peoples, and contemporary life as well are also taught. On successful completion of the course, the student should manage with confidence, at the theoretical level, the fundamental aspects of the subject, and also have a deeper understanding of the most important reactions in the biosynthesis of secondary metabolites in the cell, and of their importance for the living organism itself as a whole, and in its peculiar biosystem and environment. The student will also be aware of their implications and role for our life in the world.
2	Course content and Learning outcomes (Dublin descriptors)	Topics of the course include: Origine and history of the discipline, secondary metabolism in general; scheme of the secondary metabolism. Enzymes and cofactors in secondary metabolism: structure and chemical reactions of ATP, CoASH, $NAD(P)^+/NAD(P)H$, $FAD/FADH_2$, SAM; elucidation of a secondary metabolic pathway. Fatty acid metabolites: metabolic pathways to and function of saturated and unsaturated fatty acids and derivatives, polyacetilenes, pheromones; arachidonic acid cascade. Phenols of poliketide origin: metabolic pathways to and function of tetraketides (salycilates), aflatoxins, anthraquinones, tetracyclins (study by mutants), macrocyclic antibiotics. Isoprenoids: metabolic pathways (from AcSCoA) to and function of mono-, sesqui- and di-terpenes (pheromones), steroids and derivatives, carotenoids, vitamins. Shikimic acid derivatives: metabolic pathways to and function of aromatic amino acids, phenols, coumarins, lignins. Alcaloids: general aspects and implications, metabolic pathways to and function of belladonna and coca alcaloids, opioids, tryptophan alcaloids, curare. More secondary metabolites from amino acids: melanins and melanogenesis, cianogenic glycosides, linear and cyclic peptides, β-lactam antibiotics (biosynthesis and mechanism of action), vancomycin. On successful completion of this module, the student should - have profound knowledge of the subject fundamentals; - have knowledge and understanding of the main biosynthetic pathways for secondary metabolites and of their importance; - understand and explain fundamentals as well importance for the cell, the organism, and the biosphere of secondary metabolites, using the appropriate, technical language; - understand the fundamental concepts of secondary metabolism, and its connections with general organic chemistry and biochemistry; - demonstrate skill in managing biosynthetic pathways, and ability to conceive the implications of secondary metabolites for life; - demonstrate capacity for reading and understanding other texts on related topics.
3	Prerequisites and learning activities	The student must know the fundamental notions of General Chemistry, basic and advanced Organic Chemistry, basic methods for molecular structure investigations.
4	Teaching methods and language	Lectures (by writing on the board – sometimes ppt presentations on selected items), homework, reports, seminars. Language: Italian and English. Ref. Text Books: - J. Mann, "*Secondary Metabolism*", Oxford Science Publications. - J.B. Harborne, "*Introduction to Ecological Biochemistry*", Academic Press.
5	Assessment methods and criteria	Oral exam.

Programme of "CHIMICA DELL'ATMOSFERA" *"CHEMISTRY OF THE ATMOSPHERE "*		
F0101, Optional **Second Cycle Degree in "CHEMISTRY" 1st or 2nd year, 1st semester**		
Number of ECTS credits: 6 (workload is 150 hours; 1 credit = 25 hours)		
Teacher: Antonio Arcadi		
1	Course objectives	This course provides an introduction to the chemistry of the atmosphere. The aim is the application of fundamental principles of chemistry to study the pollution problems of our atmosphere.
2	Course content and Learning outcomes (Dublin descriptors)	Topics include: • Atmosphere layers, biogeochemical cycles of gaseous nitrogen, oxygen, carbon and sulfur compounds, aerosols; • Application of the techniques of thermodynamics, kinetics, spectroscopy, and photochemistry to atmospheric gases and particles; • Troposphere air pollutions, ozone hole and stratosphere ozone depletion. On successful completion of this module, the student should - understand sources of atmospheric trace gases and particles and their chemical and physical transformations; - be aware of causes, effects and control of air pollution; - demonstrate skill in the application of chemistry principles to pollution removal processes.
3	Prerequisites and learning activities	The student must know the basic notions of General and Inorganic Chemistry, General Physics, Physical Chemistry and Organic Chemistry.
4	Teaching methods and language	Lectures Language: Italian Ref. Text books *"Introduction to Atmospheric Chemistry"* Daniel J. Jacob, Princeton University Press, 1999. "*Chemistry of the upper and lower atmosphere : theory, experiments and applications*" Barbara J. Finlayson-Pitts, James N. Pitts, Jr, San Diego, Calif. : Academic Press 2000 "*Atmospheric chemistry and physics : from air pollution to climate change*" John H. Seinfeld, Spyros N. Pandis, New York : Wiley, 1998.
5	Assessment methods and criteria	Oral exam

Programme of
"COMPUTER MODELLING AND SIMULATIONS OF BIOMOLECULES"

F1140, Optional
Second Cycle Degree in "CHEMISTRY", 1st or 2nd year, 1st semester

Number of ECTS credits: 6 (workload is 150 hours; 1 credit = 25 hours)

Teacher: Leonardo Guidoni

1	Course objectives	The objective of the present course is to establish the foundations of the computer modelling of biological macromolecules. Students will learn the basics of the structural biology and graphical visualization of macromolecules. The underlying statistical mechanics of computer simulations will be introduced, with special focus on biomolecular applications. They will be also introduced to computer modelling techniques through the use of practical examples in Linux environment.
2	Course content and Learning outcomes (Dublin descriptors)	Topics of the module include: - Introduction to structural biology of proteins and nucleic acids. - Introduction to Lagrangian and Hamiltonian mechanics. Statistical mechanics in the microcanonical and canonical ensembles. The basic algorithms of molecular dynamics simulations. - Force-fields for biomolecules. Long range interactions. Static and dynamical properties. - Monte Carlo methods. - Practical computer exercises On successful completion of this module, the student should - have knowledge of biomolecular structures, molecular visualization programs and biological data bases - have knowledge and understanding the theory at the basis of molecular dynamics simulations and Monte Carlo methods - demonstrate skill in molecular simulations and ability to set up and to interpret classical molecular dynamics simulations - demonstrate capacity for reading and understand other texts on related topics.
3	Prerequisites and learning activities	The student must know the bases of general chemistry.
4	Teaching methods and language	Lectures, exercises, home works and a final report on the practical part. Language: English Ref. Text books L. Stryer, *Biochemistry*, Freeman 2002. T. Schlick, *Molecular Modelling and Simulation*, Springer-Verlag, New York, 2002. D. Frenkel & B. Smit, *Understanding Molecular Simulations*, Academic Press 2002. A.R. Leach, *Molecular Modelling Principles and Applications*, Addison Wesley Longman 2001, 2nd edition. K. Huang, *Statistical mechanics*, John Wiley & Sons, 1987. W. Greiner, *Classical Mechanics,* Springer-Verlag, New York, 2003.
5	Assessment methods and criteria	Oral exam, short report for the practical part