PhD Program in Chemical Sciences

A PhD Program of the Dipartimento di Chimica, Biologia e Biotecnologie (DCBB) of the Università degli Studi di Perugia

Ad-Hoc Courses Offered for the Academic Years
2020-2021
2021-2022
2022-2023

Coordinator: Prof. Luigi Vaccaro

DIPARTIMENTO 2018 di ECCELLENZA 2022 progetto AMIS

Ministero dell'Istruzione, dell'Università e della Ricerca

Lectures will be held in room A and the exact time will be updated on the webpage and communicated via email to all PhD students.
Final schedule will be also advertised on the screens in the main entrance of the DCBB.

January 11-15, 2021
Catalytic approaches in the synthesis of biologically relevant molecules (12h, 2 CFU)*

In the era of a green new deal and given the importance of catalysis for the development of sustainable synthetic processes, the aim of the course is to provide an overview of the most recent advancements regarding biomimetic and metal-based approaches. Particular emphasis will be devoted to biomimetic approaches in oxidative transformations, and metal catalysts employed in C-C bond formation and activation of otherwise unreactive C-H groups.

January 18-29, 2021
Theoretical modelling of reactivity and energy transfer in astrochemistry and planetary atmospheres *(*18 h, 3 CFU)
Prof. Andrea Lombardi, Università degli Studi di Perugia

The amount of data sent by the probes exploring the solar system and planetary atmospheres, and the astronomical discovery of numerous molecules of increasing complexity in interstellar space, implicates a remarkable relevance of the modern chemistry for the science of the Universe. The interpretation of the resulting ample phenomenology needs to be assisted by theoretical and computational modelling of energy exchanges and reactions involving chemical species to set up data bases and improve kinetic models.
In this course the theoretical grounds of quantum and classical molecular dynamics and a number of computational applications to astrochemistry will be reviewed.

February 1-14, 2021

Homogeneous catalysis by theoretical chemistry *(*18 h, 3 CFU)

Prof. Paola Belanzoni, Università degli Studi di Perugia

The enormous challenge of moving our societies to a more sustainable future offers several exciting opportunities for computational chemists. The first principles approach to "catalysis by design" will enable new and much greener chemical routes to produce vital fuels and fine chemicals. This prospective outlines a wide variety of case studies to underscore how the use of theoretical techniques can be applied to biocatalysis and homogeneous catalysts to provide invaluable insights into the reaction mechanisms. In particular, homogeneous catalysis by transition metal complexes and biomimetic catalysts will be addressed through a density functional theory (DFT) approach, based on the state-of-the-art computational protocols.

February, 2021

Process Analytical Technology and Chemometrics in the Pharmaceutical Industry (2h, 2CFU)*

Prof. Emidio Camaioni, Università degli Studi di Perugia

Dr. Remo Simonetti, Janssen

The course will show some recent PAT (Process Analytical Technology) implementations in the drug oral solid pharmaceutical industry. Examples of spectroscopic and non-spectroscopic applications will be discussed such as:

• PAT for the real-time evaluation of the particle size distribution during fluidized bed granulation;

• PAT for real-time evaluation of blending uniformity;

• PAT for real-time evaluation of the API content uniformity in the tablets.

February-March, 2021
Concepts in Metabolomic Analysis. Applications to the analysis of medicinal plants and complex natural products (12h, 2CFU)
Dr. Luisa Mattoli, Aboca

Course description: Natural substances and plant metabolites. Mass spectrometry in the Metabolomic Analysis. Identification of metabolites. Targeted and untargeted metabolomics. Identification of metabolites and their quantitative determination. Regulatory implications and study of biological activity. Analysis of metabolites by phytochemical class: the case of alkaloids and phenols. Research applications and examples for quality control.

April 12-16, 2021
X-Ray powder diffraction for pharmaceutical applications in drug discovery (12h, 2 CFU)*
Prof. Riccardo Vivani, Università degli Studi di Perugia

Course description. Introduction to the solid state: crystals and amorphous state, crystal lattice, unit cell and asymmetric unit, elements of symmetry in crystals, forms of crystals, energetics of crystals and relationships with the main chemical-physical properties, polymorphism. Introduction to diffraction techniques. Basic theory of powder diffraction. Sample preparation. Description of the instrumentation. Phase recognition. Determination of the unit cell. Profile fitting, structure refinement (Rietveld). Hints on structural resolution. Crystallographic databases and description of the CIF file. Quantification of mixtures: tutorial session at the computer room

March 20-May 15 2021
Data Scientist with R **(**18 h, 3 CFU)
Dr. Gianandrea La Porta, Università degli Studi di Perugia

Data science is the practice of transforming data into knowledge, and R is one of the most popular programming language used by scientists. The course aims to provide students with: i) the skills necessary to use the R programming language, ii) the principles of statistics to analyze and transform data, and iii) the functions to create and interpret descriptive and multivariate statistics, graphic representations, and statistical models.
Note: Lectures will be held on Monday at 3pm.

February 1-15, 2022
Raman micro-spectroscopy: theory and applications *(*18 h, 3 CFU)
Prof. Paola Sassi, Università degli Studi di Perugia

The course aims to provide students with the tools necessary to use Raman spectroscopy in the microscopic characterization of different types of materials, from clays to cells. Starting from the description of the Resonant Raman and Raman effect (6 h), passing through the concepts that underlie microspectroscopy (2 h), the theoretical and experimental aspects of the most recent techniques of light scattering spectroscopy will be illustrated. In particular, the following techniques will be presented: SERS (Surface Enhanced Raman Scattering; 2 h); TERS (Tip Enhanced Raman scattering; 2 h); ROA (Raman Optical Activity; 2 h) and EDLS (Extended Depolarized Rayleigh Scattering; 2 h). A two-hour practice exercise will also give the students the possibility to analyze different samples with the micro-Raman instrumentation available in the “Molecular Spectroscopy” Lab of this Department.

January 17-26, 2022
Introduction to retrosynthetic analysis and its application to the synthesis of antiviral drugs (12h, 2 CFU)*
Prof. Andrea Temperini, Università degli Studi di Perugia

The aim of the course is to provide a rational approach to organic synthesis through disconnections and interconversions of functional groups. Synthons and synthetic equivalents as well as evaluation of the flexibility and convenience of a linear or convergent synthesis and together with the comparative study of industrial and laboratory synthetic strategies for the preparation of Oseltamivir phosphate will be discussed.

10-20 February, 2022
Multiple applications of enantioselective liquid chromatography: from the control of asymmetric synthesis to the study of biological matrices (12h, 2 CFU)*
Prof. Roccaldo Sardella, Università degli Studi di Perugia

Course description. The Course intends to provide information on the different fields of application of enantioselective liquid chromatography. Focus will be mostly given on the way to identify the best chiral stationary phase-mobile phase combination, according to the matrix of interest, and the detection system. in this framework, the basic principles of the method development process will be given. The basic notions of the preparative-scale chiral chromatography will be given as well.

March, 2022
Nuclear magnetic resonance for structure elucidation of organic compounds, (12h, 2 CFU)*
Prof. Claudio Santi, Università degli Studi di Perugia

Focusing on novel aspects of method and instrumentation development, applications in emerging fields and new techniques and technologies, the course will illustrate the main relevant advances in the field of NMR. The aim is to facilitate greater understanding and encourage wider use of NMR techniques in structural elucidation of small and macromolecules as well as in metabolomics and host-

guest interactions. Particular enphasis will be given on the relevance of this techniques in the early phase drug discovery.

June 1-15, 2022
Computational Chemistry and Classical Molecular Dynamics: carbon-nano structures applications *(*18 h, 3 CFU)
Dr. Noelia Faginas Lago, Università degli Studi di Perugia

This course treats advanced molecular dynamics (MD) methodology for classical simulations in order to evaluate uptake and adsorption properties of small gases on carbon based materials like graphene, γ-graphynes, COFs. MD simulations provide atomistically detailed information on structural and dynamic quantities, but often at a high computational cost. This course introduces to programming and numerical methods that are useful to solve problems in chemistry. Classical molecular dynamics simulations are performed using the public domain software Dl_POLY.

February 1 -15, 2023
Cosmochemistry (18 h, 3 CFU)
Prof. Nadia Balucani, Università degli Studi di Perugia

March 20-June 15, 2023
The theory of Complex Systems to address the XXI Century Challenges **(**18 h, 3 CFU)
Dr. Pier Luigi Gentili, Università degli Studi di Perugia

Despite significant achievements in science and technology, humankind still needs to win compelling challenges. Whenever we face the XXI century challenges, we deal with Complex Systems. Complex Systems are natural systems that science is unable to describe exhaustively. This course presents the features of Complex

Systems by using the theories of Out-of-Equilibrium Thermodynamics, Non-linear Dynamics, and Natural Computing. The contents are interdisciplinary. Subjects regarding chemistry, biology, physics, economy, and philosophy are presented. This course intends to give the Ph.D. students new tools and ideas to face their specific research.
Note: Lectures will be held on Friday at 3pm.

March-May 2023
Data Scientist with R **(**18 h, 3 CFU)
Dr. Gianandrea La Porta, Università degli Studi di Perugia

Data science is the practice of transforming data into knowledge, and R is one of the most popular programming language used by scientists. The course aims to provide students with: i) the skills necessary to use the R programming language, ii) the principles of statistics to analyze and transform data, and iii) the functions to create and interpret descriptive and multivariate statistics, graphic representations, and statistical models.
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June 19-30, 2023
Advances in biogeochemistry (18 h, 3 CFU)
Prof. David Cappelletti, Università degli Studi di Perugia

Interdisciplinary course, applying concepts from chemistry, physics, biology and geology to Earth systems including terrestrial, ocean and freshwater environments; water and energy cycles; carbon, nitrogen, phosphorus and sulfur cycles; biogeochemical cycles through Earth history. Advanced examples from state-of-the-art research work will be illustrated and discussed.

July 3–14, 2023

Continuous flow technologies for the preparation of pharmaceutically relevant molecules (18 h, 3 CFU)

Prof. Luigi Vaccaro, Università degli Studi di Perugia

Modern chemical production relies on the development of innovative technologies that could allow the preparation of the desired chemicals at the highest chemical and economic efficiency.

Flow technologies have proved to be powerful synthetic tools for accessing complex molecular entities in a faster and user friendly manner. The use of flow reactors has also proven to be very effective for the definition of protocols featuring easier purification of the pure products leading to a minimal waste production and consequently a lower cost of the synthetic process. In this course, the student will be introduced to the fundamental aspects of flow chemistry and some examples of application of this technology to relevant target will be also presented.

September 11-23, 2023

Introducton to Nanophotonics (18 h, 3 CFU)

Prof, Loredana Latterini, Università degli Studi di Perugia

This course presents the fundamental aspects of the interactions between radiation and nanomaterials and the criteria to prepare and engineer materials to achieve tailored optical responses. Examples of ordered nanostructures to harvest, guide, shift and concentrate the radiation in the nanometer-scale are going to be presented.

** Course organized in collaboration with the Dipartimento di Scienze Farmaceutiche (DSF) with the PhD Programme in Pharmaceutical Sciences.*