




A.D. 1308  
**unipg**

DEPARTMENT  
OF PHARMACEUTICAL SCIENCES

## DOCTORATE IN PHARMACEUTICAL SCIENCES

### Course Program (XXXVI cycle)

*[...ut civitas Perusii sapientia valeat elucere...]*

Partner of the European Pharmacoinformatic Initiative   
Partner of the Paul Ehrlich Euro-PhD Network

DOCTORATE IN PHARMACEUTICAL SCIENCES  
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VICE COORDINATOR: PROF. FRANCESCA MARINI  
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## AA 2020-2021

January 11-18, 2021

*Dr. Luca Sancineto, University of Perugia*

*Catalytic approaches in the synthesis of biologically relevant molecules (2 CFU, 12h)*

*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..*

February 5-19, 2021

*Prof. Emidio Camaioni, University of Perugia*

*Dr. Remo Simonetti, Janssen*

*Process Analytical Technology and Chemometrics in the Pharmaceutical Industry  
(2 CFU, 12h)*

*The course will show some recent PAT (Process Analytical Technology) implementations in the drug oral solid pharmaceutical industry. Examples of spectroscopic and nonspectroscopic 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.*

June 18,25-July 2,9, 2021

*Dr. Luisa Mattoli, Aboca*

*Concepts in Metabolomic Analysis. Applications to the analysis of medicinal plants and complex natural products (2 CFU, 12h)*

*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

*Prof. Riccardo Vivani, University of Perugia*

*X-Ray powder diffraction for pharmaceutical applications in drug discovery (2 CFU, 12h)*

*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 emphasis will be given on the relevance of this techniques in the early phase drug discovery.*

*Room and timetable, as well as any change, will be communicated to PhD students by e-mail and published on the website.*

## AA 2021-2022

January 17-26, 2022

*Prof. Andrea Temperini, University of Perugia*

Introduction to retrosynthetic analysis and its application to the synthesis of antiviral drugs (2 CFU, 12h)

*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.*

February 1-15, 2022

*Prof. Paola Sassi, University of Perugia*

Raman micro-spectroscopy: theory and applications (3 CFU, 18 h)\*

*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.*

February 24–March 11,18,25, 2022

*Prof. Roccoaldo Sardella, University of Perugia*

Multiple applications of enantioselective liquid chromatography: from the control of asymmetric synthesis to the study of biological matrices (2 CFU, 12h)

*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 28-31, 2022

*Prof. Claudio Santi, University of Perugia*

Nuclear magnetic resonance for structure elucidation of organic compounds (2 CFU, 12h)

*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 emphasis will be given on the relevance of this techniques in the early phase drug discovery.*

**\*Course organized in collaboration with the Department of Chemistry, Biology and Biotechnology (DCBB) of the University of Perugia.**

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June 1-15, 2022

Dr. Noelia Faginas Lago, University of Perugia

Computational chemistry and classical molecular dynamics: carbon-nano structures applications (3 CFU, 18 h)\*

*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,  $\gamma$ -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.*

\*Course organized in collaboration with the Department of Chemistry, Biology and Biotechnology (DCBB) of the University of Perugia.

Room and timetable, as well as any change, will be communicated to PhD students by e-mail and published on the website.

## AA 2022-2023

January-February 2023

*Prof. Francesco Galli, University of Perugia*

Omics technologies in drug discovery (2 CFU, 12h)

*The term "omics" refers to the set of sciences and technologies that essentially derived from the completion of the genome project in 2000. It deals with the complexity of biological phenomena in all their manifestations and applications, including identification of therapeutic targets and drug development using a holistic approach. In these two decades, a growing number of software and hardware tools have developed to address "omics" problems. These involve bioinformatics for the management and interpretation of "big data" that are produced in every "omics" domain. The evolution of this area and its importance in the pharmaceutical sector will be discussed in this short course in their main aspects, also giving particular emphasis to the technical and practical aspects and to the laboratory approach and sector research projects.*

March-May 2023

*Dr. Gianandrea La Porta, University of Perugia*

Data Scientist with R (3 CFU, 18 h)\*

*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.*

Room and timetable, as well as any change, will be communicated to PhD students by e-mail and published on the website.

March 20-June 15, 2023

*Dr. Pier Luigi Gentili, University of Perugia*

The theory of complex systems to address the XXI century challenges (3 CFU, 18 h)\*

*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.*

July 3-14, 2023

*Prof. Luigi Vaccaro, University of Perugia*

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

*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.*

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