

A.D. 1308 UNIPS DEPARTMENT OF PHARMACEUTICAL SCIENCES

# DOCTORATE IN PHARMACEUTICAL SCIENCES

Course Program (XXXV cycle)

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

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

DOCTORATE IN PHARMACEUTICAL SCIENCES COORDINATOR: PROF. ANTONIO MACCHIARULO VICE COORDINATOR: PROF. FRANCESCA MARINI CONTACT : francesca.marini@unipg.it April 14-17, 2020 Prof. Serge van Calenbergh, University of Gent New approaches in medicinal chemistry (2 CFU, 12h) The course has been canceled

May 8,1, 2020 Dr. Andrea Capotorti

Precourses of statistics

Dr. Paolo Cerea Design of Experiments (DoE) in the development of new processes (2 CFU) (Pre-courses of Statistics are mandatory)

Room and timetable, as well as any change, will be communicated to PhD students by e-mail and published on the website. June 3-10, 2020 Prof. Vittorio Pace, University of Wien

Advanced Methods for Chemical Synthesis (2 CFU)

The course has been postponed to November 18 - December 16, 2020.

September 23-25, 2020 Dr. Andrea Astolfi, University of Perugia

In silico drug discovery: from theory to practice (2 CFU)

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

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# 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 Scatterina: 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 "MolecularSpectroscopy" Lab.

#### February 24–March 11,18,25, 2022 Prof. Roccaldo 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 Chermistry, 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.

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