

A.D. 1308 UNIPS DEPARTMENT OF PHARMACEUTICAL SCIENCES

# DOCTORATE IN PHARMACEUTICAL SCIENCES

# Course Program (XXXVIII 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

# AA 2022-2023

January, 13- February 2, 2023 Dr. Remo Simonetti, Janssen Prof. Emidio Camaioni, University of Perugia

Advanced analytics tools supporting pharmaceutical oral solid dosages manufacturing (2 CFU, 12h)

Over the past few years, the role of advanced analytics tools in the pharmaceutical oral solid dosages manufacturing has become crucial. Starting from the process analytical technology (PAT) applications passing through the process modeling in use for the batch manufacturing this course will also elucidate the control strategy based on a combined use of PAT and Residence Time Distribution into continuous manufacturing. The course will also focus on integrated quality strategies where the combination of multivariate data analysis, spectroscopic analytical techniques and surrogate models are used for the Real Time Release of the product on the market allowing significant timing reductions.

#### 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.

### July , 2023

#### Dr. Valerio Mammoli, Aptuit (Verona) Srl, an Evotec Company

Pharmacokinetics: theories and techniques to explore in vivo characterization (2 CFU, 12h)

Pharmacokinetics and pharmacodynamics are the essential components of pharmacology. To obtain in vivo robust data, sample preparation and sample analysis can be a challenge and therefore extraction and analytical method development are vital to allow an adequate bioanalysis. Due to, an increasing use of PK prediction tools, the use of in vivo experiments in animals is slowly decreasing, on the other hand, in vitro ADMET is essential to ensure reliability of insilico prediction. The high demand of in vitro data has increased the volume of the throughput, the use of automation can definitely play a crucial role in supporting the high demand as well as ensure precision, limiting human errors.

Room and timetable, as well as any change, will be communicated to PhD students by e-mail and published on the website. Courses organized in collaboration with the Department of Chermistry, Biology and Biotechnology (DCBB) of the University of Perugia.\*

### 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.

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.

# AA 2023-2024

#### January 8-24, 2024 Prof. Andrea Carotti, University of Perugia

Introduction to open source and free *in silico* tools useful in drug discovery (2 CFU, 12h)

Nowadays the drug discovery process is a complex workflow full of risks that even the majority of the big pharma company cannot deal with. In this view a big opportunity is given by the computational approaches. In the last 25 years the molecular modeling scenario was enriched by the release of open source and free modeling software. The course will provide some theoretical basis to deeper understand the applications to perform molecular visualization, docking and use artificial intelligence (AI) algorithms. Moreover, with hands-on tasks, some practical and standard scenarios in the drug discovery process will be reproduced.

#### February, 2024

Dr. Silvia Vernotico, Farmaceutica Younger-GUNA S.p.A. Dr. Giovanni Maurizi, Dompè Farmaceutici Dr. Anna Tolomeo, Itelpharma Dr. Michele Cianchini, Baxter/Takeda Prof. Vittorio Maio, Thomas Jefferson University, Philadelphia

Medicines: from the rules of production to therapy (2 CFU, 12h)

This course aims to follow the path of the drug from its production to its use in therapy. The rigid rules of production must guarantee efficacy and safety, while the rules of politics and economics guide medicine use in therapy. The five speakers will discuss the following topics: introduction to GMP, production of proteins in GMP, preparation and quality control of radio pharmaceuticals, health and pharmaceutical outcomes.

### March, 2024 Dr. Anna Donnadio, University of Perugia

Solid state characterization of pharmaceuticals (2 CFU, 12h)

The course will be addressed to introduce some of the solid state characterization techniques (X-ray diffraction, thermogravimetric analysis, differential calorimetry scanning, scanning electron microscopy and hot stage microscopy) routinely utilized in the pharmaceutical field, together with examples of the information provided by each. The aim is to provide the basic principles and typical applications of these commonly employed analytical tools for characterization of pharmaceutical solids for understanding the physical properties and ensure optimal physical form.

#### May-June 2024

#### Prof. Antimo Gioiello, University of Perugia

Integrated technology platforms for medicinal chemistry and organic synthesis (2 CFU, 12h)

Over last years, innovations in synthetic chemistry have areatly enabled the discovery and development of important life-changing medicines. Recent developments in enabling chemical technologies including new synthetic methods, flow chemistry, biocatalysis, chemoinformatics, and automation have the power to accelerate the pace and improve the quality of products in pharmaceutical research. Indeed, the application of new synthetic methods is rapidly expanding the realm of accessible chemical matter and there is a growing recognition that innovations in synthetic chemistry are changing the practice of drug discovery. These seminal lessons will showcase some of the most enabling recent advances in synthetic chemistry and related technologies as well as opportunities that are believed to transform the practice of drug discovery and development in the coming vears.

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# February, 2025

Prof. Alessandro Fatica, Sapienza University of Rome Prof. Mariangela Morlando, University of Perugia Prof. Serena Massari, University of Perugia

Emerging Approaches using Nucleic Acids as target or therapeutic molecules for the treatment of complex diseases (2 CFU, 12h)

Small-molecules proteins/antibodies and have represented for long time the major form of drugs for medical use and the preferred modes in drug development, mainly acting on protein targets such as enzymes, receptors and ion channels. However, there are number of proteins, RNAs and genes that cannot be targeted by these conventional approaches, while they can be selectively targeted by RNA molecules. Moreover, a growing number of evidences have highlighted the contribution of altered RNA and DNA metabolism in the pathogenesis of many complex diseases, thus expanding the repertoire of suitable targets for therapeutic purposes. This course aims to provide students with knowledge of the most advanced methodologies employing RNA and DNA as novel drugs and of the most promising therapeutic strategies targeting the pathological alteration of the RNA and DNA metabolism occurring in complex diseases such as neurological disorders and cancer.

#### May, 2025

#### 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.

# May-June, 2025

Prof. Anna K. H. Hirsch, Helmholtz Institute for Pharmaceutical Research Saarland (HIPS), Germany Prof. Sabatini Stefano, University of Perugia

Classical and innovative approaches to address Anti-Microbial Resistance (2 CFU, 12 h)

Antimicrobial resistance (AMR) represents a global health issue threatening our social lifestyle and the world economy. The course will show the results of some recent approaches, both classical and innovative, aimed to contrast microbial resistance. Among the innovative approaches, a particular focus will entail Target-guided synthesis (TGS), a powerful approach in which the target selects its own inhibitors, and its two main methods: kinetic target-guided synthesis (KTGS) and dynamic combinatorial chemistry (DCC).

June 23-27, 2025

Prof. Francesca Blasi, University of Perugia Prof. Aurélie Schoubben, University of Perugia

Bioactives from Agri-Food Waste (2 CFU, 12h)

The course intends to provide information on the valorization of agri-food waste as source of bioactive compounds. Lectures will focus on bioactive compounds and their functional properties, paying particular attention on: ecofriendly methods for their extraction, analytical methods to evaluate their composition, spectrophotometric methods to determine their in vitro bioactivity. The use of bioactives from agri-food waste suffers from several hurdles such as poor stability and solubility. In the second part of the course knowledge on technological strategies proposed to overcome these limitations will be reviewed according to the hydrophilic or lipophilic nature of the bioactives. Advantages of using encapsulation approaches to solve stability problems and at the same time improve bioactive delivery will be illustrated. July , 2025 Prof. Claudia Zadra, University of Perugia Prof. Maria Carla Marcotullio, University of Perugia

Plant extracts (2 CFU, 12h)

Plant secondary metabolites are important leads in the drug discovery and the formulation of food supplements, and to use plant metabolites for these purposes is fundamental the correct preparation of plant extracts. Besides the traditional extracting methods, in these last years, new eco-friendly techniques have been developed with the aim of reducing the use of polluting solvents and energy-consuming strategies. Plant extracts are often used as such for the preparation of plant-based medicines and food supplements, so the occurrence of residues and contaminants in medicinal herbs and their products is of great importance. Different classes of contaminants (natural toxicants, heavy metals, pesticides, mycotoxins..) could have adverse effects on human health and also represent an index of quality for the product. In this context, information will be provided about the legislation and the requirements for the safety assessment of these materials.

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