A.D. 1308
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DIPARTIMENTO
DI SCIENZE FARMACEUTICHE

**DOCTORAL PROGRAM**
IN PHARMACEUTICAL
SCIENCES

# Frontal teaching provided by the doctoral course
## a.a. 2024-25

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| **Prof. Ecker Gerhard -** Department of Pharmaceutical Sciences , University of Vienna, Vienna (Austria) | 2 CFU, 12h | CC | **April, 1-3 2025** |

**In silico prediction of toxicity**
Besides lack of efficacy, unforeseen toxicity still is one of the major causes for failure in drug discovery. In this course I will provide an overview on computational methods and approaches to predict the toxicity potential of small, drug like molecules. These include both compound centric methods such as QSAR, machine learning, pharmacophore modeling, and docking, as well as biology-oriented approaches such as off-target prediction tools and the Adverse Outcome Pathway concept.

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| **Prof. Anna K. H. Hirsch -** Helmholtz Institute for Pharmaceutical Research Saarland (HIPS), Saarbrücken (Germany)<br>**Prof. Sabatini Stefano -** University of Perugia | 2 CFU, 12h | EPDD | **April, 14-17 2025** |

**Classical and innovative approaches to address Anti-Microbial Resistance**
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).

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| **Prof. Elwira Lasoń -** Faculty of Chemical Engineering and techonolgy - Cracow University of Technology, Kraków (Poland)<br>**Prof. Aurelie Schoubben -** University of Perugia<br>**Prof. Francesca Blasi -** University of Perugia | 2 CFU, 12h | EPDD | **May 2025** |

**Bioactives from Agri-Food Waste**
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: eco-friendly 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.

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| **Prof. Claudio Santi -** University of Perugia | 2 CFU, 12h | EPDD | **May, 20-23 2025** |

**Modern NMR techniques for structure elucidation**

NMR spectroscopy is a very relevant technique for characterization of organic compounds, during the last couple of decades tremendous improvements have been made on the application of two-dimensional spectroscopy for the purpose of structural elucidation of organic compounds. Similarly new modern tools enable to study the interaction of small molecules with macromolecules, the reaction kinetics improving the possibility to define a reliable reaction mechanism. Course Outline: The course topics are organized 4 units: a) brief remind of basic concepts, principles and terminologies associated with NMR spectroscopy, b) introduction of various strategies and experiments in interpreting complex spectra and assign 3D-structures, c) interpretation of various 1D and 2D NMR spectra of simple and complex organic molecules, d) novel tools in early phase drug discovery and mechanistic investigation.

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| **Prof. Maria Carla Marcotullio -** University of Perugia<br>**Prof. Claudia Zadra -** University of Perugia | 1 CFU, 6h | PTN | **June, 11-12 2025** |

**Plant extracts**

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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| **Dr. Luisa Mattoli** – Aboca S.p.a. | 2 CFU, 12h | CC | **October 2025** |

**Concepts in Metabolomic Analysis. Applications to the analysis of medicinal plants and complex natural products**

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 metabolites by biological activity. Analysis of phytochemical class: the case of alkaloids and phenols. Research applications and examples for quality control.