



PhD Advanced Course

Advanced Topics in Medicinal Chemistry and Chemical Biology

July 5-9, 2021

Online Course through the Zoom Platform

Course Coordination:

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Short Introduction

The advanced specialization course in Medicinal Chemistry and Chemistry Biology is intended to frame the training of students who have been admitted to the PhD program in Pharmacy. It is a highly flexible programme covering a wide range of courses taught by chemists, pharmacists, biologists and industrial medicinal chemists. It provides a strong foundation in core chemistry, supplemented by specialist knowledge of medicinal chemistry and chemical biology.

Goals and Goals and Learning Outcomes

The course on Advanced Topics on Medicinal Chemistry and Chemical Biology covers the critical aspects of drug discovery ranging from target identification to lead identification and lead optimization strategies. Hands-on training using state-of-the-art molecular simulation software is included. In addition, a unique overview of the drug discovery process in the pharmaceutical industry is also provided. The training program is aimed at PhD students and has slots allocated to seminars and practical workshops, including discussions with lecturers.

Programme

The program is organized around four major topics: (i) chemical tools and computational approaches for target identification, (ii) drug discovery to tackle infection and cancer, (iii) artificial intelligence and computer-assisted drug discovery, (iv) Chemical Biology and Medicinal Chemistry approaches for drug targeting

Assessment

Assessment of the course consists in the preparation and submission of a research project, 10 000 characters long (including spaces). Students are grouped to build multidisciplinary teams. Each group works throughout the week on a research project that should reflect the topic of the

course, including methodologies and strategies to solve an innovative research question. The project is expected to adhere to the following general structure: a) Title; b) Conceptual hurdle and innovative idea to be tested; c) Plan and methods; d) Relevance of the project (scientific and social impact).

The students will select a broad topic of research in Medicinal Chemistry and are expected to propose a specific project. This project will be evaluated according to the following criteria and weight: a) Novelty and relevance (30%); b) approach to the problem (40%); c) multidisciplinary of the research plan (30%).

Registration and Fees

The registration is made through the [FenixEdu Platform](#) until **June 29, 2021**.

- Registration with evaluation: 125€
- Registration without evaluation: 100€

This course is free for 1st year PhD students of FFUL Doctoral Program.

PROGRAMME

Advanced Topics on Medicinal Chemistry and Chemical Biology

Sessions				
Medicinal chemistry and infectious diseases	Medicinal chemistry and cancer	Chemical biology	New technologies for medicinal chemistry	Novel therapeutic modalities

Advanced Topics on Medicinal Chemistry and Chemical Biology

Hour	July 5	July 6	July 7	July 8	July 9
9:00	Opening				
9:15	MedChem & infectious diseases Opening (F Lopes)		Chemical biology: Opening (P Góis)	MedChem Technologies: Opening (T Rodrigues)	Novel Therapeutic Modalities: Opening (R Moreira)
9:30	Digby Warner (Cape Town) <i>Targeting Mycobacterium tuberculosis for new TB drug discovery</i>		Pedro Góis (Lisbon) <i>New chemical methods for bioconjugation</i>	Fátima Lucas (Zymvol) <i>Expanding the use of drug design modeling tools to industrial biocatalysts</i>	Maria Duca (Nice) <i>Targeting of non-coding RNAs using synthetic small molecules: scope and applications</i>
10:15		MedChem & cancer: Opening (MJ Ferreira)			

10:30	Marco Pieroni (Parma) <i>Spotlight on the TB drug pipeline: comments and medchem perspectives</i>	Thomas Efferth (Mainz) <i>Prognostic value of ABC transporter expression and mutations on survival of cancer patients</i>	Seah-Ling (MaxPlank) <i>Protein Therapeutics by Chemical Design</i>	Nadine Schneider (Novartis) Nikolaus Stiefl (Novartis) <i>Integrating predictive models and drug discovery data to enable MedChem 2.0</i>	Alberto Dal Corso (Milan) <i>Chemical Design of Tumor-Targeted Drug Conjugates</i>
11:30	Coffee break	Coffee break	Coffee break	Coffee break	Coffee break
12:00	Ana Martinez (CISC, Madrid) <i>Therapeutic targets and emerging drugs for COVID19</i>	Elisa Giovannetti (Amsterdam) <i>Molecular mechanisms underlying resistance and advances in pancreatic cancer translational research</i>	David Peralta (Wiley) <i>Publishing talk: Optimizing scientific manuscripts</i>	Thierry Langer (Vienna) <i>Pharmacophores: Versatile Tools for Computer-assisted Molecular Design</i>	Ranganath Gopalakrishnan (AstraZeneca) <i>New Modality Therapeutics: Revolutionizing Drug Discovery'</i>
13:00	End of morning session	End of morning session	End of morning session	End of morning session	End of morning session
14:15	MedChem Technologies: Opening (R Guedes)				Ola Engkvist (AstraZeneca) <i>Deep learning based molecular de novo design (from 14 to 15h)</i>
14:30	Bill Jorgensen (Yale) <i>Rapid Discovery of Potent Inhibitors of the Main Protease of SARS-CoV-2</i>	Romano Silvestri (Roma) <i>Agents that Modulate the Cancer Drug Resistance</i>	Pat Walters (Relay Tx) <i>Challenges and Opportunities for AI in Drug Discovery</i>	Maria Santos (Lisbon) Tiago Rodrigues (Lisbon) <i>Writing project and postdoc applications</i>	
15:30	End of afternoon session	End of afternoon session	End of afternoon session	End of afternoon session	Round Table & Closing remarks