



i3du

PhD Programme in Medicines
and Pharmaceutical Innovation

Course

ADVANCED TOPICS IN MEDICINAL CHEMISTRY

February 04 - 08, 2019

Faculty of Pharmacy

Amphitheatre B

Universidade de Lisboa, Portugal

The FCT PhD Programme in Medicines and Pharmaceutical Innovation (i3DU; <http://www.ff.ul.pt/phd3duul/>) trains students in target discovery, drug design, pre-clinical development, and drug safety, bridging the translational gap from discoveries on disease targets and mechanisms into novel diagnostic and therapeutic agents.

The i3DU Programme offers a training course in Advanced Topics in Medicinal Chemistry that will be held at the Research Institute for Medicines (iMed.Ulissboa), Faculdade de Farmácia, Universidade de Lisboa, in Lisbon, 4-8 February 2019.

Course outline

The course on Medicinal Chemistry 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. The training program welcomes the participation of external academic and scientific community members. [Registration](#) is free but mandatory.

Program

The program is organized around four major topics: (i) target identification and screening, (ii) strategies for lead compound discovery, (iii) drug discovery in oncology, (iv) drug discovery for infectious diseases, and (v) drug discovery and development in the pharmaceutical industry:

4 February 2019

9h15 **Opening**

Topic: Target Identification and Screening

9h30 **Medicinal Chemistry: from target to drug discovery and development**

Rui Moreira

iMed.Ulisboa, Faculdade de Farmácia, Universidade de Lisboa

10h30 **NMR toolbox to decipher protein-ligand interactions**

Filipa Marcelo

UCBIO, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa

11h30 **Break**

12h00 **Cellular Assays in Drug Discovery**

Cecília Rodrigues

iMed.Ulisboa, Faculdade de Farmácia, Universidade de Lisboa

13h00 **Lunch**

14h00 **GRPR-Targeted Radioconjugates for Cancer Theranostics**

António Paulo

Instituto Superior Técnico, Universidade de Lisboa

15h00 **How can structural biology contribute to drug design?**

Margarida Archer

ITQB, Universidade Nova de Lisboa

16h00 **End of day**

5 February 2019

Topic: Drug Discovery in Infectious Diseases

9h30 **Multitarget drugs to tackle resistance. The case of malaria**

Francisca Lopes

iMed.Ulisboa, Faculdade de Farmácia, Universidade de Lisboa

10h30 **Design, synthesis and antimicrobial mode of action of deoxy glycosides**

Amélia Rauter

CQE, Faculdade de Ciências, Universidade de Lisboa

11h30 **Break**

12h00 **iLiquids vs iDiseases - Ionic liquids against infectious diseases**

Ricardo Ferraz

CISA, Porto; LAQV-REQUIMTE

13h00 **Lunch**

14h00 **How to prepare a project in Medicinal Chemistry**

15h00 **End of day**

6 February 2019

Topic: Drug Discovery in Oncology

9h30 **Design of protein-protein interaction inhibitors to activate the tumor suppressor protein p53**

Maria M. Santos

iMed.Ulisboa, Faculdade de Farmácia, Universidade de Lisboa

10h30 **Natural Products as leads for tackling multidrug resistance in cancer**

Maria José Ferreira

iMed.Ulisboa, Faculdade de Farmácia, Universidade de Lisboa

11h30 **Break**

12h00 **Optimizing therapeutic molecules - A never ending story!**

Maria Jesus Perry

iMed.Ulisboa, Faculdade de Farmácia, Universidade de Lisboa

13h00 **Lunch**

14h00 **Targeting oncogene expression with small molecules: challenges & achievements**

Alexandra Paulo

iMed.Ulisboa, Faculdade de Farmácia, Universidade de Lisboa

15h00 **Translational research from the university to clinical trials: the example of redaporfin**

Luís Arnaut

Faculdade de Ciências e Tecnologia, Universidade de Coimbra

16h00 **End of day**

7 February 2019

Keynote Lectures

9h30 **Multi-target drug discovery strategies for Alzheimer's disease**

Maria Laura Bolognesi

University of Bologna

10h30 **Chemical physiology of antibody conjugates and natural products**

Gonçalo Bernardes

IMM, Faculdade de Medicina, Universidade de Lisboa & University of Cambridge

11h30 **Break**

Topic: *In Silico* Strategies in Drug Discovery

12h00 **Discovery of 2-thioxothiazolidin-4-ones as potent transthyretin stabilizers: a story of pride and prejudice in the quest for a better drug**
Carlos Simões
BSIM & Universidade de Coimbra

13h00 **Lunch**

14h00 ***In Silico* Strategies in Drug Discovery**
Rita Guedes
iMed.Ulisboa, Faculdade de Farmácia, Universidade de Lisboa

15h00 **Hands-on (i3DU PhD students ONLY)**
Rita Guedes
iMed.Ulisboa, Faculdade de Farmácia, Universidade de Lisboa

16h00 **End of day**

8 February 2019

Keynote Lecture

9h30 **Sustainable drug discovery for trypanosomatid neglected tropical diseases**
Maria Laura Bolognesi
University of Bologna

Topic: *In Silico* Strategies in Drug Discovery

10h30 **Hands-on (i3DU PhD students ONLY)**
Rita Guedes
iMed.Ulisboa, Faculdade de Farmácia, Universidade de Lisboa

11h30 **Break**

12h00 **Machine learning as a multipurpose tool for drug discovery**
Tiago Rodrigues
IMM, Faculdade de Medicina, Universidade de Lisboa

13h00 **Lunch**

14h00 **Peer-Review: Why, How-To, and What Not To Do**
Maria Laura Bolognesi
University of Bologna

15h00 **Closing & Networking**

Assessment

(3DU 1st Year PhD students ONLY)

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%).