



PhD program in Pharmaceutical Sciences

- *Advanced courses* -

*Faculdade de Farmácia
Universidade de Coimbra*

Coordinator

Fernanda Maria Fernandes Roleira,
FFUC/CIEPQPF

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ADVANCED COURSE

“Principles of Drug Design, Synthesis and Structure-Activity Relationships in Medicinal Chemistry”

24-28 May, 2021

OBJECTIVES AND SIGNIFICANCE

According to IUPAC, “Medicinal chemistry is a chemistry-based discipline, also involving aspects of biological, medical and pharmaceutical sciences. It is concerned with the invention, discovery, design, identification and preparation of biologically active compounds, the study of their metabolism, the interpretation of their mode of action at the molecular level and the construction of structure-activity relationships.” In this course, the components of drug design and synthesis as well as of structure-activity relationships of the medicinal chemistry discipline will be particularly explored, focusing on aspects such as molecular modeling, rational strategies of drug design, synthesis and retrosynthesis of drugs, and examples of research on structure-activity relationships. An overview of the toxicological analysis of drugs will be also addressed.

This course comprises six classes, two lecturers and one seminar during a total of 12 h with Professors and Researchers from the University of Coimbra, University of Porto, University of Açores and from the Pharmaceutical Industry (BIAL), which will address the above-mentioned topics. The seminar will be held by an international invited speaker from the University of Santiago de Compostela, Spain at the end of the course.

Due to the multidisciplinary nature of medicinal chemistry the course will be considered a way to share knowledge on aspects of drug design and discovery. Students will have the opportunity to put questions in the final ten minutes of each class, lecture or seminar and will carry out a final test. A certificate of course attendance and of test approval will be delivered. The course will be online, in Portuguese, English or Spanish language.

PROGRAM

Monday, 24 May

15.30h- Introduction

Fernanda Maria Fernandes Roleira

Faculdade de Farmácia da Universidade de Coimbra

16.00h- Computational drug design

Marco Neves

BIAL



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18.00h- Rational strategies for drug design

Fernanda Maria Fernandes Roleira

Faculdade de Farmácia da Universidade de Coimbra

Tuesday, 25 May

16.00h- Some central synthetic reactions in organic chemistry – a mechanistic perspective

Elisário José Tavares da Silva

Faculdade de Farmácia da Universidade de Coimbra

18.00h- Retrosynthesis in drug discovery I

Saul Campos Costa

Faculdade de Farmácia da Universidade de Coimbra

Wednesday, 26 May

16.00h- Retrosynthesis in drug discovery II

Saul Campos Costa

Faculdade de Farmácia da Universidade de Coimbra

17.00h- Toxicological analysis of drugs

Isabel Rita Barbosa

Faculdade de Farmácia da Universidade de Coimbra

Thursday, 27 May

16.00h- Lecture: Evaluation of a flavonoids library for inhibition of enzymes involved in Diabetes Mellitus pathophysiology towards a structure–activity relationship

Marisa Andreia Carvalho de Freitas

Faculdade de Farmácia da Universidade do Porto

17.00h- Lecture: Anti-inflammatory activity of flavonoids and 2-styrylchromones: exploring their structure-activity relationships

Daniela Sofia Almeida Ribeiro

Faculdade de Ciências Agrárias e do Ambiente, Universidade dos Açores

Friday, 28 May

16.00h- Seminar: Medicinal Chemistry: Opportunities, Challenges and Strategies

Eugenio Uriarte

University of Santiago de Compostela, Spain



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Professor Eugenio Uriarte



Eugenio Uriarte Villares, PhD in Organic Chemistry in 1983, is Professor of Organic and Medicinal Chemistry since 1989 at the Organic Chemistry Department, Faculty of Pharmacy, University of Santiago de Compostela, Spain. He is academic coordinator of European program Socrates-Erasmus from 1996. He spent one year at the Institut de Chimie des Substances Naturelles (CNRS, Gif-sur-Yvette, France), six months at the Università degli Studi di Napoli (Italia), fifteen months at the Università di Padova (Italia), and tree months at the Department of Chemistry, University of Wales (Bangor, United Kingdom) performing organic synthesis methodologies, as well as isolation, purification, and structural determination of natural products, in the medicinal chemistry context. He authored more than 350 publications in international journals and presented over 250 communications in congresses. He serves as an official reviewer for more than 50 international journals and other national and international research agencies. He was director of 28 Doctoral Thesis and heads an active research group since many years with large international collaboration.

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Monday, 31 May

17.30h- Evaluation