

**Drug Design & Discovery Summer School**

**Organizing Committee**

Prof. Emmanuel Mikros  
National & Kapodistrian University of Athens

Prof. Rino Ragno  
Sapienza University of Rome

Prof. Francois Devred  
Aix-Marseille Université

Prof. Sandrine Alibert  
Aix-Marseille Université

Prof. Frank M. Boeckler  
Eberhard Karls University

Assoc. Professor Luminita Marutescu  
Bucharest University

**4-8<sup>th</sup> July 2022**  
**Panepistimiopolis Zografou, Greece**

HELENIC REPUBLIC National and Kapodistrian University of Athens | SAPIENZA UNIVERSITÀ DI ROMA | Aix-Marseille université | EBERHARD KARLS UNIVERSITÄT TUBINGEN | UNIVERSITY OF BUCHAREST

## PROGRAMME

Student's Week July 4-8 2022	
Monday, 4 July 2022	
09:00-10:00	Kinases structural insights for drug development Ass. Prof. Vasilios Myrianthopoulos, Faculty of Pharmacy, National Kapodistrian University of Athens
10:00-11:00	Recent advances in Anticancer agents Prof. Panagiotis Marakos, Faculty of Pharmacy, National Kapodistrian University of Athens
11:00-12:00	Recent advances in Antiviral agents Prof. Nicole Pouli, Faculty of Pharmacy, National Kapodistrian University of Athens
14:00-15:00	Practical aspects in building (3D-) QSAR models and their validation Prof. Rino Ragno Faculty of Pharmacy, La Sapienza University,
15:00-16:00	Understanding and Applying Halogen-Bonds in Molecular Design and Lead Discovery Prof. Dr. Frank M. Boeckler Lab for Molecular Design & Pharm. Biophysics Chair for Medicinal Chemistry Department of Pharmacy and Biochemistry Eberhard Karls University Tuebingen
16:00-17:00	Methods for the in vitro assessment of antimicrobial activity

	Assoc. Prof. Luminita Marutescu Bucharest University Faculty of Biology Department of Microbiology and Immunology luminita.marutescu@bio.unibuc.ro
17:00-18:00	In vitro and in silico cardiac safety drug testing: advancing the CiPA paradigm
	Professor Bogdan Amuzescu, Faculty of Biology, Department of Biophysics Bucharest University
Tuesday, 5 July 2022	
09:00-10:00	New strategies to develop drugs for neurodegenerative diseases Prof. María F. Cano Abad Facultad de Medicina. Universita Autonoma Madrid
10:00-11:00	Introduction to physiologically-based modelling Prof. Florence Gattacceca Faculty of Pharmacy Aix-Marseille Université,
11:00-12:00	Using physicochemical properties to understand molecule behaviour in environment pertinent to pharmacological activity. Prof. Sandrine Alibert Faculty of Pharmacy Aix-Marseille Université
14:00-15:00	SGLT-2 inhibitors: the newest antidiabetic drugs with pleotropic effects Prof. Ioanna Andreadou, Faculty of Pharmacy, National Kapodistrian University of Athens
15:00-16:00	Natural Products in Drug Discovery Prof. Maria Halabalaki Faculty of Pharmacy, National Kapodistrian University of Athens
16:00-17:00	TBA Prof. Antonello Mai Faculty of Pharmacy, La Sapienza University
17:00-18:00	Lab Visit Faculty of Pharmacy National Kapodistrian University of Athens
Wednesday, 6 July 2022	
09:00-12:00	3D QSAR practical course Coordinator Prof. Rino Ragno Faculty of Pharmacy, La Sapienza University
14:00-17:00	Gastroplus ADMET predictor to screen gastro-intestinal absorption and metabolism properties Coordinator Prof. Florence Gattacceca Faculty of Pharmacy Aix-Marseille Université
Thursday, 7 July 2022	
09:00-12:00	DSF High-Throughput Screening Coordinator Prof. V. Myrianthopoulos Faculty of Pharmacy, NKUA NMR practical course Coordinator Dr D. Benaki, Faculty of Pharmacy, National Kapodistrian University of Athens,
14:00-17:00	Molecular Modeling-Docking calculations -Virtual screening Coordinator Dr G Lambrinidis Faculty of Pharmacy NKUA
Friday, 8 July 2022	
09:00-12:00	Student oral presentation -Discussion
14:00-17:00	Student oral presentation -Discussion