



## PROGRAMME

Spring Semester 2022	
Friday, 4 March 2022	Molecular Interactions: Classical (Charges, H-Bonds, v.d.Waals, $\pi$ -int.) Molecular Interactions: Non-Classical (Weak H-Bonds, Orthogonal Multipolar Interactions, Sigma hole Interactions / Halogen Bonds) Thermodynamics in drug discovery (in Hit2Lead / LeadOpt)
	Prof. Dr. Frank M. Boeckler Lab for Molecular Design & Pharm. Biophysics Chair for Medicinal Chemistry Department of Pharmacy and Biochemistry Eberhard Karls University Tuebingen
Friday, 11 March 2022	Molecular Complexity / Drug, Discovery Process and Technologies - Strategies, Issues, Costs, Outlook. Fragment-based Drug Discovery Hit-to-Lead optimization, Co-optimizing Ligand Properties, Avoiding late Attrition
	Prof. Dr. Frank M. Boeckler Lab for Molecular Design & Pharm. Biophysics Chair for Medicinal Chemistry Department of Pharmacy and Biochemistry Eberhard Karls University Tuebingen
Friday, 18 March 2022	Animal models (ethical considerations, experimental design, in vivo analysis of drug effects)
	In vitro cell culture models and evaluation of drug effects

	<p>Prof. María F. Cano Abad Facultad de Medicina. Universita Autonoma Madrid</p> <p>Dr. Gratiela Gradisteanu, Research Institute of Bucharest University</p> <p>Dr. Miruna Stan, Bucharest University Faculty of Biology</p>
Friday, 25 March 2022	<p>Immunomodulation</p> <p>Drug impact on cytokine production and on the M1/M2 macrophage phenotype</p> <p>Evaluation drug-induced responses in cultured cells at specific time points (cell cycle analysis and apoptosis).</p> <p>Screening of drug-induced reactive oxygen species production in leukocytes subpopulations in whole blood (ex-vivo)</p> <p>Assoc Prof. Luminita Marutescu Bucharest University Faculty of Biology</p> <p>Dr. Gratiela Gradisteanu, Research Institute of Bucharest University</p>
Friday, 1 April 2022	<p>Biophysical assays for high throughput screening</p> <p>Microcalorimetry ITC, DSC nanoDSF analytical Ultracentrifugation, SPR</p> <p>Prof. Francois Devred, Faculty of Pharmacy Aix-Marseille Université,</p>
Friday, 8 April 2022	<p>Introduction to NMR</p> <p>NMR screening in drug discovery</p> <p>Introduction to NMR based metabolomics</p> <p>Prof. Emmanuel Mikros, Faculty of Pharmacy, National Kapodistrian University of Athens,</p>
Friday, 15 April 2022	<p>Pharmacokinetics</p> <p>ADME properties</p> <p>Prof. Florence Gattacceca Faculty of Pharmacy Aix-Marseille Université,</p>
Friday, 22 April 2022	<p>Facts, and principles in drug discovery and development: the molecular drug space selection and optimization</p> <p>Prof. Sandrine Alibert Faculty of Pharmacy Aix-Marseille Université,</p>
Friday, 29 April 2022	<p>Introduction to ligand-based methods: Pharmacophore modeling, QSAR</p> <p>Prof. Rino Ragno Faculty of Pharmacy, La Sapienza University,</p>
Friday, 6 May 2022	<p>Advanced ligand-based method: 3-D QSAR with some cross-talking to structure-based techniques.</p> <p>Prof. Rino Ragno Faculty of Pharmacy, La Sapienza University,</p>
Friday, 13 May 2022	<p>Introduction to epigenetics and related drugs</p> <p>Antonello Mai Faculty of Pharmacy, La Sapienza University</p>
Friday, 20 May 2022	<p>Clinical Trials</p> <p>Prof. Evangelos Terpos, School of Medicine, National Kapodistrian University of Athens</p>
Friday, 27 May 2022	<p>Regulatory Affairs</p> <p>Prof. Pietro Matricardi Faculty of Pharmacy, La Sapienza University</p> <p>Patent writing and Application</p> <p>Dr Dimitris Roukounas Patent Attorney</p>

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	TBA
	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	Cardiovascular Pharmacology
	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	DSF in Hightroughput Screening
	Coordinator Prof. Francois Devred, Faculty of Pharmacy Aix-Marseille Université

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	3D QSAR practical course
	Coordinator Prof. Rino Ragno Faculty of Pharmacy, La Sapienza University
14:00-17:00	NMR practical course
	Coordinator Prof. Emmanuel Mikros, Faculty of Pharmacy, National Kapodistrian University of Athens,
Friday, 8 July 2022	
09:00-12:00	Student oral presentation -Discussion
14:00-17:00	Student oral presentation -Discussion