



Aix-Marseille  
université  
Socialement engagée

HELLENIC REPUBLIC  
National and Kapodistrian  
University of Athens  
EST. 1837

UNIVERSITY OF  
BUCHAREST  
— VIRTUTE ET SAPIENTIA —

UAM Universidad Autónoma  
de Madrid



SAPIENZA  
UNIVERSITÀ DI ROMA

EBERHARD KARLS  
UNIVERSITÄT  
TÜBINGEN



Virtual component of the CIVIS Blended Intensive Program: D<sub>3</sub>HT<sub>5</sub>

3<sup>rd</sup> BIP Drug Design and Discovery: Hot Topics, Tools, Technologies, and  
Translation @ Tübingen 2024



Planned Program (as of 4<sup>th</sup> Sept. 2023)

		Time slots (CEST)	Lectures, Speakers
Week 1	Tuesday, 30 <sup>th</sup> April	14:00-17:00	From Charges to $\pi$ -systems: Classical Molecular Interactions – Familiar, yet still Surprising Non-Classical Molecular Interactions: New Tools, New Rules <b>Prof. Dr. Frank M. Boeckler</b> <i>Molecular Design &amp; Pharm. Biophysics, Department of Pharmacy and Biochemistry, Eberhard Karls University Tübingen</i>
	Friday, 3 <sup>rd</sup> May	14:00-17:00	The Drug Discovery Process & Technologies - Strategies, Issues, Costs, Outlook Thermodynamics in Drug Discovery (in Hit2Lead / LeadOpt) Molecular Complexity & Fragment-based Drug Discovery Hit-to-Lead optimization, Co-optimizing Ligand Properties, Avoiding late Attrition <b>Prof. Dr. Frank M. Boeckler</b> <i>Lab for Molecular Design &amp; Pharm. Biophysics, Department of Pharmacy and Biochemistry, Eberhard Karls University Tübingen</i>



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<b>Week 2</b>	Wednesday, 8 <sup>th</sup> May	14:00-15:30	<i>In Vitro</i> Cell Culture Models and Evaluation of Drug Effects <b>Dr. Miruna Stan</b> , Faculty of Biology, Bucharest University
		15:30-17:00	Neurodegenerative Diseases and Drug Discovery <b>Prof. Dr. Maria Cano-Abad</b> , Facultad de Medicina, Universita Autonoma Madrid
	Friday, 10 <sup>th</sup> May	14:00-15:00	Immunomodulation and Drug Impact on Cytokine Production and on the M1/M2 Macrophage Phenotype <b>Dr. Gratiela Gradisteanu</b> , Research Institute of Bucharest University
		15:00-17:00	Evaluation Drug-induced Responses in Cultured Cells at Specific Time Points (Cell Cycle Analysis and Apoptosis). Screening of Drug-induced Reactive Oxygen Species Production in Leukocytes Subpopulations in Whole Blood ( <i>Ex-vivo</i> ) <b>Prof. Dr. Luminita Marutescu</b> , Faculty of Biology, Bucharest University
<b>Week 3</b>	Wednesday, 15 <sup>th</sup> May	14:00-17:00	Microcalorimetry (ITC, DSC) and NanoDSF : Application to Anticancer Drugs Screening and Thermodynamic Characterization <b>Prof. Dr. Francois Devred</b> , Faculty of Pharmacy, Aix-Marseille Université
	Friday, 17 <sup>th</sup> May	14:00-17:00	Introduction to NMR Spectroscopy and Related Screening Methods <b>Prof. Dr. Emmanuel Mikros</b> , Faculty of Pharmacy, National Kapodistrian University of Athens
<b>Week 4</b>	Wednesday, 22 <sup>th</sup> May	14:00-17:00	Pharmacokinetics in Drug Discovery and Development: Physiologically-based PK (PBPK) Models <b>Prof. Dr. Florence Gattacceca</b> , Faculty of Pharmacy, Aix-Marseille Université
	Friday, 24 <sup>th</sup> May	14:00-17:00	Facts and Principles in Drug Discovery and Development: the Molecular Drug Space Selection and Optimization <b>Prof. Dr. Sandrine Alibert</b> , Faculty of Pharmacy, Aix-Marseille Université
<b>Week 5</b>	Wednesday, 29 <sup>th</sup> May	14:00-15:00	Animal Models (Ethical Considerations, Experimental Design, <i>In vivo</i> Analysis of Drug Effects) <b>Dr. Gratiela Gradisteanu</b> , Research Institute of Bucharest University
		14:00-17:00	Visualizing K <sup>+</sup> Ion Signaling Pathways in Cell Metabolism <b>Prof. Dr. Robert Lukowski</b> , Experimental Pharmacology, Department of Pharmacy and Biochemistry, Eberhard Karls University Tübingen
	Friday, 31 <sup>st</sup> May	14:00-15:30	Nanobody Technology Platform <b>Prof. Dr. Ulrich Rothbauer</b> , Pharm. Biotechnology, Department of Pharmacy and Biochemistry, Eberhard Karls University Tübingen
		15:30-17:00	Mass Spectrometry and Bioanalytics <b>Prof. Dr. Michael Lämmerhofer</b> , Pharm. Analytics, Department of Pharmacy and Biochemistry, Eberhard Karls University Tübingen



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<b>Week 6</b>	Wednesday, 5 <sup>th</sup> June	14:00-15:30	Peptides by Design – RiPP Engineering Technology <b>JProf. Dr. Silja Mordhorst</b> , Pharm. Biology, Department of Pharmacy and Biochemistry, Eberhard Karls University Tübingen
		15:30-17:00	Genome Mining Enables a Renaissance of Natural Product Drug Discovery <b>Prof. Dr. Harald Groß</b> , Pharm. Biology, Department of Pharmacy and Biochemistry, Eberhard Karls University Tübingen
	Friday, 7 <sup>th</sup> June	14:00-15:30	Targeted Covalent Inhibitors in Drug Discovery <b>JProf. Dr. Matthias Gehringer</b> , Medicinal Chemistry, Department of Pharmacy and Biochemistry, Eberhard Karls University Tübingen
		15:30-17:00	Academic Drug Discovery: Fiction, Facts or Fantasy <b>Prof. Dr. Stefan Laufer</b> , Medicinal Chemistry, Department of Pharmacy and Biochemistry, Eberhard Karls University Tübingen
<b>Week 7</b>	Wednesday, 12 <sup>th</sup> June	14:00-15:30	Introduction to Epigenetics and Related Drugs <b>Prof. Dr. Antonello Mai</b> , Faculty of Pharmacy, La Sapienza University
		15:30-17:00	Introduction to Ligand-based Methods: Pharmacophore Modeling, (3D) QSAR <b>Prof. Dr. Rino Ragno</b> Faculty of Pharmacy, La Sapienza University, Rome
	Friday 14 <sup>th</sup> June	14:00-15:30	Introduction to Structure-based Methods in Drug Design: Molecular Docking <b>Prof. Dr. Rino Ragno</b> Faculty of Pharmacy, La Sapienza University, Rome
		15:30-17:00	Machine Learning and Artificial Intelligence in Drug Discovery <b>Dr. Markus Zimmermann</b> , Molecular Design & Pharm. Biophysics, Department of Pharmacy and Biochemistry, Eberhard Karls University Tübingen
<b>Week 8</b>	Wednesday, 19 <sup>th</sup> June	14:00-15:30	Case Studies in Industrial Anti-cancer Drug Discovery: KRAS G12C and HIF2 $\alpha$ <b>Dr. Rainer Wilcken</b> , Senior Principal Scientist, Computer-Aided Drug Design and Project Leader at Novartis
		15:30-17:00	Fragment-based Approaches towards PROTAC Development and Free Energy Methods in Industry <b>Dr. Matthias R. Bauer</b> , Senior Expert II Data Science at Novartis Institutes for BioMedical Research (NIBR)



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		Time slots (CEST)	Lectures, Speakers
	Friday 21 <sup>st</sup> June	14:00-15:30	Embedding of Nanoparticles in Solid (Orodispersible) Matrices <b>JProf. Dr. Denise Steiner</b> , Medicinal Chemistry, Department of Pharmacy and Biochemistry, Eberhard Karls University Tübingen
		15:30-17:00	Clinical Trials <b>Prof. Dr. Evangelos Terpos</b> , School of Medicine, National Kapodistrian University of Athens