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UNIVERSITY OF
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— VIRTUTE ET SAPIENTIA

UAM Universidad Autónoma
de Madrid



SAPIENZA
UNIVERSITÀ DI ROMA

EBERHARD KARLS
UNIVERSITÄT
TÜBINGEN



Virtual component of the CIVIS Blended Intensive Program: D₃ 4th BIP Drug Design and Discovery @ Madrid 2025

| | | Time slots (CEST) | Lectures, Speakers |
|---------------|-----------------------------------|----------------------|---|
| Week 1 | Wednesday, 7 th May | 14:00-17:00 | From Charges to π -systems: Classical Molecular Interactions – Familiar, yet still Surprising Non-Classical Molecular Interactions: New Tools, New Rules Prof. Dr. Frank M. Boeckler <i>Molecular Design & Pharm. Biophysics, Department of Pharmacy and Biochemistry, Eberhard Karls University Tübingen</i> |
| | Friday, 9 th 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 Prof. Dr. Frank M. Boeckler <i>Lab for Molecular Design & Pharm. Biophysics, Department of Pharmacy and Biochemistry, Eberhard Karls University Tübingen</i> |



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|---------------|------------------------------------|----------------------|---|
| Week 2 | Wednesday, 14 th May | 14:00-15:30 | <i>In Vitro</i> Cell Culture Models and Evaluation of Drug Effects Dr. Miruna Stan , Faculty of Biology, Bucharest University |
| | | 15:30-17:00 | Neurodegenerative Diseases and Drug Discovery Prof. Dr. Maria Cano-Abad , Facultad de Medicina, Universita Autonoma Madrid |
| | Friday, 16 th May | 14:00-15:00 | Immunomodulation and Drug Impact on Cytokine Production and on the M1/M2 Macrophage Phenotype Dr. Gratiela Gradisteanu , 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>) Prof. Dr. Luminita Marutescu , Faculty of Biology, Bucharest University |
| Week 3 | Wednesday, 21 st May | 14:00-17:00 | Microcalorimetry (ITC, DSC) and NanoDSF : Application to Anticancer Drugs Screening and Thermodynamic Characterization Prof. Dr. Francois Devred , Faculty of Pharmacy, Aix-Marseille Université |
| | Friday, 23 rd May | 14:00-17:00 | Introduction to NMR Spectroscopy and Related Screening Methods Prof. Dr. Emmanuel Mikros , Faculty of Pharmacy, National Kapodistrian University of Athens |
| Week 4 | Wednesday, 28 th May | 14:00-17:00 | Pharmacokinetics in Drug Discovery and Development: Physiologically-based PK (PBPK) Models Prof. Dr. Florence Gattacceca , Faculty of Pharmacy, Aix-Marseille Université |
| | Friday, 30 th May | 14:00-17:00 | Facts and Principles in Drug Discovery and Development: the Molecular Drug Space Selection and Optimization Prof. Dr. Sandrine Alibert , Faculty of Pharmacy, Aix-Marseille Université |
| Week 5 | Wednesday, 4 th June | 14:00-15:30 | Animal Models (Ethical Considerations, Experimental Design, <i>In vivo</i> Analysis of Drug Effects) Dr. Gratiela Gradisteanu , Research Institute of Bucharest University Animal models for metabolism diseases |
| | | 15:03-17:00 | Animal models for metabolism diseases Dr. Javier Blanco , Physiology Department, Medicine School, Universidad Autónoma de Madrid |
| | Friday, 6 th June | 14:00-17:00 | Controlled Drug Delivery Systems for Parenteral Administration. Microparticles and Nanoparticles for Drug Delivery. Dr. Juan Aparicio Blanco , Pharmacy and Food Technology. Universidad Complutense de Madrid |



| | | Time slots (CEST) | Lectures, Speakers |
|---------------|-------------------------------------|----------------------|---|
| Week 6 | Wednesday, 11 th June | 14:00-15:30 | Screening methodologies for the identification of new drugs Dr. Adrian Girona Martinez , Pharmacology Department Medicine School, Universidad Autónoma de Madrid |
| | | 15:30-17:00 | Drug repurposing and repositioning: A new life for old drugs Dr. Adrian Girona Martinez , Pharmacology Department, Medicine School, Universidad Autónoma de Madrid |
| | Friday, 13 rd June | 14:00-15:30 | Case Studies in Industrial Anti-cancer Drug Discovery: KRAS G12C and HIF2 α Dr. Rainer Wilcken , Drug Design at Flare Therapeutics. Director, Computational Chemistry / Computer-Aided Therapeutics |
| | | 15:30-17:00 | Fragment-based Approaches towards PROTAC Development and Free Energy Methods in Industry Dr. Matthias Bauer , Senior Expert II Data Science at Novartis Institutes for BioMedical Research (NIBR) |
| Week 7 | Wednesday, 18 th June | 14:00-15:30 | Introduction to Epigenetics and Related Drugs Prof. Dr. Antonello Mai , Faculty of Pharmacy, La Sapienza University |
| | | 15:30-17:00 | Introduction to Ligand-based Methods: Pharmacophore Modeling, (3D) QSAR Prof. Dr. Rino Ragno Faculty of Pharmacy, La Sapienza University, Rome |
| | Friday 20 th June | 14:00-15:30 | Introduction to Structure-based Methods in Drug Design: Molecular Docking Prof. Dr. Rino Ragno Faculty of Pharmacy, La Sapienza University, Rome |
| | | 15:30-17:00 | Machine Learning and Artificial Intelligence in Drug Discovery Dr. Markus Zimmermann , Molecular Design & Pharm. Biophysics, Department of Pharmacy and Biochemistry, Eberhard Karls University Tübingen |
| Week 8 | Wednesday, 25 th June | 14:00-15:30 | New targets and potential drug candidates for refractory epilepsy Dr. Carmen Ovejero , Pharmacology Department, Pharmacy, Universidad San Pablo Ceus. Madrid. |
| | | 15:30-17:00 | Introduction to ligand-based methods: Pharmacophore modeling, Prof. Dr. Thilo Stehle , Dean of the Faculty of Science Department of Pharmacy and Biochemistry Eberhard Karls University Tübingen |



| | | Time slots (CEST) | Lectures, Speakers |
|--|---------------------------------|----------------------|--|
| | Friday 27 th June | 14:00-15:30 | Bioequivalence clinical Trials Prof. Dr. Alberto Borobia , Pharmacology Department, School of Medicine, Universidad Autónoma de Madrid |
| | | 15:30-17:00 | Clinical Trials Prof. Dr. Evangelos Terpos , School of Medicine, National Kapodistrian University of Athens |

María Cano Abad, PhD
CIVIS COORDINATOR
maria.cano@uam.es.

Madrid, mobility calendar

| | Monday, 30 th June 2025 | Tuesday, 1 st July 2025 | Wednesday, 2 nd July 2025 | Thursday, 3 rd July 2025 | Friday, 4 th July 2025 | Saturday, 5 th July 2025 |
|---------------|--|---|---|--|--|---|
| 09:30 - 10:00 | Coffee Bar / Snack | Coffee Bar / Snack | Coffee Bar / Snack | Coffee Bar / Snack | Coffee Bar / Snack | Optional Social Program Prado Museum |
| 10:00 - 11:00 | Arrival / Opening Session | Prof. Dra. Manuela García López Pharmacology Department Facultad de Medicina, Universidad Autónoma Madrid: From the laboratory to the patient | Prof. Dr. Rino Ragno, Faculty of Pharmacy, La Sapienza University, Rome: Practical Aspects in Validating Molecular Docking | Prof. Dr. Florence Gattacceca, Faculty of Pharmacy, Aix-Marseille Université: Introduction to physiologically-based modelling | Student oral presentation** - Discussion | |
| 11:00 - 12:00 | Prof. Dr. María F. Cano Abad, Pharmacology Department Facultad de Medicina, Universidad Autónoma Madrid: New strategies to develop drugs for neurodegenerative diseases | Epigenetics: a Med Chem Perspective Prof. Dr. Antonello Mai, Istituto Pasteur - Fondazione Cenci Bolognetti, Dipartimento di Chimica e Tecnologie del Farmaco, Sapienza University, Rome | Prof. Dr. Rino Ragno*, Faculty of Pharmacy, La Sapienza University, Rome: Molecular Docking in Action | Prof. Dr. Florence Gattacceca*, Faculty of Pharmacy, Aix-Marseille Université: Gastroplus ADMET Predictor to Screen Gastro-intestinal absorption and metabolism properties | Student oral presentation** - Discussion | |
| 12:00 - 13:00 | Prof. Dr. María F. Cano Abad, Pharmacology Department Facultad de Medicina, Universidad Autónoma Madrid: Methods to measure calcium - Tools for drug discovery | Prof. Dr. Emmanuel Mikros, Faculty of Pharmacy, National Kapodistrian University of Athens: NMR-based Metabolomics | Prof. Dr. Rino Ragno*, Faculty of Pharmacy, La Sapienza University, Rome: Molecular Docking in Action | Prof. Dr. Florence Gattacceca*, Faculty of Pharmacy, Aix-Marseille Université: Gastroplus ADMET Predictor to Screen Gastro-intestinal absorption and metabolism properties | Student oral presentation** - Discussion | |
| 13:00 - 14:00 | Lunch Break | Lunch Break | Lunch Break | Lunch Break | Lunch Break | |
| 14:00 - 15:00 | Prof. Dr. Frank M. Böckler, Dept. Pharmacy and Biochemistry, Eberhard Karls Universität Tübingen: The Versatility of Halogen Bonding | Dr. Markus O. Zimmermann, Dept. Pharmacy and Biochemistry, Eberhard Karls Universität Tübingen: Machine Learning Approaches - The Long Path to Artificial Intelligence | Prof. Dr. Rino Ragno*, Faculty of Pharmacy, La Sapienza University, Rome: Molecular Docking in Action | Prof. Dr. Florence Gattacceca*, Faculty of Pharmacy, Aix-Marseille Université: Gastroplus ADMET Predictor to Screen Gastro-intestinal absorption and metabolism properties | Student oral presentation** - Discussion | |
| 15:00 - 16:00 | Dr. Markus O. Zimmermann, Dept. Pharmacy and Biochemistry, Eberhard Karls Universität Tübingen: Principles and Applications of Chalcogen Bonding | Prof. Dr. Frank M. Böckler, Dept. Pharmacy and Biochemistry, Eberhard Karls Universität Tübingen: Methods in CompChem - Choose wisely and apply with care! | Prof. Dr. Javier Blanco Rivero*, Dept. Physiology, Universidad Autónoma de Madrid: Hands-on-Animals models for metabolic diseases in drug discovery | Visit Laboratory | Student oral presentation** - Discussion | |
| 16:00 - 16:30 | Coffee Break | Coffee Break | Coffee Break | Coffee Break | Coffee Break | |
| 16:30 - 17:30 | Prof. Dr. Carmen Chifriuc, University of Bucharest: Microbicidal versus antipathogenic strategies in antimicrobial drug discovery | Dra. Elena Tortosa Pharmacology Department Facultad de Medicina, Universidad Autónoma Madrid: Hands-on-Animals models in neurodegenerative disease- Tools for drug discovery | Prof. Dra. Ana Isabel Torres, Pharmacy faculty Department of Galenic Pharmacy and Food Technology.Universidad Complutense de Madrid Hands-on-Microparticles and Nanoparticles for drug administration | Dr. Carlos Herrero, EMA Head. Early Development & Clinical Pharmacology. Global Clinical Operations The Janssen Pharmaceutical Companies of Johnson & Johnson Drug development | Feedback BIP & Discussion with Students** | |
| 17:30 - 18:30 | Prof. Dr. Luminita Marutescu, Faculty of Biology, University of Bucharest: Methods for the <i>In vitro</i> Assessment of Antimicrobial Activity | Dra. Elena Tortosa Pharmacology Department Facultad de Medicina, Universidad Autónoma Madrid: Hands-on-Animals models in neurodegenerative disease- Tools for drug discovery | Prof. Dra. Ana Isabel Torres, Pharmacy faculty Department of Galenic Pharmacy and Food Technology.Universidad Complutense de Madrid Hands-on-Microparticles and Nanoparticles for drug administration | Mentoring for students' projects presentations** | Internal Meeting / Discussion**: Organizers - Preview 2025 | |
| 20:00 - 22:00 | Welcome Reception | | | Speakers' dinner | Dinner | |

* Supported by other CIVIS lecturers / ** All CIVIS lecturers