

Program – Day 1

European Conference on Allostery in Drug Discovery

Day 1 9.4.2025	10:00 – 10:15	Opening Remarks Zoe Cournia
	10:15 – 11:15	Opening Plenary Lecture: Jean-Pierre Changeux (Institute Pasteur, France) - The concept of allosteric interaction and its usefulness to understand the higher brain functions and their pathology
	11:15 – 15:30	Session 1: Towards a global understanding of allostery Chair: Christoph Rademacher
	11:15 – 11:45	Charalampos G. Kalodimos (St Jude’s Hospital, USA) - Leveraging the dynamic conformational ensemble to develop kinase inhibitors
	11:45 – 12:15	Coffee Break
	12:15 – 12:45	Simone Fulle (Novo Nordisk, Denmark) - Generative Protein Design for Therapeutic Applications
	12:45 – 13:15	Christoph Rademacher (University of Vienna, Austria) - Allostery of C-type lectins
	13:15 – 13:45	Antoine Taly (CNRS, France) - The opportunities and limitations of AlphaFold to model allosteric proteins: A case study on P2X receptors
	13:45 – 14:00	Francho Nerin Fonz (BRFAA, Greece) - Machine Learning for allosteric site prediction
	14:00 – 15:00	Lunch Break
	15:00 – 15:30	Yiorgo Skiniotis (St. Jude Children's Research Hospital, USA) - Non-Equilibrium Structural Pharmacology of the μ -Opioid Receptor
	15:30 – 18:00	Session 2: Identification of allosteric pockets and ligands Chair: Marco Cecchini
	15:30 – 15:45	Sonja Peter (Nxera, UK) - Comparative Study of Allosteric GPCR Binding Sites and Their Ligandability Potential
	15:45 – 16:00	David Sotillo Núñez (University of Urbino, Italy) -Automatic detection of cholesterol hot spots in GPCR-membrane systems
	16:00 – 17:00	Coffee Break
	17:00 – 17:30	Efstratios Stratikos (University of Athens, Greece) - Targeting the regulatory site of ER aminopeptidase 1 for the development of next-generation immunomodulatory agents
	17:30 – 18:00	Demetres D. Leonidas (University of Thessaly, Greece) - Structure driven drug discovery targeting allosteric sites of glycogen phosphorylase
	18:00 – 19:00	Poster Session



Program – Day 2 (Part 1)

European Conference on Allostery in Drug Discovery

Day 2 10.4.2025	9:30 – 17:00	Session 2: Identification of allosteric pockets and ligands Chair: Ijen Chen
	9:30 – 10:00	Reto Walser (Astex, UK) - Fragment screening for the identification of allosteric binding sites
	10:00-10:15	Varbina Ivanova (University of Barcelona, Spain) - Multiple-copies Association Studies (MAS) – a computational approach for binding mode elucidation
	10:15 – 10:45	Steven Jerome (Schrodinger, Europe) - A Novel Workflow for the In-Silico Identification and Prioritization of Potential Allosteric Binding Sites based on Mixed Solvent Simulations and SiteMap
	10:45 – 11:15	Coffee Break
		Chair: Patrick Scheerer
	11:15 – 11:45	George Spyroulias (University of Patras, Greece) - NMR evaluation of ligand binding among protein players in the ADP-ribosylation pathway
	11:45 – 12:00	Nina-Louisa Efrém (FMP, Germany) - From active site- to allosteric SHP2 inhibitors: Discovery and structure-activity relationship of N-aryl-1H-azaindazoles
	12:00 – 12:15	Vincenzo di Lorenzo (RCNS, Hungary) - Advancing Covalent Allosteric Inhibitors: Insights into SHP2 Modulation on the Latch side
	12:15 – 12:30	Hryhory Sinenka (University of Strasbourg, France) - Towards the accurate prediction of modulatory ligands activity in synaptic receptors
	13:00 – 14:00	Lunch Break



Program – Day 2 (Part 2)

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		Chair: György Keserü
	14:00 – 14:30	Athanasios Papakyriakou (National Research Center Demokritos, Greece) - Discovery of novel allosteric inhibitor hits for Insulin-Regulated Aminopeptidase provides insights on enzyme mechanism and regulation
	14:30 – 15:00	Anastassis Perrakis (National Cancer Institute, Netherlands) - Allosteric Autotaxin inhibitors: a key to clinical success?
	15:00 – 15:30	Marco De Vivo (Italian Institute of Technology, Italy) - Protein-protein and protein-nucleic acid interactions through alchemical free energy calculations
	15:30 – 16:00	Coffee Break
	16:00 – 16:30	Petros Giastas (Agricultural University of Athens, Greece) - Allosteric Activation of ACE2: Structural Insights and Future Perspectives in Drug Discovery
	16:30 – 17:00	Xavier Barril (Boehringer-Ingelheim, Germany) - Virtual Screening for Allosteric Drugs: Where are We?"
	17:00 – 20:00	Free time
	20:00	Conference Dinner



Program – Day 3

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Day 3 11.4.2025	9:30 – 12:30	Session 3: Understanding allosteric response Chair: Giulia Rossetti
	9:30 – 10:00	Judith Günther (Bayer, Germany) - Joys and tribulations pursuing allosteric inhibitors – an industry perspective
	10:00 – 10:15	Enrico Guarnera (Merck KGaA, Germany) - Hijacking EGFR Signaling: Computational Insights into Allosteric Antibodies Engineering
	10:15 – 10:45	Minos Matsoukas (University of Western Attica, Greece) - Exploring Allosteric Modulation through Virtual Screening: From GPCR Heteromers to a Cancer-linked Target
	10:45 – 11:00	Sigrid Pedersen (Charité, Germany) - Elucidating the structure and dynamics of the Melanocortin-4 receptor (MC4R)
	11:00 – 11:30	Coffee Break
		Chair: Marc Nazaré
	11:30 – 12:00	Adnan Sljoka (RIKEN, Japan) - Probing allosteric activation and biased signaling with rigidity transmission allostery (RTA) theory, NMR, and geometric Monte-Carlo simulations
	12:00 – 12:15	Simone Mariani (Forschungszentrum Jülich, Germany) - Predicting Binding Affinity and Kinetics in GPCR Oligomers: Insights from Enhanced Sampling Simulation
	12:15 – 12:30	Bohdana Sokolova (Karolinska Institute) - Above-Filter Digestion Proteomics Identifies Drug targets and estimates ligand binding site
	12:30	Closing remarks and farewell - End of conference

