



The ALLODD Journal Club takes place monthly 3-4.30pm CET (45min presentation + 45min discussion).

Date	ESR	Journal Club Title, DOI of paper
May 25, 2022, 2pm CET (exceptionally)	ESR13 Martijn Bemelmans	Understanding Cryptic pocket Formation in Protein Targets by enhanced Sampling Simulations
June 23, 2022	ESR2 Jonathan Lefèbre	Divergent allostery reveals critical differences between structurally homologous regulatory domains of Plasmodium falciparum and human protein kinase G
July 28, 2022	ESR3 Varbina Ivanova	How Effectively Can Adaptive Sampling Methods Capture Spontaneous Ligand Binding?
August 25, 2022	ESR7 Vincenzo Di Lorenzo	Mapping the energetic and allosteric landscapes of protein binding domains
September 22, 2022	ESR12 Léxane Fournier	Conformational dynamics and allosteric modulation of the SARS-CoV-2 spike
October 27, 2022	ESR5 Simone Mariani	Rethinking Metadynamics: From Bias Potentials to Probability Distributions
November 24, 2022	ESR8 Nina-Louisa Efrém	Discovery of Novel Allosteric EGFR L858R Inhibitors for the Treatment of Non-Small-Cell Lung Cancer as a Single Agent or in Combination with Osimertinib
December 15, 2023	ESR4 Özge Ergun	Photoprogramming Allostery in Human Serum Albumin
January 26, 2023	ESR10 Sonja Peter	Membrane Lipids Are an Integral Part of Transmembrane Allosteric Sites in GPCRs: A Case Study of Cannabinoid CB1 Receptor Bound to a Negative Allosteric Modulator, ORG27569, and Analogs
February 27, 2023	ESR6 Sigrid Pedersen	MRAP2 regulates energy homeostasis by promoting primary cilia localization of MC4R
March 24, 2023 (Friday) (exceptionally)	ESR1 Francho Nerín Fonz	Neural relational inference to learn long-range allosteric interactions in proteins from molecular dynamics simulations
April 27, 2023	ESR14 David Sotillo Núñez	Lipid–Protein Interactions Are Unique Fingerprints for Membrane Proteins
May 24, 2023 16:40 – 17:40	ESR9 Bohdana Sokolova	Combining Small-Molecule Bioconjugation and Hydrogen–Deuterium Exchange Mass Spectrometry (HDX-MS) to Expose Allostery: the Case of Human Cytochrome P450 3A4
June 29, 2023	ESR11 Hryhory Sinenka	Accurate absolute free energies for ligand–protein binding based on non-equilibrium approaches
July 27, 2023	ESR13 Martijn Bemelmans	OneOPES, a combined enhanced sampling method to rule them all
August 24, 2023	ESR2 Jonathan Lefèbre	Dual mechanisms of cholesterol-GPCR interactions that depend on membrane phospholipid composition
September 28, 2023	ESR3 Varbina Ivanova	Discovery of Nanomolar DCAF1 Small Molecule Ligands
October 26, 2023	ESR7 Vincenzo di Lorenzo	An inverse agonist of orphan receptor GPR61 acts by a G protein-competitive allosteric mechanism



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November 23, 2023	ESR12 Léxane Fournier	Conformation-locking antibodies for the discovery and characterization of KRAS inhibitors
December 14, 2023	ESR5 Simone Mariani	Protein–ligand binding with the coarse-grained Martini model
January 25, 2024	ESR8 Nina-Louisa Efrém	Development of allosteric and selective CDK2 inhibitors for contraception with negative cooperativity to cyclin binding
February 22, 2024	ESR4 Özge Ergun	Biophysical Mechanism of Allosteric Regulation of Actin Capping Protein
March 28, 2024	ESR10 Sonja Peter	GPCR activation mechanisms across classes and macro/microscales
April 25, 2024	ESR1 Francho Nerín Fonz	Deciphering interaction fingerprints from protein molecular surfaces using geometric deep learning
May 23, 2024	ESR6 Sigrid Pedersen	MRAP2 inhibits β-arrestin-2 recruitment to the prokineticin receptor 2
June 27, 2024	ESR14 David Sotillo Núñez	Allosteric Cholesterol Site in Glycine Receptors Characterized through Molecular Simulations
July 25, 2024	ESR9 Bohdana Sokolova	Hybrid Mass Spectrometry Approaches to Determine How L-Histidine Feedback Regulates the Enzyme MtATP-Phosphoribosyltransferase
August 29, 2024	ESR11 Hryhory Sinenka	