



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



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