

Category	Poster number	Poster Title	Name
1. Molecular dynamics	1	Helix stabilizing cyclic peptides with mixed stereochemistry as anti-cancer drugs	Julen Aduriz-Arrizabalaga
1. Molecular dynamics	2	Deciphering promiscuity of HUWE1 for protein degradation using Molecular Dynamic Simulations	Ritika Aggarwal
1. Molecular dynamics	3	Molecular dynamics simulations of a protein-micelle complex to model contrast-variation SAXS experiments	Noora Aho
1. Molecular dynamics	4	The molecular dynamics data bank: bridging gaps in bio-molecular simulation interoperability	Adam Bellaiche
1. Molecular dynamics	5	Prediction of unknown binding sites in proteins by biased molecular dynamics simulations	Jan Beránek
1. Molecular dynamics	6	Molecular Dynamics Simulation of High-Mobility Group Box Protein 2: Insights into the Conformational Dynamics of Auto-Inhibition	Hao-Ting Chang
1. Molecular dynamics	7	Computational Design and Optimization of Aptamer-Based Biosensor for Enhanced West Nile Virus Detection	Schiffino Gioacchino
1. Molecular dynamics	8	Facilitating Non-Equilibrium Molecular Dynamics Simulations with POP-MD	Jackson Crowley
1. Molecular dynamics	9	MDaRes: An R tool for the Analysis of Protein Residue Dynamics from Molecular Simulations	Nancy D'Arminio
1. Molecular dynamics	10	De novo design of peptides that form transmembrane $\alpha$ -helical barrel pores with potent antimicrobial activity and optimization for coiled-coil nanopore formation	Rahul Deb
1. Molecular dynamics	11	Molecular Mechanism of Calcium Block in the MthK Potassium Channel	Reinier deVries
1. Molecular dynamics	12	Exploring the dynamics, allostery, and unresolved structure of the PEBP1/LC3 complex in cell death mechanisms	Julia Duda
1. Molecular dynamics	13	Speeding up sampling in molecular dynamics simulations with fast-TIP3P water	Balázs Fábrián
1. Molecular dynamics	14	P2Y12 receptor goes towards activation: insights by Principal Component Analysis	Francesco Fontanive
1. Molecular dynamics	15	High-Pressure Response of the Coupled Dynamics of Lipids and Membrane Proteins	Yanna Gautier
1. Molecular dynamics	16	Investigating Nanodiscs as a Membrane Protein Environment	Veera Hägg
1. Molecular dynamics	17	Are membraneless organelles truly membrane-less?	Art Hoti
1. Molecular dynamics	18	Molecular Dynamics Simulations Coupled On-the-fly to Experimentally Determined Helical Content for Interpretation of Circular Dichroism Data	Leonie Chatzimagas
1. Molecular dynamics	19	Transcription factors meet chromatin under the computational nanoscope	Jan Huertas
1. Molecular dynamics	20	Martini 3 Oligomers: A Scalable Approach for Multimers and Fibrils in GROMACS	Ksenia Korshunova
1. Molecular dynamics	21	Influence of the Drug Disulfiram on the Dimer Stability of Gasdermin D	Paul Kretschmer
1. Molecular dynamics	22	Computational analysis of flavonoid deglycosylation to enhance antibiotic activity: Predicting substrate affinity by different methods	Natalia Kulik
1. Molecular dynamics	23	Lipid composition regulates membrane association and the activity of the human ubiquitin conjugating enzyme UBE2J2.	Florian Leidner
1. Molecular dynamics	24	How Binding Site Flexibility Promotes RNA Scanning in TbRGG2 RRM: A Molecular Dynamics Simulation Study	Toon Lemmens
1. Molecular dynamics	25	Antimicrobial Action of Essential Oils and CuO Nanoparticles Against Pathogenic Proteins: Elucidation of the Inhibitory Mechanism through Molecular Dynamics and Free Energy Calculations	Georgios Leonis

1. Molecular dynamics	26	An integrated protocol for relating Hydrogen-Deuterium exchange data to protein conformational ensembles	Valentin Loux
1. Molecular dynamics	27	Simulations of immunity receptors and more: from micelles to membranes and liposomes.	Sonsoles Martin-Santamaria
1. Molecular dynamics	28	Evolutionary Molecular Dynamics: Physics-based inverse design of functional peptides	Jeroen Methorst
1. Molecular dynamics	29	Effective Inclusion of Electronic Polarization in Molecular Dynamics of the Human Insulin Receptor–Insulin Complex	Ngoc Nguyen
1. Molecular dynamics	30	Oligomerization of G-protein coupled receptors across different classes: structural insights from computational methods	Urszula Orzeł
1. Molecular dynamics	31	Effect of two activators on the gating of a K2P channel	Edward Otalvaro
1. Molecular dynamics	32	Can Amphipathic Helices Sense Negative Membrane Curvature?	Peter Pajtinka
1. Molecular dynamics	33	Molecular dynamics simulation of keratin-derived antimicrobial peptides (KAMPs) in solution and of their interaction with bacterial membranes	Panagiotis Panagopoulos
1. Molecular dynamics	35	Rationalizing the tridimensional structure of Hyaluronan and Heparin based on their monosaccharide sequence and sulfation pattern	Miguel Riopedre-Fernandez
1. Molecular dynamics	36	Investigating Collectivity in Self-Assembled Protein Filaments Involved in Homologous Recombination	Afra Sabei1
1. Molecular dynamics	37	Exploring interactions in between Pep-1 peptide and Hyaluronan with molecular simulations	Mariia Savenko
1. Molecular dynamics	38	The capacity of GM1 to modulate the properties of biomembranes	Cecilie Soennichsen
1. Molecular dynamics	39	Exploring Photodynamic Cycle of EL222 Transcription Factor: A Molecular Dynamics Approach	Zahra Tehrani
1. Molecular dynamics	40	In silico characterization of a rare disease that affects the dynamics and function of linker histone H1	Serhan Turunç
1. Molecular dynamics	41	Design Guidelines for Antimicrobial Peptides that Kill Antibiotic-Resistant Bacteria via Transmembrane Pores	Robert Vacha
1. Molecular dynamics	42	Lys716 in the transmembrane domain of yeast mitofusin Fzo1 modulates anchoring and fusion	Raphaëlle Versini
1. Molecular dynamics	43	DISRUPTION OF MONOAMINE OXIDASE ENZYMES BY SARS-COV-2 SPIKE PROTEIN: IMPLICATIONS FOR NEURODEGENERATIVE DISEASES	Lucija Vrban
2. Free energy calculations	44	On the challenge of predicting the conformational ensembles of unordered biomolecules	Lucio Bremen
2. Free energy calculations	45	Unraveling Heme flipping in biological transport phenomena with an effective data-driven collective variable	MINA EBRAHIMI
2. Free energy calculations	46	Targeting RNA with Small Molecules - Absolute Binding Free Energy Calculations on a Riboswitch-like RNA-ligand complex from the Hepatitis C Virus Internal Ribosome Entry Site	Krystal EL
2. Free energy calculations	47	Comparing Free Energy Profiles of PFKL and PFKP Isoform Interfaces: A Multiscale MD Simulation Study	Mehrnoosh Hazrati
2. Free energy calculations	48	Binding of arginine peptides to non-planar lipid bilayers	Zuzana Janáčková
2. Free energy calculations	49	Impact of Charged Residue Distribution on Peptide Translocation	Ivo Kabelka
2. Free energy calculations	50	Absolute binding free energy calculations: a systematic force field comparison by a newly designed computational pipeline	Alejandro León
2. Free energy calculations	51	Applications of Ligand-Based Grand Canonical Nonequilibrium Candidate Monte Carlo to Drug Design	William Poole
2. Free energy calculations	52	Elucidating the mechanism of ligand control of PAR1 receptor activation by molecular dynamics simulations	Inken Schwerin

2. Free energy calculation	53	Hydrothermal scenario of the amino acids formation	Sofia Slavova
2. Free energy calculation	54	Calculation of errorbars only from numbers of transitions: molecular dynamics and parallel tempering	Vojtěch Spiwok
3. Force field development	55	Refinement of ionic force fields through electronic continuum correction utilizing a global optimization method	Shujie Fan
3. Force field development	56	Influencing calcium-membrane binding in classical molecular dynamics simulations by varying dielectric constant of water models	Mikulas Klenor
3. Force field development	57	Combining CHARMM36m and OPC to improve accuracy	Nicolai Kozłowski
3. Force field development	58	Bringing the last decade of AMBER force field improvements to GROMACS	Vedran Miletic
3. Force field development	59	Incorporating Electronic Polarization into All-Atom Molecular Dynamics Simulations of Glycans: From Simple Saccharides to Glycosaminoglycans and Lipopolysaccharides	Denys Biriukov
4. Integrative modelling	60	Computational modelling driven biosynthetic protein materials design	Adam Harmat
4. Integrative modelling	61	Transient Non-local Interactions of the Measles Virus Nucleocapsid Tail Domain	Gabor Nagy
4. Integrative modelling	62	Intuitive, three-dimensional agent-based simulation of complex molecular mechanisms: application to the dynein walk cycle	Margot Riggi
4. Integrative modelling	63	Combining Computational and Experimental Approaches for Unraveling the Molecular Mechanisms of Phase Behavior of Intrinsically Disordered Proteins.	Dmitry Tolmachev
4. Integrative modelling	64	Molecular architecture of the plant callose synthase complex	David Ušák
5. Coarse graining	65	A coarse-grained model for disordered and multi-domain proteins	Fan Cao
5. Coarse graining	66	In Silico Activation of Arrestin by Means of Small Molecules	Zeynep Cinviz
5. Coarse graining	67	Modelling mechanical properties of nucleic acid structural motifs	Eva Matoušková
5. Coarse graining	68	Untangling the Network Interactions Inside a Model of Transcriptional Condensate	William Morton
5. Coarse graining	69	Development of a coarse-grained model of disordered RNA for protein–RNA phase separation	Ikki Yasuda
6. AI	70	A Data-Driven Approach to Enhancing Cell-Penetrating Peptide Uptake Predictions	Ana Caniceiro
6. AI	71	Machine Learning Applied to Drug Discovery for the Treatment of Colorectal Cancer	Marcia Castillo
6. AI	72	Sampling-friendly MD Dimensionality Reduction with Autoencoders	Aleš Křenek
6. AI	73	Analysis and Sampling of Molecular Simulations by Adversarial Autoencoders	Guglielmo Tedeschi
7. QM/MM	74	Substrate Positioning and Mechanism of Non-Heme Fe(II)/ $\alpha$ -Ketoglutarate-Dependent Hydroxylases and Epoxidases: A QM/MM Study	Kosala Amarasinghe
7. QM/MM	75	Comparative study of MnmE GTPase catalysis mechanisms	Evgenia Elizarova
8. Applications	76	Salicylic Acid Binding to Redox-Related Enzymes: Insights from Arabidopsis Catalase 2	Lucas Amokrane
8. Applications	77	Insertases scramble lipids: Molecular simulations of MTCH2	Ladislav Bartoš

8. Applications	78	Mechanistic insights into P-glycoprotein ligand transport and inhibition revealed by enhanced molecular dynamics simulations.	Ahmad Elbahnsi
8. Applications	79	Structural and Functional Insights of a Novel Bacterial Copper Radical Oxidase	Tomás Frazão
8. Applications	80	Rest assured: programmed translational stalling studied by means of MDsimulations	Sara Gabrielli
8. Applications	81	Molecular dynamics-driven selection of vectors for targeted delivery of doxorubicin	Gergana Gocheva
8. Applications	82	Crucial role of the correlation between glycan conformations and ring distortion in the catalytic reaction of CAZymes	Isabell Grothaus
8. Applications	83	Collaborative Rotamer Network Guides Mutation-Driven Multi-State Switch in EGFR Kinase Domain	Yazan Haddad
8. Applications	84	Self-assembly of sucrose esters studied by molecular dynamics simulations	Fatmegyul Mustan
8. Applications	85	Aggregation, binding and phase separation of disordered proteins from short model peptides	David Sancho University
8. Applications	86	Exploration of intermolecular interactions between folate-based vectors and the folate receptor- $\alpha$	Marianna Vasilaki
9. Other	87	The shape of the endocytic TPLATE complex drives vesicle formation	Michaela Neubergerová
9. Other	88	Beyond Metadata: Leveraging Similarity Search in Molecular Dynamics Data	Adrián Rošinec