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#	**Last Name,** First Name	**Poster Title**	**On-site**	**online**
129	**Badillo**, Joel A.	Potential of Mean Force for the Acetylation of Glucose in Choline-Chloride Ethylene Glycol Deep Eutectic Solvent from QM/MM MD Simulations		**X**
133	**Padmanaban**, Rajashree	Interaction of Hydroxyapatite and TLR-4 Using In Vitro and In Silico Approaches		**X**
142	**Kolář**, Michal H.	Gating of the Ribosome Exit Tunnel by Constriction-Site Proteins	**X**	**X**
158	**Cofas-Vargas**, Luis Fernando	Molecular Basis for FOF1-ATP Synthase Allosteric Drug Development: Aurovertin Binding Site		**X**
159	**Munguía Salazar**, Paloma	F1 sector of the F1Fo-ATP Synthase of Staphylococcus Aureus: Conformational Characterization and Inhibitor Development		**X**
163	**Velarde**, Marco Vinicio	Comparison of Different Force Fields in the Determination of the Excess Chemical Potential of Thiophene in the [C4MIM] [BF4, Cl, Br, CH3COO] ILs		**X**
183	**V. Guzman**, Horacio	Quantitative Electrostatic Force Tomography for Proteinaceous Capsids in Interaction with an Approaching Nanoscale Substrate	**X**	
195	**Scherer**, Katharina	Effect of Transmembrane Domains on the Free Energy of Stalk Formation during Membrane Fusion	**X**	**X**
200	**Matthes**, Dirk	Interactions of Anle138b with α-Synuclein Fibrils in the Presence of Phospholipids	**X**	**X**
202	**Aldakul**, Yessenbek	Investigation of Non-Canonical Voltage-Sensing Mechanism in K2P Channels Using Molecular Dynamics Simulations	**X**	**X**
207	**Szöllösi**, Daniel	Investigation of the Altered Folding Kinetics of the N-terminal Transactivation Domain of p53 due to the Mutation P27A	**X**	**X**
218	**Riedmiller**, Kai	Predicting Reaction Barriers of Hydrogen Atom Transfer in Proteins	**X**	**X**
221	**Acharya**, Abhishek	L3 Loop Mediated Translocation of Charged Molecules Through the OmpF Channel	**X**	**X**

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232	**Kambaine**, Naserian	Conformations and Stability of Capsaicin in Bulk Solvent: A Molecular Dynamic (MD) Simulation Study		**X**
236	**Jung**, Hendrik	"asyncmd" - A Python Library for Parallel Setup, Control and Analysis of Molecular Dynamics Simulations	**X**	**X**
239	**Ping**, Xiaofei	Coarse-Grained Simulation Model of TDP43 Liquid-liquid Phase Separation Behavior	**X**	**X**
240	**Das**, Chandan K.	Computer Simulations of Porphyrin-Based Nanomachines	**X**	**X**
245	**Palacio-Rodriguez**, Karen	Estimation of Kinetic Rates and Collective Variable Quality From Time-Dependent Biased Simulations	**X**	**X**
247	**Qian**, Xuliang	Molecular Mechanisms of a Novel Insect Cuticle Peptide-Based Nano-Capsule Platform		**X**
248	**Mukherjee**, Saumyak	Molecular Thermodynamics of Protein Condensate Formation from All-Atom MD Simulations	**X**	**X**
268	**Lytje**, Kristian	Combining MD and SAXS in Rigid-Body Optimizations	**X**	**X**
272	**Fatafta**, Hebah	The Effects of Lipid Binding, Neuronal Membrane, Oxidative Stress and Molecular Crowding on Amyloid Aggregation	**X**	**X**
275	**Martínez-León**, Alejandro	Overcoming Hysteresis in Ligand Binding Potential of Mean Force Calculations	**X**	**X**
283	**Sohraby**, Farzin	Characterization of Ligand Unbinding Mechanisms and Kinetics for NiFe Hydrogenase Mutants Using τRAMD	**X**	**X**
296	**Monego**, Debora *	Size-dependent Sedimentation of Nanocrystals: The Role of the Ligand Shell Structure		**X**
298	**Claveras Cabezudo**, Ainara	Scaling Protein-Water Interactions in the Martini 3 Coarse-Grained Force Field to Simulate Transmembrane Helix Dimers in Different Lipid Environments	**X**	**X**

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299	**Schäfer**, Stefan	Atomistic Molecular Dynamics Simulations of Gasdermin Pores	**X**	**X**
300	**Maihöfer**, Michael	Bayesian Methods for Fluctuation X-Ray Scattering	**X**	**X**
303	**Chatzimagas**, Leonie	Simulation of Liquid Jet Explosions and Shock Waves Induced by X-Ray Free-Electron Lasers	**X**	**X**
306	**Sritharan**, Sujith	Molecular Modeling of Plasmodesm Organization by MCTP Proteins	**X**	**X**
314	**Schultze**, Steffen	Bayesian Structure Determination of Multiple Conformational Structures from Single-Molecule X-ray Scattering Images	**X**	**X**
316	**Briand**, Eliane	Constant pH Molecular Dynamics in GROMACS using λ-dynamics and the Fast Multipole Method	**X**	**X**
318	**Leidner**, Florian	Regulation of the Fungal Fatty Acid Synthase Through Conformational Selection	**X**	**X**
329	**Schäffner**, Malte	Conditions for the Occurrence of Michaelis-Menten Kinetics in Markov Models	**X**	
331	**Hui**, Chenggong	Potassium Channel Force Field Development Using ab Initio MD	**X**	**X**
332	**Kalutskii**, Maksim	Multiscale Mechanochemical Model of Microtubule Dynamics	**X**	**X**
333	**Boushehri**, Saber	Effect of O-Glycans on Structure and Friction of the Intrinsically Disordered Synovial Joint Protein Lubricin	**X**	
334	**Kozlowski**, Nicolai	Evaluation of the CHARMM36m Force Field Combined with the OPC Water Model for Protein Simulations	**X**	**X**
336	**Kasparyan**, Gari	Electroporation: Free Energy Landscape and Methods for Imposing Transmembrane-Potentials	**X**	**X**
337	**Rennekamp**, Benedikt	How Collagen is Designed to Tame its Radicals	**X**	**X**
344	**Chen**, Yixin *	A Minimal Markov Model for Rotary Catalysis of F1-ATPase		**X**

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368	**Brosz**, Matthias	Martini 3 Coarse-Grained Force Field for Collagen	**X**	**X**
381	**Schmidt**, Lisa	Active vs Inactive - Using Alchemical Free Energy Simulations to Probe Stabilizational Effects within the Human Dopamine 2 Receptor	**X**	**X**
391	**Lam**, Chun Kei	Ion Conduction Mechanisms in Potassium Channels Revealed by Permeation Cycles	**X**	**X**
394	**Forget**, Selene	Impact of Conformational Shifts on the Hairpin Ribozyme Reactivity	**X**	**X**
406	**Bodosa**, Jessica	Metadynamics Study of Benzyltrimethylammonium Binding Free Energy to Emre Protein		**X**
408	**Castillo Tarazona**, Marcia Yineth	Understanding the Interaction Between Gold Nanoparticles Functionalized with Amino Acid Derivatives and Proteins with Positively Charged Residues.		**X**
414	**Heinz**, Frederick	Structure and Dynamics of a Biomimetic Hydrogel: Coiled-Coil Monomers Self-Assemble into Chains	**X**	**X**
419	**Teuffel**, Jonathan	Effects of Conformational Transitions and Redox Protein Binding on the Catalytic Properties of Cytochrome P450s Revealed by Ligand Egress Patterns	**X**	**X**
421	**Chavarria Rivera**, Joel	Free Energies of Stalk Formation - Comparison between All Atomistic and Martini Simulations	**X**	**X**
432	**Versini**, Raphaëlle	Molecular Dynamics Based Prediction of Fzo1's Transmembrane Domains Structure	**X**	**X**
437	**Schäfer**, Joana-Lysiane	Rare Event Simulation for Bioactive Peptides	**X**	**X**
442	**Shylendran**, Ardhra	Ion-Cluster Morphology and Impact on the Structure and Dynamics of Diglyme Based Sodium-Ion Battery Electrolyte - A Molecular Simulation Study		**X**
452	**Rauda-Ceja**, Jesus Antonio	Cavity Hydration in MUP-1 and Influence on Nonclassical Hydrophobic Effect		**X**

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458	**Ali**, Ahmed	Allosteric Communication in Photoswitchable PDZ3 Domain	**X**	**X**
460	**Sorout**, Nidhi	Effects of Boron Nitride Nanoparticles and Selected Osmolytes on the Secondary Structure of Aβ-Peptide in Aqueous Medium: Prevention of β-Sheet Formation.	**X**	**X**
464	**Buhr**, Jannik	KIMMDY 2.0: A Kinetic Monte Carlo Reactive Molecular Dynamics Framework	**X**	**X**
465	**Gabrielli**, Sara	Conformational Dynamics of Elongation Factor G: Looking for Unresolved Intermediates in Ribosomal Translation	**X**	**X**
466	**de Maeyer**, Annke	Viral mRNA Secondary Structures Affect the Thermodynamics of Frameshifting	**X**	**X**
470	**Dorbath**, Emanuel	Hierarchical Dynamics as Result of Log-Periodic Oscillations in Proteins	**X**	**X**
473	**Heß**, Lisa-Marie	Base-Pair Free-energy Differences Estimated from Frameshifting Efficiencies for SARS Coronavirus	**X**	**X**
476	**Jones**, Jesse	Simulations of the Proton Exit Channel in Cytochrome c Oxidase	**X**	**X**
479	**Tusha**, Gers	Exploring the Reactivity of Supramolecular Helicates as Confining Catalysts	**X**	**X**
480	**De Vecchis**, Dario	The Functional Interplay of the ABC Transporter Pgp with its Lipid Substrates	**X**	**X**
488	**Shakibi**, Saber *	A One-Bead-Per-Saccharide (1BPS) Model for Multiscale Modelling of the Brain ECM		**X**
491	**Kim**, Hyuntae (Henry)	Unexpected Challenges in Molecular Dynamics Simulations of Large Systems	**X**	**X**
492	**Nagy**, Gabor	Role of disordered regions beyond the binding motif of the Measles virus NTAIL	**X**	**X**
494	**Gaurav**, Kumar	Multiscale Simulations of Molecular Recoginition by Phase Separated Mut-16: A Scaffolding Protein of Mutator Foci	**X**	**X**
495	**de Vries**, Reinier	Gating Transitions in the MthK Potassium Channel	**X**	**X**

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497	**Mendez Otalvaro**, Edward Francisco	Pharmacological Modulation of Trek1 Channel	**X**	**X**
503	**Farcas**, Alexandra	Computational Design Optimization of Nanoparticle Based Delivery Vectors for the CRISPR/Cas9 System		**X**
518	**Stuke**, Jan Felix Maximilian	SUMO in Dense Protein Solutions	**X**	**X**
523	**Torres Constante**, Karen Odalys	Characterizing the Transport Pathway of ABCG36 Substrates Using Metadynamics	**X**	**X**
524	**Pietrek**, Lisa Maria	Structural Ensembles of Disordered Proteins and RNA from Hierarchical Chain Growth	**X**	**X**
525	**Finn**, Lauren	Investigating Allostery of a Bacterial Toxin	**X**	**X**
527	**Zschau**, Richard	Mechanism of Beta-Hairpin Formation in Azochignolin	**X**	**X**
528	**Diez**, Georg	Comparing Correlation Measures to Study Protein Dynamics	**X**	**X**
534	**Hegedus**, Tamas	Modeling the Soluble and Membrane-Bound Conformations of Syntaxin 17 SNARE Proteins	**X**	**X**
535	**Scherlo**, Marvin	Structural Insights into Conformational Changes During Protein Aggregation and Refolding by Combining Theoretical and Experimental Infrared Spectroscopy of Amid Bands	**X**	**X**
538	**Gunes**, Sude	In Silico Identification of Potential Ligand Binding Sites of Galactokinase 1 (GALK1) to Treat Classic Galactosemia		**X**
541	**Jäger**, Miriam	Finding Unbinding Pathways in the A1 and A2 Adenosine Receptor Combining Targeted MD and Leiden Clustering	**X**	**X**
543	**Leitmann**, Katharina *	Refining Active Sites of Proteins to Sub-Ångström Resolution by Combining Theoretical and Experimental Infrared Spectroscopy		**X**
545	**Reboul**, Etienne	In Silico Study of Protease Activated Receptor 1 (PAR1) and Thrombin Receptor Activator Peptide 6 (TRAP-6)	**X**	**X**

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546	**Ezat**, Ahmed	Study of The Binding Site Dynamics, Druggability and Cryptic Pocket Formation in Different Human Coronaviruses' Main Protease (Mpro)		**X**
547	**Kopec**, Wojciech	Identification of Metastable States of a Large-Conductance Mechanosensitive Channel (MscL) Using Enhanced Sampling Methods		**X**
555	**Althoff**, Philipp	Tracking Water Molecules and Ions: Investigating Channelrhodopsin Gate Opening with Molecular Dynamics Simulations	**X**	**X**
556	**Post**, Matthias *	Path Separation of Dissipation-Corrected Targeted Molecular Dynamics Simulations of Protein-Ligand Unbinding		**X**
557	**Sartore**, Sofia	Importance of Feature Selection for Markov State Models: A Case Study on HP35	**X**	**X**
559	**Jana**, Kalyanashis	Demonstrating the Function of the Surface-Exposed Lipoprotein BtuG in Efficient B12 Transport in Association with the Outer-Membrane BtuB Protein	**X**	**X**
560	**Böckmann**, Rainer	mRNA Lipid Nanoparticle Phase Transition	**X**	**X**
573	**Jamal**, Sehrish	Computational Structure Modelling and Dynamics of Influenza Encoded Viroporin in Host Lipid Membrane System	**X**	**X**
576	**Kuntze**, Ricarda	Exploration of Ion Permeation in the Gramicidin A Channel Using a Charge Scaling MD Approach	**X**	**X**
581	**Goeppert**, Simone	Peptide Binding in MHC Receptors	**X**	**X**
582	**Ramírez**, Marco	Conformational Selection in the CBD Domain of Cre Recombinase		**X**
583	**Kohnke**, Bartosz	GROMACS Meets FMM - The Path to Highly Scalable Constant pH Electrostatics	**X**	**X**
586	**Barbieri**, Mariano	Reinforcement and Competition Between RNAPolII-Enhancer-Promoter Contacts and Cohesin-CTCF Loop Extrusion	**X**	**X**

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588	**Öztürk**, Mehmet Ali	ReverseDock: A Web Server to Dock a Single Ligand to Multiple Protein Targets		**X**
590	**Popov**, Cristian	Role of Receptor-Receptor Interaction as Checkpoint in Immune Signaling	**X**	**X**
591	**Sucerquia**, Daniel	How a Stretching Force Differently Destabilizes Chemical Bonds on a Protein Backbone	**X**	**X**
593	**Trollmann**, Marius F. W.	One Ring to Rule Them All: Lugdunin's Disruptive Effects	**X**	**X**
596	**Stelzl**, Lukas	From the Integrative Atomic Resolution Ensembles of Disordered Proteins to Simulations of Phase Separated Condensates	**X**	
606	**Atik**, Seref Berk	Computational Analysis of the Interaction of HIV-1 Capsid and Nanobody Complex Structure with a Potential for Diagnostic Applications		**X**
607	**Aponte-Santamaría,** Camilo	Energetics and Permeation of Small Molecules Used for 3D-Laser Printing Across Biological Lipid Bilayers	**X**	**X**
774	**Beierlein**, Frank	DNA-Repair Mechanisms: Molecular Simulations and Computational Alchemy		**X**
810	**Stachowicz-Kusnierz**, Anna	Molecular Dynamics Study of Interactions between Nanoplasics and Lipid Membranes		**X**

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