COMPUTER SIMULATION AND THEORY OF MACROMOLECULES

Hünfeld, April 19-20, 2024, Hybrid

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2024-04-16

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159	Matthes, Dirk	Amyloid-β Oligomer Conformations and Membrane Permeabilization
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307	Kumar, Akhil	Peripheral linker mediates ACP's recognition of DH and stabilizes Mycobacterium tuberculosis FAS-I
317	Wasim, Abdul	Modulation of α-Synuclein Aggregation Amid Diverse Environmental Perturbation
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393	Akkus, Ebru	Elucidating the Exciton Transfer Mechanism in LHCII Through ML
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435	Patel, Smit	Deciphering Niemann-Pick C Disease: Structural and Functional Perspectives on NPC2-Mediated Cholesterol Transport using Molecular Dynamics Simulations
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552	Prass, Tobias Marcel	Fine-Tuning Martini3: Protein-Cosolvent Interactions
556	Bock, Lars V.	Ribosome Stalling in Presence and Absence of Antiobiotics studied by MD Simulations
558	Wolf, Nicolas	SE(3)^N Equivariant Diffusion Models for the Design of a Small Protein with Trivalent Crosslink
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579	McGrath, Hugo	Nascent Peptide Presence in Ribosomal Tunnel Linked to Long-range Allostery
587	Betz, Johannes	Efficient Generation of Disordered Protein Ensembles at Atomic Resolution: An Easy-to-Use Implementation of Hierarchical Chain Growth
590	Mašek, Martin	Exploring the Evolutionary Stability of the Peptidyl Transferase Center in Ribosomes Using All-Atom and Coarse Grained Simulations
600	Ezat, Ahmed	Study of the Binding Site Dynamics, Druggability and Cryptic Pocket Formation in Different Human Coronaviruses' Main Protease (Mpro)
606	Polverini, Eugenia	The C282Y Mutation in Hereditary Hemochromatosis: Structural and Functional Implications Investigated by Molecular Dynamics Simulations
614	Jahani, Kiana	Superoxide Production in Protein Complexes
735	Sayed, Azmy Mohammed	Unveiling the TP53-CDK1 Axis to Target CDK1 in Breast and Lung Cancer via Integrative Multi-Omics, Molecular Docking and Molecular Dynamics Simulation
742	Tummeley, Marco Andreas Malte	Calculating Mössbauer Parameters of Iron Centers in Macromolecules with Density Functional Theory
743	Knauer, Lukas	Vibrational Properties and Protonation States of the [2Fe-2S] Cluster of Apd1 Protein and its Ligands

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