Abhishek Singharoy

List of Publications by Year
in descending order

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50	3,359	331259	223531
papers	citations	21 h-index	46 g-index

60	60	60	4255
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Anionic Lipids Confine Cytochrome c₂ to the Surface of Bioenergetic Membranes without Compromising Its Interaction with Redox Partners. Biochemistry, 2022, 61, 385-397.	1.2	4
2	Energy landscape of the SARS-CoV-2 reveals extensive conformational heterogeneity. Current Research in Structural Biology, 2022, 4, 68-77.	1.1	8
3	Exploring cryo-electron microscopy with molecular dynamics. Biochemical Society Transactions, 2022, 50, 569-581.	1.6	10
4	The ugly, bad, and good stories of large-scale biomolecular simulations. Current Opinion in Structural Biology, 2022, 73, 102338.	2.6	25
5	Revealing a Hidden Intermediate of Rotatory Catalysis with X-ray Crystallography and Molecular Simulations. ACS Central Science, 2022, 8, 915-925.	5.3	3
6	Poor Personâ€™s pH Simulation of Membrane Proteins. Methods in Molecular Biology, 2021, 2315, 197-217.	0.4	1
7	Large-Scale Molecular Dynamics Simulations of Cellular Compartments. Methods in Molecular Biology, 2021, 2302, 335-356.	0.4	2
8	Cryo-EM model validation recommendations based on outcomes of the 2019 EMDataResource challenge. Nature Methods, 2021, 18, 156-164.	9.0	73
9	Antimicrobial Peptide-Membrane Interactions: Insights from Molecular Simulations. Biophysical Journal, 2021, 120, 141a.	0.2	0
10	Total predicted MHC-I epitope load is inversely associated with population mortality from SARS-CoV-2. Cell Reports Medicine, 2021, 2, 100221.	3.3	17
11	CryoFold: Determining protein structures and data-guided ensembles from cryo-EM density maps. Matter, 2021, 4, 3195-3216.	5.0	26
12	Mucin-mimetic glycan arrays integrating machine learning for analyzing receptor pattern recognition by influenza A viruses. CheM, 2021, 7, 3393-3411.	5.8	9
13	ChAdOx1 interacts with CAR and PF4 with implications for thrombosis with thrombocytopenia syndrome. Science Advances, 2021, 7, eabl8213.	4.7	112
14	Cryo-EM and MD infer water-mediated proton transport and autoinhibition mechanisms of V _o complex. Science Advances, 2020, 6, .	4.7	51
15	Scalable molecular dynamics on CPU and GPU architectures with NAMD. Journal of Chemical Physics, 2020, 153, 044130.	1.2	1,548
16	Retrieving functional pathways of biomolecules from single-particle snapshots. Nature Communications, 2020, 11, 4734.	5.8	76
17	Data-guided Multi-Map variables for ensemble refinement of molecular movies. Journal of Chemical Physics, 2020, 153, 214102.	1.2	12
18	Hydrogen bond network analysis reveals the pathway for the proton transfer in the E-channel of T. thermophilus Complex I. Biochimica Et Biophysica Acta - Bioenergetics, 2020, 1861, 148240.	0.5	20

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19	XFEL and NMR Structures of Francisella Lipoprotein Reveal Conformational Space of Drug Target against Tularemia. Structure, 2020, 28, 540-547.e3.	1.6	8
20	Flexible Fitting of Small Molecules into Electron Microscopy Maps Using Molecular Dynamics Simulations with Neural Network Potentials. Journal of Chemical Information and Modeling, 2020, 60, 2591-2604.	2.5	24
21	Antimicrobial Peptide Functionalized Biomaterials Investigated by Molecular Dynamics Simulations. Biophysical Journal, 2020, 118, 380a-381a.	0.2	1
22	Charge Transfer and Chemo-Mechanical Coupling in Respiratory Complex I. Journal of the American Chemical Society, 2020, 142, 9220-9230.	6.6	22
23	Molecular Dynamics Simulations for Improving Crystal Quality and Illuminating the Function of Taspase1: A Therapeutic Target. Biophysical Journal, 2020, 118, 507a.	0.2	0
24	Molecular Dynamics Flexible Fitting: All You Want to Know About Resolution Exchange. Methods in Molecular Biology, 2020, 2165, 301-315.	0.4	5
25	Atoms to Phenotypes: Molecular Design Principles of Cellular Energy Metabolism. Cell, 2019, 179, 1098-1111.e23.	13.5	122
26	Rotational Mechanism Model of the Bacterial V1 Motor Based on Structural and Computational Analyses. Frontiers in Physiology, 2019, 10, 46.	1.3	7
27	Constructing atomic structural models into cryo-EM densities using molecular dynamics â€“ Pros and cons. Journal of Structural Biology, 2018, 204, 319-328.	1.3	9
28	Inchworm movement of two rings switching onto a thread by biased Brownian diffusion represent a three-body problem. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 9391-9396.	3.3	19
29	Chemomechanical Coupling in Hexameric Proteinâ€“Protein Interfaces Harnesses Energy within V-Type ATPases. Journal of the American Chemical Society, 2017, 139, 293-310.	6.6	44
30	CHARMM-GUI MDFF/xMDFF Utilizer for Molecular Dynamics Flexible Fitting Simulations in Various Environments. Journal of Physical Chemistry B, 2017, 121, 3718-3723.	1.2	24
31	Methodology for the Simulation of Molecular Motors at Different Scales. Journal of Physical Chemistry B, 2017, 121, 3502-3514.	1.2	20
32	Overall energy conversion efficiency of a photosynthetic vesicle. ELife, 2016, 5, .	2.8	63
33	Computational Methodologies for Real-Space Structural Refinement of Large Macromolecular Complexes. Annual Review of Biophysics, 2016, 45, 253-278.	4.5	67
34	Binding Site Recognition and Docking Dynamics of a Single Electron Transport Protein: Cytochrome c₂. Journal of the American Chemical Society, 2016, 138, 12077-12089.	6.6	15
35	Conserved methionine dictates substrate preference in Nramp-family divalent metal transporters. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 10310-10315.	3.3	72
36	Crystal Structure and Conformational Change Mechanism of a Bacterial Nramp-Family Divalent Metal Transporter. Structure, 2016, 24, 2102-2114.	1.6	56

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37	Advances in the molecular dynamics flexible fitting method for cryo-EM modeling. Methods, 2016, 100, 50-60.	1.9	82
38	Flexibility Coexists with Shape-Persistence in Cyanostar Macrocycles. Journal of the American Chemical Society, 2016, 138, 4843-4851.	6.6	53
39	Atomic detail visualization of photosynthetic membranes with GPU-accelerated ray tracing. Parallel Computing, 2016, 55, 17-27.	1.3	37
40	Molecular dynamics-based refinement and validation for sub-5 Ã... cryo-electron microscopy maps. ELife, 2016, 5, .	2.8	136
41	New Perspectives on Quinol Binding Motifs at the bc1 Complex Based on MD Simulations. Biophysical Journal, 2015, 108, 602a-603a.	0.2	0
42	Macromolecular Crystallography for Synthetic Abiological Molecules: Combining xMDFF and PHENIX for Structure Determination of Cyanostar Macrocycles. Journal of the American Chemical Society, 2015, 137, 8810-8818.	6.6	29
43	Structural mechanism of voltage-dependent gating in an isolated voltage-sensing domain. Nature Structural and Molecular Biology, 2014, 21, 244-252.	3.6	228
44	xMDFF: molecular dynamics flexible fitting of low-resolution X-ray structures. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 2344-2355.	2.5	50
45	A structural model of the active ribosome-bound membrane protein insertase YidC. ELife, 2014, 3, e03035.	2.8	69
46	Epitope Fluctuations in the Human Papillomavirus Are Under Dynamic Allosteric Control: A Computational Evaluation of a New Vaccine Design Strategy. Journal of the American Chemical Society, 2013, 135, 18458-18468.	6.6	19
47	Space Warping Order Parameters and Symmetry: Application to Multiscale Simulation of Macromolecular Assemblies. Journal of Physical Chemistry B, 2012, 116, 8423-8434.	1.2	16
48	Hierarchical Order Parameters for Macromolecular Assembly Simulations. 1. Construction and Dynamical Properties of Order Parameters. Journal of Chemical Theory and Computation, 2012, 8, 1379-1392.	2.3	12
49	Multiscale simulation of microbe structure and dynamics. Progress in Biophysics and Molecular Biology, 2011, 107, 200-217.	1.4	29
50	Multiscale analytic continuation approach to nanosystem simulation: Applications to virus electrostatics. Journal of Chemical Physics, 2010, 132, 174112.	1.2	10