Diwakar Shukla

List of Publications by Year
in descending order

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103	4,493	159525	128225
papers	citations	30 h-index	60 g-index

143	143	143	4784
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	OpenMM 4: A Reusable, Extensible, Hardware Independent Library for High Performance Molecular Simulation. Journal of Chemical Theory and Computation, 2013, 9, 461-469.	2.3	583
2	Cloud-based simulations on Google Exacycle reveal ligand modulation of GPCR activation pathways. Nature Chemistry, 2014, 6, 15-21.	6.6	388
3	To milliseconds and beyond: challenges in the simulation of protein folding. Current Opinion in Structural Biology, 2013, 23, 58-65.	2.6	331
4	Activation pathway of Src kinase reveals intermediate states as targets for drug design. Nature Communications, 2014, 5, 3397.	5.8	300
5	Markov State Models Provide Insights into Dynamic Modulation of Protein Function. Accounts of Chemical Research, 2015, 48, 414-422.	7.6	231
6	Interaction of Arginine with Proteins and the Mechanism by Which It Inhibits Aggregation. Journal of Physical Chemistry B, 2010, 114, 13426-13438.	1.2	183
7	Arginine and the Hofmeister Series: The Role of Ionâ€“Ion Interactions in Protein Aggregation Suppression. Journal of Physical Chemistry B, 2011, 115, 7447-7458.	1.2	125
8	Crops In Silico: Generating Virtual Crops Using an Integrative and Multi-scale Modeling Platform. Frontiers in Plant Science, 2017, 8, 786.	1.7	102
9	Molecular level insight into intra-solvent interaction effects on protein stability and aggregation. Advanced Drug Delivery Reviews, 2011, 63, 1074-1085.	6.6	83
10	Reinforcement Learning Based Adaptive Sampling: REAPing Rewards by Exploring Protein Conformational Landscapes. Journal of Physical Chemistry B, 2018, 122, 8386-8395.	1.2	82
11	Molecular Computations of Preferential Interaction Coefficients of Proteins. Journal of Physical Chemistry B, 2009, 113, 12546-12554.	1.2	79
12	Dynamic-template-directed multiscale assembly for large-area coating of highly-aligned conjugated polymer thin films. Nature Communications, 2017, 8, 16070.	5.8	78
13	Degradation of complex arabinoxylans by human colonic Bacteroidetes. Nature Communications, 2021, 12, 459.	5.8	68
14	Transition path theory analysis of c-Src kinase activation. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 9193-9198.	3.3	67
15	Understanding the Synergistic Effect of Arginine and Glutamic Acid Mixtures on Protein Solubility. Journal of Physical Chemistry B, 2011, 115, 11831-11839.	1.2	66
16	The shape of water in zeolites and its impact on epoxidation catalysis. Nature Catalysis, 2021, 4, 797-808.	16.1	66
17	Engineered ACE2 decoy mitigates lung injury and death induced by SARS-CoV-2 variants. Nature Chemical Biology, 2022, 18, 342-351.	3.9	63
18	Cloud computing approaches for prediction of ligand binding poses and pathways. Scientific Reports, 2015, 5, 7918.	1.6	54

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19	Preferential Interaction Coefficients of Proteins in Aqueous Arginine Solutions and Their Molecular Origins. Journal of Physical Chemistry B, 2011, 115, 1243-1253.	1.2	53
20	Molecular Basis of the Glucose Transport Mechanism in Plants. ACS Central Science, 2019, 5, 1085-1096.	5.3	52
21	Conformational heterogeneity of the calmodulin binding interface. Nature Communications, 2016, 7, 10910.	5.8	49
22	Free Energy Landscape of the Complete Transport Cycle in a Key Bacterial Transporter. ACS Central Science, 2018, 4, 1146-1154.	5.3	49
23	Structural architecture of a dimeric class C GPCR based on co-trafficking of sweet taste receptor subunits. Journal of Biological Chemistry, 2019, 294, 4759-4774.	1.6	48
24	Enhanced unbiased sampling of protein dynamics using evolutionary coupling information. Scientific Reports, 2017, 7, 12700.	1.6	47
25	Allosteric Control of a Plant Receptor Kinase through S-Glutathionylation. Biophysical Journal, 2017, 113, 2354-2363.	0.2	47
26	Molecular dynamics simulations reveal the conformational dynamics of Arabidopsis thaliana BRI1 and BAK1 receptor-like kinases. Journal of Biological Chemistry, 2017, 292, 12643-12652.	1.6	45
27	Dewetting Controls Plant Hormone Perception and Initiation of Drought Resistance Signaling. Structure, 2019, 27, 692-702.e3.	1.6	44
28	Complex Pathways in Folding of Protein G Explored by Simulation and Experiment. Biophysical Journal, 2014, 107, 947-955.	0.2	41
29	Universality of the Sodium Ion Binding Mechanism in Classâ€…A Gâ€Proteinâ€Coupled Receptors. Angewandte Chemie - International Edition, 2018, 57, 3048-3053.	7.2	41
30	Understanding the Role of Arginine as an Eluent in Affinity Chromatography via Molecular Computations. Journal of Physical Chemistry B, 2011, 115, 2645-2654.	1.2	40
31	A network of molecular switches controls the activation of the two-component response regulator NtrC. Nature Communications, 2015, 6, 7283.	5.8	40
32	Universality of the Sodium Ion Binding Mechanism in Classâ€…A Gâ€Proteinâ€Coupled Receptors. Angewandte Chemie, 2018, 130, 3102-3107.	1.6	38
33	Complex Interactions between Molecular Ions in Solution and Their Effect on Protein Stability. Journal of the American Chemical Society, 2011, 133, 18713-18718.	6.6	37
34	Markov State Models and tICA Reveal a Nonnative Folding Nucleus in Simulations of NuG2. Biophysical Journal, 2016, 110, 1716-1719.	0.2	34
35	When SWEETs Turn Tweens: Updates and Perspectives. Annual Review of Plant Biology, 2022, 73, 379-403.	8.6	31
36	Structure and Potentialâ€Dependent Selectivity in Redoxâ€Metallopolymers: Electrochemically Mediated Multicomponent Metal Separations. Advanced Functional Materials, 2021, 31, 2009307.	7.8	30

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37	Heat dissipation guides activation in signaling proteins. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 10377-10382.	3.3	27
38	Using molecular simulation to explore the nanoscale dynamics of the plant kinome. Biochemical Journal, 2018, 475, 905-921.	1.7	27
39	Role of substrate recognition in modulating strigolactone receptor selectivity in witchweed. Journal of Biological Chemistry, 2021, 297, 101092.	1.6	27
40	Recruiting machine learning methods for molecular simulations of proteins. Molecular Simulation, 2018, 44, 891-904.	0.9	26
41	Distinct Substrate Transport Mechanism Identified in Homologous Sugar Transporters. Journal of Physical Chemistry B, 2019, 123, 8411-8418.	1.2	26
42	How do antiporters exchange substrates across the cell membrane? An atomic-level description of the complete exchange cycle in NarK. Structure, 2021, 29, 922-933.e3.	1.6	24
43	Automatic Selection of Order Parameters in the Analysis of Large Scale Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2014, 10, 5217-5223.	2.3	23
44	Modeling Shell Formation in Coreâ˜Shell Nanocrystals in Reverse Micelle Systems. Langmuir, 2006, 22, 9500-9506.	1.6	22
45	TLmutation: Predicting the Effects of Mutations Using Transfer Learning. Journal of Physical Chemistry B, 2020, 124, 3845-3854.	1.2	21
46	The substrate import mechanism of the human serotonin transporter. Biophysical Journal, 2022, 121, 715-730.	0.2	21
47	Mechanistic origin of partial agonism of tetrahydrocannabinol for cannabinoid receptors. Journal of Biological Chemistry, 2022, 298, 101764.	1.6	21
48	Coagulation of Nanoparticles in Reverse Micellar Systems:Â A Monte Carlo Model. Langmuir, 2005, 21, 11528-11533.	1.6	20
49	Chiral emergence in multistep hierarchical assembly of achiral conjugated polymers. Nature Communications, 2022, 13, 2738.	5.8	20
50	Effects of PAMAM Dendrimer Salt Solutions on Protein Stability. Journal of Physical Chemistry Letters, 2011, 2, 1782-1788.	2.1	19
51	Effects of Solute-Solute Interactions on Protein Stability Studied Using Various Counterions and Dendrimers. PLoS ONE, 2011, 6, e27665.	1.1	18
52	Predicting Optimal DEER Label Positions to Study Protein Conformational Heterogeneity. Journal of Physical Chemistry B, 2017, 121, 9761-9770.	1.2	18
53	Role of internal loop dynamics in antibiotic permeability of outer membrane porins. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	3.3	18
54	Identification and analysis of sugar transporters capable of coâ€transporting glucose and xylose simultaneously. Biotechnology Journal, 2021, 16, e2100238.	1.8	17

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55	CaCO3nanoparticle synthesis by carbonation of lime solution in microemulsion systems. Nanotechnology, 2007, 18, 035607.	1.3	16
56	Inhibition of lung microbiota-derived proapoptotic peptides ameliorates acute exacerbation of pulmonary fibrosis. Nature Communications, 2022, 13, 1558.	5.8	16
57	Elucidating Ligand-Modulated Conformational Landscape of GPCRs Using Cloud-Computing Approaches. Methods in Enzymology, 2015, 557, 551-572.	0.4	15
58	Characterizing Conformational Dynamics of Proteins Using Evolutionary Couplings. Journal of Physical Chemistry B, 2018, 122, 1017-1025.	1.2	15
59	Distinct Binding Mechanisms for Allosteric Sodium Ion in Cannabinoid Receptors. ACS Chemical Neuroscience, 2022, 13, 379-389.	1.7	15
60	Recent Advances in Machine Learning Variant Effect Prediction Tools for Protein Engineering. Industrial & Engineering Chemistry Research, 2022, 61, 6235-6245.	1.8	15
61	Conserve Water: A Method for the Analysis of Solvent in Molecular Dynamics. Journal of Chemical Theory and Computation, 2015, 11, 1094-1101.	2.3	14
62	Molecular Mechanism of Brassinosteroid Perception by the Plant Growth Receptor BRI1. Journal of Physical Chemistry B, 2020, 124, 355-365.	1.2	14
63	A Monte Carlo Model for the Formation of Coreâ"Shell Nanocrystals in Reverse Micellar Systems. Industrial & Engineering Chemistry Research, 2006, 45, 2249-2254.	1.8	13
64	Modeling of Formation of Nanoparticles in Reverse Micellar Systems: Ostwald Ripening of Silver Halide Particles. Langmuir, 2009, 25, 3786-3793.	1.6	13
65	SAXS-guided Enhanced Unbiased Sampling for Structure Determination of Proteins and Complexes. Scientific Reports, 2018, 8, 17748.	1.6	13
66	Markov state modeling of membrane transport proteins. Journal of Structural Biology, 2021, 213, 107800.	1.3	13
67	Ion Gel Dynamic Templates for Large Modulation of Morphology and Charge Transport Properties of Solution-Coated Conjugated Polymer Thin Films. ACS Applied Materials & Interfaces, 2019, 11, 22561-22574.	4.0	12
68	FingerprintContacts: Predicting Alternative Conformations of Proteins from Coevolution. Journal of Physical Chemistry B, 2020, 124, 3605-3615.	1.2	12
69	Impact of Increased Membrane Realism on Conformational Sampling of Proteins. Journal of Chemical Theory and Computation, 2021, 17, 5342-5357.	2.3	12
70	Molecular basis of the activation and dissociation of dimeric PYL2 receptor in abscisic acid signaling. Physical Chemistry Chemical Physics, 2022, 24, 724-734.	1.3	12
71	Structural Rearrangement of the Serotonin Transporter Intracellular Gate Induced by Thr276 Phosphorylation. ACS Chemical Neuroscience, 2022, 13, 933-945.	1.7	11
72	Application of Hidden Markov Models in Biomolecular Simulations. Methods in Molecular Biology, 2017, 1552, 29-41.	0.4	10

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73	A model for particle coagulation in reverse micelles with a size dependent coagulation rate. Nanotechnology, 2006, 17, 261-267.	1.3	9
74	Maximizing Kinetic Information Gain of Markov State Models for Optimal Design of Spectroscopy Experiments. Journal of Physical Chemistry B, 2018, 122, 10793-10805.	1.2	9
75	Structural Consequences of Multisite Phosphorylation in the BAK1 Kinase Domain. Biophysical Journal, 2020, 118, 698-707.	0.2	9
76	Activation Mechanism of Strigolactone Receptors and Its Impact on Ligand Selectivity between Host and Parasitic Plants. Journal of Chemical Information and Modeling, 2022, 62, 1712-1722.	2.5	9
77	Pricing policy for declining demand using item preservation technology. SpringerPlus, 2016, 5, 1957.	1.2	7
78	Dodine as a Kosmo-Chaotropic Agent. Journal of Physical Chemistry Letters, 2019, 10, 2600-2605.	2.1	7
79	Divalent cations promote TALE DNA-binding specificity. Nucleic Acids Research, 2020, 48, 1406-1422.	6.5	6
80	Automatic Feature Selection in Markov State Models Using Genetic Algorithm. Journal of Computational Science Education, 2018, 9, 14-22.	0.3	6
81	Predicting the Activities of Drug Excipients on Biological Targets using One-Shot Learning. Journal of Physical Chemistry B, 2022, 126, 1492-1503.	1.2	5
82	Dual Role of Strigolactone Receptor Signaling Partner in Inhibiting Substrate Hydrolysis. Journal of Physical Chemistry B, 2022, 126, 2188-2195.	1.2	5
83	Inventory model for convertible item with deterioration. Communications in Statistics - Theory and Methods, 2016, 45, 1137-1147.	0.6	4
84	Understanding the Conformational Diversity of Proton-Coupled Oligopeptide Transporter (POT) Family. Biophysical Journal, 2017, 112, 16a-17a.	0.2	3
85	Machine Learning Guided Ligand-Protein Simulation Approach Elucidates the Binding Mechanism of Abscisic Acid. Biophysical Journal, 2017, 112, 349a.	0.2	2
86	Understanding the Role of Arginine and Citrate as Eluents in Affinity Chromatography. ACS Symposium Series, 2013, , 67-86.	0.5	1
87	Simulation Guided Design of Spectroscopy Experiments via Maximizing Kinetic Information Gain. Biophysical Journal, 2019, 116, 183a-184a.	0.2	1
88	How does evolution design functional free energy landscapes of proteins? A case study on the emergence of regulation in the Cyclin Dependent Kinase family. Molecular Systems Design and Engineering, 2020, 5, 392-400.	1.7	1
89	Integration of machine learning with computational structural biology of plants. Biochemical Journal, 2022, 479, 921-928.	1.7	1
90	Activation Pathways of Kinases Reveal Intermediate States as Novel Targets for Drug Design. Biophysical Journal, 2014, 106, 308a.	0.2	0

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91	Toward a Global View of the Conformational Landscape of the Human Kinome. Biophysical Journal, 2014, 106, 655a-656a.	0.2	0
92	Investigating Ligand-Modulation of GPCR Activation Pathways. Biophysical Journal, 2014, 106, 14a.	0.2	0
93	Optimal Probes: An Efficient Method to Select Deer Distance Restraints using Machine Learning. Biophysical Journal, 2017, 112, 328a.	0.2	0
94	Frontispiece: Universality of the Sodium Ion Binding Mechanism in Classâ€…A Gâ€Proteinâ€Coupled Receptors. Angewandte Chemie - International Edition, 2018, 57, .	7.2	0
95	Frontispiz: Universality of the Sodium Ion Binding Mechanism in Classâ€…A Gâ€Proteinâ€Coupled Receptors. Angewandte Chemie, 2018, 130, .	1.6	0
96	Investigating the Conformational Dynamics of Plant Protein Kinases. Biophysical Journal, 2018, 114, 582a-583a.	0.2	0
97	Efficient Unbiased Sampling of Protein Dynamics using Reinforcement Learning. Biophysical Journal, 2018, 114, 673a.	0.2	0
98	Elucidating Mechanisms of Substrate Transport in Membrane Transporters. Biophysical Journal, 2019, 116, 347a.	0.2	0
99	Is Dodine a Protein Stabilizer or Destabilizer? It'S Complicated!. Biophysical Journal, 2020, 118, 199a.	0.2	0
100	Reconciling Membrane Protein Simulations with Experimental Spectroscopic Data. Biophysical Journal, 2020, 118, 231a.	0.2	0
101	Mechanistic Origin of Partial Agonism of Î”9-Tetrahydrocannabinol for Cannabinoid Receptors. Biophysical Journal, 2021, 120, 131a-132a.	0.2	0
102	Establishing an Idealized Plant Plasma Membrane for Biomolecular Simulation. Biophysical Journal, 2021, 120, 224a.	0.2	0
103	Electrosorption: Structure and Potentialâ€Dependent Selectivity in Redoxâ€Metallopolymers: Electrochemically Mediated Multicomponent Metal Separations (Adv. Funct. Mater. 15/2021). Advanced Functional Materials, 2021, 31, 2170103.	7.8	0