Diwakar Shukla

List of Publications by Year
in descending order

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103 papers	4,493 citations	159585 30 h-index	128289 60 g-index
143 all docs	143 docs citations	143 times ranked	4784 citing authors

#	Article	IF	Citations
1	Molecular basis of the activation and dissociation of dimeric PYL2 receptor in abscisic acid signaling. Physical Chemistry Chemical Physics, 2022, 24, 724-734.	2.8	12
2	Distinct Binding Mechanisms for Allosteric Sodium Ion in Cannabinoid Receptors. ACS Chemical Neuroscience, 2022, 13, 379-389.	3.5	15
3	Engineered ACE2 decoy mitigates lung injury and death induced by SARS-CoV-2 variants. Nature Chemical Biology, 2022, 18, 342-351.	8.0	63
4	The substrate import mechanism of the human serotonin transporter. Biophysical Journal, 2022, 121, 715-730.	0.5	21
5	Predicting the Activities of Drug Excipients on Biological Targets using One-Shot Learning. Journal of Physical Chemistry B, 2022, 126, 1492-1503.	2.6	5
6	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.	5.4	9
7	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, .	7.1	18
8	Structural Rearrangement of the Serotonin Transporter Intracellular Gate Induced by Thr276 Phosphorylation. ACS Chemical Neuroscience, 2022, 13, 933-945.	3.5	11
9	Inhibition of lung microbiota-derived proapoptotic peptides ameliorates acute exacerbation of pulmonary fibrosis. Nature Communications, 2022, 13, 1558.	12.8	16
10	Dual Role of Strigolactone Receptor Signaling Partner in Inhibiting Substrate Hydrolysis. Journal of Physical Chemistry B, 2022, 126, 2188-2195.	2.6	5
11	Mechanistic origin of partial agonism of tetrahydrocannabinol for cannabinoid receptors. Journal of Biological Chemistry, 2022, 298, 101764.	3.4	21
12	Recent Advances in Machine Learning Variant Effect Prediction Tools for Protein Engineering. Industrial & Engineering Chemistry Research, 2022, 61, 6235-6245.	3.7	15
13	When SWEETs Turn Tweens: Updates and Perspectives. Annual Review of Plant Biology, 2022, 73, 379-403.	18.7	31
14	Integration of machine learning with computational structural biology of plants. Biochemical Journal, 2022, 479, 921-928.	3.7	1
15	Chiral emergence in multistep hierarchical assembly of achiral conjugated polymers. Nature Communications, 2022, 13, 2738.	12.8	20
16	Degradation of complex arabinoxylans by human colonic Bacteroidetes. Nature Communications, 2021, 12, 459.	12.8	68
17	Mechanistic Origin of Partial Agonism of Î”9-Tetrahydrocannabinol for Cannabinoid Receptors. Biophysical Journal, 2021, 120, 131a-132a.	0.5	0
18	Establishing an Idealized Plant Plasma Membrane for Biomolecular Simulation. Biophysical Journal, 2021, 120, 224a.	0.5	0

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19	Structure and Potentialâ€Dependent Selectivity in Redoxâ€Metallopolymers: Electrochemically Mediated Multicomponent Metal Separations. Advanced Functional Materials, 2021, 31, 2009307.	14.9	30
20	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.	14.9	0
21	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.	3.3	24
22	Impact of Increased Membrane Realism on Conformational Sampling of Proteins. Journal of Chemical Theory and Computation, 2021, 17, 5342-5357.	5.3	12
23	Identification and analysis of sugar transporters capable of coâ€transporting glucose and xylose simultaneously. Biotechnology Journal, 2021, 16, e2100238.	3.5	17
24	Markov state modeling of membrane transport proteins. Journal of Structural Biology, 2021, 213, 107800.	2.8	13
25	The shape of water in zeolites and its impact on epoxidation catalysis. Nature Catalysis, 2021, 4, 797-808.	34.4	66
26	Role of substrate recognition in modulating strigolactone receptor selectivity in witchweed. Journal of Biological Chemistry, 2021, 297, 101092.	3.4	27
27	Structural Consequences of Multisite Phosphorylation in the BAK1 Kinase Domain. Biophysical Journal, 2020, 118, 698-707.	0.5	9
28	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.	3.4	1
29	Molecular Mechanism of Brassinosteroid Perception by the Plant Growth Receptor BRI1. Journal of Physical Chemistry B, 2020, 124, 355-365.	2.6	14
30	Divalent cations promote TALE DNA-binding specificity. Nucleic Acids Research, 2020, 48, 1406-1422.	14.5	6
31	Is Dodine a Protein Stabilizer or Destabilizer? It'S Complicated!. Biophysical Journal, 2020, 118, 199a.	0.5	0
32	Reconciling Membrane Protein Simulations with Experimental Spectroscopic Data. Biophysical Journal, 2020, 118, 231a.	0.5	0
33	TLmutation: Predicting the Effects of Mutations Using Transfer Learning. Journal of Physical Chemistry B, 2020, 124, 3845-3854.	2.6	21
34	FingerprintContacts: Predicting Alternative Conformations of Proteins from Coevolution. Journal of Physical Chemistry B, 2020, 124, 3605-3615.	2.6	12
35	Distinct Substrate Transport Mechanism Identified in Homologous Sugar Transporters. Journal of Physical Chemistry B, 2019, 123, 8411-8418.	2.6	26
36	Dewetting Controls Plant Hormone Perception and Initiation of Drought Resistance Signaling. Structure, 2019, 27, 692-702.e3.	3.3	44

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37	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.	8.0	12
38	Molecular Basis of the Glucose Transport Mechanism in Plants. ACS Central Science, 2019, 5, 1085-1096.	11.3	52
39	Simulation Guided Design of Spectroscopy Experiments via Maximizing Kinetic Information Gain. Biophysical Journal, 2019, 116, 183a-184a.	0.5	1
40	Dodine as a Kosmo-Chaotropic Agent. Journal of Physical Chemistry Letters, 2019, 10, 2600-2605.	4.6	7
41	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.	3.4	48
42	Elucidating Mechanisms of Substrate Transport in Membrane Transporters. Biophysical Journal, 2019, 116, 347a.	0.5	0
43	Frontispiece: Universality of the Sodium Ion Binding Mechanism in Classâ€…A Gâ€Proteinâ€Coupled Receptors. Angewandte Chemie - International Edition, 2018, 57, .	13.8	0
44	Universality of the Sodium Ion Binding Mechanism in Classâ€…A Gâ€Proteinâ€Coupled Receptors. Angewandte Chemie - International Edition, 2018, 57, 3048-3053.	13.8	41
45	Universality of the Sodium Ion Binding Mechanism in Classâ€…A Gâ€Proteinâ€Coupled Receptors. Angewandte Chemie, 2018, 130, 3102-3107.	2.0	38
46	Characterizing Conformational Dynamics of Proteins Using Evolutionary Couplings. Journal of Physical Chemistry B, 2018, 122, 1017-1025.	2.6	15
47	Recruiting machine learning methods for molecular simulations of proteins. Molecular Simulation, 2018, 44, 891-904.	2.0	26
48	Using molecular simulation to explore the nanoscale dynamics of the plant kinome. Biochemical Journal, 2018, 475, 905-921.	3.7	27
49	Frontispiz: Universality of the Sodium Ion Binding Mechanism in Classâ€…A Gâ€Proteinâ€Coupled Receptors. Angewandte Chemie, 2018, 130, .	2.0	0
50	Investigating the Conformational Dynamics of Plant Protein Kinases. Biophysical Journal, 2018, 114, 582a-583a.	0.5	0
51	Efficient Unbiased Sampling of Protein Dynamics using Reinforcement Learning. Biophysical Journal, 2018, 114, 673a.	0.5	0
52	SAXS-guided Enhanced Unbiased Sampling for Structure Determination of Proteins and Complexes. Scientific Reports, 2018, 8, 17748.	3.3	13
53	Maximizing Kinetic Information Gain of Markov State Models for Optimal Design of Spectroscopy Experiments. Journal of Physical Chemistry B, 2018, 122, 10793-10805.	2.6	9
54	Free Energy Landscape of the Complete Transport Cycle in a Key Bacterial Transporter. ACS Central Science, 2018, 4, 1146-1154.	11.3	49

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55	Reinforcement Learning Based Adaptive Sampling: REAPing Rewards by Exploring Protein Conformational Landscapes. Journal of Physical Chemistry B, 2018, 122, 8386-8395.	2.6	82
56	Automatic Feature Selection in Markov State Models Using Genetic Algorithm. Journal of Computational Science Education, 2018, 9, 14-22.	0.3	6
57	Application of Hidden Markov Models in Biomolecular Simulations. Methods in Molecular Biology, 2017, 1552, 29-41.	0.9	10
58	Machine Learning Guided Ligand-Protein Simulation Approach Elucidates the Binding Mechanism of Abscisic Acid. Biophysical Journal, 2017, 112, 349a.	0.5	2
59	Molecular dynamics simulations reveal the conformational dynamics of Arabidopsis thaliana BRI1 and BAK1 receptor-like kinases. Journal of Biological Chemistry, 2017, 292, 12643-12652.	3.4	45
60	Understanding the Conformational Diversity of Proton-Coupled Oligopeptide Transporter (POT) Family. Biophysical Journal, 2017, 112, 16a-17a.	0.5	3
61	Optimal Probes: An Efficient Method to Select Deer Distance Restraints using Machine Learning. Biophysical Journal, 2017, 112, 328a.	0.5	0
62	Enhanced unbiased sampling of protein dynamics using evolutionary coupling information. Scientific Reports, 2017, 7, 12700.	3.3	47
63	Predicting Optimal DEER Label Positions to Study Protein Conformational Heterogeneity. Journal of Physical Chemistry B, 2017, 121, 9761-9770.	2.6	18
64	Allosteric Control of a Plant Receptor Kinase through S-Glutathionylation. Biophysical Journal, 2017, 113, 2354-2363.	0.5	47
65	Dynamic-template-directed multiscale assembly for large-area coating of highly-aligned conjugated polymer thin films. Nature Communications, 2017, 8, 16070.	12.8	78
66	Crops In Silico: Generating Virtual Crops Using an Integrative and Multi-scale Modeling Platform. Frontiers in Plant Science, 2017, 8, 786.	3.6	102
67	Conformational heterogeneity of the calmodulin binding interface. Nature Communications, 2016, 7, 10910.	12.8	49
68	Inventory model for convertible item with deterioration. Communications in Statistics - Theory and Methods, 2016, 45, 1137-1147.	1.0	4
69	Markov State Models and tICA Reveal a Nonnative Folding Nucleus in Simulations of NuG2. Biophysical Journal, 2016, 110, 1716-1719.	0.5	34
70	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.	7.1	67
71	Pricing policy for declining demand using item preservation technology. SpringerPlus, 2016, 5, 1957.	1.2	7
72	Markov State Models Provide Insights into Dynamic Modulation of Protein Function. Accounts of Chemical Research, 2015, 48, 414-422.	15.6	231

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73	Conserve Water: A Method for the Analysis of Solvent in Molecular Dynamics. Journal of Chemical Theory and Computation, 2015, 11, 1094-1101.	5.3	14
74	Heat dissipation guides activation in signaling proteins. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 10377-10382.	7.1	27
75	Cloud computing approaches for prediction of ligand binding poses and pathways. Scientific Reports, 2015, 5, 7918.	3.3	54
76	A network of molecular switches controls the activation of the two-component response regulator NtrC. Nature Communications, 2015, 6, 7283.	12.8	40
77	Elucidating Ligand-Modulated Conformational Landscape of GPCRs Using Cloud-Computing Approaches. Methods in Enzymology, 2015, 557, 551-572.	1.0	15
78	Automatic Selection of Order Parameters in the Analysis of Large Scale Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2014, 10, 5217-5223.	5.3	23
79	Activation pathway of Src kinase reveals intermediate states as targets for drug design. Nature Communications, 2014, 5, 3397.	12.8	300
80	Cloud-based simulations on Google Exacycle reveal ligand modulation of GPCR activation pathways. Nature Chemistry, 2014, 6, 15-21.	13.6	388
81	Complex Pathways in Folding of Protein G Explored by Simulation and Experiment. Biophysical Journal, 2014, 107, 947-955.	0.5	41
82	Activation Pathways of Kinases Reveal Intermediate States as Novel Targets for Drug Design. Biophysical Journal, 2014, 106, 308a.	0.5	0
83	Toward a Global View of the Conformational Landscape of the Human Kinome. Biophysical Journal, 2014, 106, 655a-656a.	0.5	0
84	Investigating Ligand-Modulation of GPCR Activation Pathways. Biophysical Journal, 2014, 106, 14a.	0.5	0
85	To milliseconds and beyond: challenges in the simulation of protein folding. Current Opinion in Structural Biology, 2013, 23, 58-65.	5.7	331
86	OpenMM 4: A Reusable, Extensible, Hardware Independent Library for High Performance Molecular Simulation. Journal of Chemical Theory and Computation, 2013, 9, 461-469.	5.3	583
87	Understanding the Role of Arginine and Citrate as Eluents in Affinity Chromatography. ACS Symposium Series, 2013, , 67-86.	0.5	1
88	Arginine and the Hofmeister Series: The Role of Ionâ€“Ion Interactions in Protein Aggregation Suppression. Journal of Physical Chemistry B, 2011, 115, 7447-7458.	2.6	125
89	Understanding the Synergistic Effect of Arginine and Glutamic Acid Mixtures on Protein Solubility. Journal of Physical Chemistry B, 2011, 115, 11831-11839.	2.6	66
90	Preferential Interaction Coefficients of Proteins in Aqueous Arginine Solutions and Their Molecular Origins. Journal of Physical Chemistry B, 2011, 115, 1243-1253.	2.6	53

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91	Complex Interactions between Molecular Ions in Solution and Their Effect on Protein Stability. Journal of the American Chemical Society, 2011, 133, 18713-18718.	13.7	37
92	Effects of PAMAM Dendrimer Salt Solutions on Protein Stability. Journal of Physical Chemistry Letters, 2011, 2, 1782-1788.	4.6	19
93	Understanding the Role of Arginine as an Eluent in Affinity Chromatography via Molecular Computations. Journal of Physical Chemistry B, 2011, 115, 2645-2654.	2.6	40
94	Effects of Solute-Solute Interactions on Protein Stability Studied Using Various Counterions and Dendrimers. PLoS ONE, 2011, 6, e27665.	2.5	18
95	Molecular level insight into intra-solvent interaction effects on protein stability and aggregation. Advanced Drug Delivery Reviews, 2011, 63, 1074-1085.	13.7	83
96	Interaction of Arginine with Proteins and the Mechanism by Which It Inhibits Aggregation. Journal of Physical Chemistry B, 2010, 114, 13426-13438.	2.6	183
97	Molecular Computations of Preferential Interaction Coefficients of Proteins. Journal of Physical Chemistry B, 2009, 113, 12546-12554.	2.6	79
98	Modeling of Formation of Nanoparticles in Reverse Micellar Systems: Ostwald Ripening of Silver Halide Particles. Langmuir, 2009, 25, 3786-3793.	3.5	13
99	CaCO3nanoparticle synthesis by carbonation of lime solution in microemulsion systems. Nanotechnology, 2007, 18, 035607.	2.6	16
100	A Monte Carlo Model for the Formation of Coreâ"Shell Nanocrystals in Reverse Micellar Systems. Industrial & Engineering Chemistry Research, 2006, 45, 2249-2254.	3.7	13
101	Modeling Shell Formation in Coreâ"Shell Nanocrystals in Reverse Micelle Systems. Langmuir, 2006, 22, 9500-9506.	3.5	22
102	A model for particle coagulation in reverse micelles with a size dependent coagulation rate. Nanotechnology, 2006, 17, 261-267.	2.6	9
103	Coagulation of Nanoparticles in Reverse Micellar Systems:Â A Monte Carlo Model. Langmuir, 2005, 21, 11528-11533.	3.5	20