Diwakar Shukla

List of Publications by Citations

97 papers	3,070 citations	26 h-index	54 g-index
143 ext. papers	3,911 ext. citations	6.6 avg, IF	5.7 L-index

#	Paper	IF	Citations
97	OpenMM 4: A Reusable, Extensible, Hardware Independent Library for High Performance Molecular Simulation. *Journal of Chemical Theory and Computation*, **2013**, 9, 461-469	6.4	440
96	Cloud-based simulations on Google Exacycle reveal ligand modulation of GPCR activation pathways. *Nature Chemistry*, **2014**, 6, 15-21	17.6	306
95	To milliseconds and beyond: challenges in the simulation of protein folding. *Current Opinion in Structural Biology*, **2013**, 23, 58-65	8.1	281
94	Activation pathway of Src kinase reveals intermediate states as targets for drug design. *Nature Communications*, **2014**, 5, 3397	17.4	244
93	Markov state models provide insights into dynamic modulation of protein function. *Accounts of Chemical Research*, **2015**, 48, 414-22	24.3	172
92	Interaction of arginine with proteins and the mechanism by which it inhibits aggregation. *Journal of Physical Chemistry B*, **2010**, 114, 13426-38	3.4	153
91	Arginine and the Hofmeister Series: the role of ion-ion interactions in protein aggregation suppression. *Journal of Physical Chemistry B*, **2011**, 115, 7447-58	3.4	99
90	Molecular computations of preferential interaction coefficients of proteins. *Journal of Physical Chemistry B*, **2009**, 113, 12546-54	3.4	70
89	Molecular level insight into intra-solvent interaction effects on protein stability and aggregation. *Advanced Drug Delivery Reviews*, **2011**, 63, 1074-85	18.5	69
88	Dynamic-template-directed multiscale assembly for large-area coating of highly-aligned conjugated polymer thin films. *Nature Communications*, **2017**, 8, 16070	17.4	66
87	Crops : Generating Virtual Crops Using an Integrative and Multi-scale Modeling Platform. *Frontiers in Plant Science*, **2017**, 8, 786	6.2	61
86	Understanding the synergistic effect of arginine and glutamic acid mixtures on protein solubility. *Journal of Physical Chemistry B*, **2011**, 115, 11831-9	3.4	53
85	Transition path theory analysis of c-Src kinase activation. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 9193-8	11.5	49
84	Reinforcement Learning Based Adaptive Sampling: REAPing Rewards by Exploring Protein Conformational Landscapes. *Journal of Physical Chemistry B*, **2018**, 122, 8386-8395	3.4	48
83	Preferential interaction coefficients of proteins in aqueous arginine solutions and their molecular origins. *Journal of Physical Chemistry B*, **2011**, 115, 1243-53	3.4	45
82	A network of molecular switches controls the activation of the two-component response regulator NtrC. *Nature Communications*, **2015**, 6, 7283	17.4	38
81	Conformational heterogeneity of the calmodulin binding interface. *Nature Communications*, **2016**, 7, 10910	17.4	38

80	Cloud computing approaches for prediction of ligand binding poses and pathways. *Scientific Reports*, **2015**, 5, 7918	4.9	37
79	Understanding the role of arginine as an eluent in affinity chromatography via molecular computations. *Journal of Physical Chemistry B*, **2011**, 115, 2645-54	3.4	36
78	Complex pathways in folding of protein G explored by simulation and experiment. *Biophysical Journal*, **2014**, 107, 947-55	2.9	34
77	Molecular dynamics simulations reveal the conformational dynamics of BRI1 and BAK1 receptor-like kinases. *Journal of Biological Chemistry*, **2017**, 292, 12643-12652	5.4	33
76	Enhanced unbiased sampling of protein dynamics using evolutionary coupling information. *Scientific Reports*, **2017**, 7, 12700	4.9	31
75	Universality of the Sodium Ion Binding Mechanism in Class A G-Protein-Coupled Receptors. *Angewandte Chemie - International Edition*, **2018**, 57, 3048-3053	16.4	31
74	Complex interactions between molecular ions in solution and their effect on protein stability. *Journal of the American Chemical Society*, **2011**, 133, 18713-8	16.4	31
73	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	5.4	30
72	Allosteric Control of a Plant Receptor Kinase through S-Glutathionylation. *Biophysical Journal*, **2017** , 113, 2354-2363	2.9	28
71	Markov State Models and tICA Reveal a Nonnative Folding Nucleus in Simulations of NuG2. *Biophysical Journal*, **2016**, 110, 1716-1719	2.9	25
70	Free Energy Landscape of the Complete Transport Cycle in a Key Bacterial Transporter. *ACS Central Science*, **2018**, 4, 1146-1154	16.8	25
69	Molecular Basis of the Glucose Transport Mechanism in Plants. *ACS Central Science*, **2019**, 5, 1085-1096	16.8	23
68	Dewetting Controls Plant Hormone Perception and Initiation of Drought Resistance Signaling. *Structure*, **2019**, 27, 692-702.e3	5.2	22
67	Heat dissipation guides activation in signaling proteins. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 10377-82	11.5	21
66	Recruiting machine learning methods for molecular simulations of proteins. *Molecular Simulation*, **2018**, 44, 891-904	2	21
65	Modeling shell formation in core-shell nanocrystals in reverse micelle systems. *Langmuir*, **2006**, 22, 9500-6		21
64	Using molecular simulation to explore the nanoscale dynamics of the plant kinome. *Biochemical Journal*, **2018**, 475, 905-921	3.8	18
63	Coagulation of nanoparticles in reverse micellar systems: a Monte Carlo model. *Langmuir*, **2005**, 21, 11528-33		18

62	Automatic Selection of Order Parameters in the Analysis of Large Scale Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2014**, 10, 5217-5223	6.4	15
61	Effects of solute-solute interactions on protein stability studied using various counterions and dendrimers. *PLoS ONE*, **2011**, 6, e27665	3.7	15
60	Degradation of complex arabinoxylans by human colonic Bacteroidetes. *Nature Communications*, **2021**, 12, 459	17.4	15
59	The shape of water in zeolites and its impact on epoxidation catalysis. *Nature Catalysis*, **2021**, 4, 797-808	36.5	14
58	TLmutation: Predicting the Effects of Mutations Using Transfer Learning. *Journal of Physical Chemistry B*, **2020**, 124, 3845-3854	3.4	13
57	Effects of PAMAM Dendrimer Salt Solutions on Protein Stability. *Journal of Physical Chemistry Letters*, **2011**, 2, 1782-1788	6.4	13
56	CaCO(3) nanoparticle synthesis by carbonation of lime solution in microemulsion systems. *Nanotechnology*, **2007**, 18, 035607	3.4	13
55	Predicting Optimal DEER Label Positions to Study Protein Conformational Heterogeneity. *Journal of Physical Chemistry B*, **2017**, 121, 9761-9770	3.4	12
54	Modeling of formation of nanoparticles in reverse micellar systems: Ostwald ripening of silver halide particles. *Langmuir*, **2009**, 25, 3786-93	4	12
53	A Monte Carlo Model for the Formation of Core‐Shell Nanocrystals in Reverse Micellar Systems. *Industrial & Engineering Chemistry Research*, **2006**, 45, 2249-2254	3.9	12
52	Elucidating Ligand-Modulated Conformational Landscape of GPCRs Using Cloud-Computing Approaches. *Methods in Enzymology*, **2015**, 557, 551-72	1.7	11
51	Universality of the Sodium Ion Binding Mechanism in Class A G-Protein-Coupled Receptors. *Angewandte Chemie*, **2018**, 130, 3102-3107	3.6	11
50	Characterizing Conformational Dynamics of Proteins Using Evolutionary Couplings. *Journal of Physical Chemistry B*, **2018**, 122, 1017-1025	3.4	11
49	SAXS-guided Enhanced Unbiased Sampling for Structure Determination of Proteins and Complexes. *Scientific Reports*, **2018**, 8, 17748	4.9	11
48	Distinct Substrate Transport Mechanism Identified in Homologous Sugar Transporters. *Journal of Physical Chemistry B*, **2019**, 123, 8411-8418	3.4	10
47	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	9.5	10
46	Conserve Water: A Method for the Analysis of Solvent in Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2015**, 11, 1094-101	6.4	10
45	Engineered ACE2 decoy mitigates lung injury and death induced by SARS-CoV-2 variants.. *Nature Chemical Biology*, **2022**,	11.7	10

44	FingerprintContacts: Predicting Alternative Conformations of Proteins from Coevolution. *Journal of Physical Chemistry B*, **2020**, 124, 3605-3615	3.4	8
43	A model for particle coagulation in reverse micelles with a size dependent coagulation rate. *Nanotechnology*, **2006**, 17, 261-267	3.4	8
42	Molecular Mechanism of Brassinosteroid Perception by the Plant Growth Receptor BRI1. *Journal of Physical Chemistry B*, **2020**, 124, 355-365	3.4	8
41	Structure and Potential-Dependent Selectivity in Redox-Metallopolymers: Electrochemically Mediated Multicomponent Metal Separations. *Advanced Functional Materials*, **2021**, 31, 2009307	15.6	7
40	Role of substrate recognition in modulating strigolactone receptor selectivity in witchweed. *Journal of Biological Chemistry*, **2021**, 297, 101092	5.4	7
39	Application of Hidden Markov Models in Biomolecular Simulations. *Methods in Molecular Biology*, **2017**, 1552, 29-41	1.4	6
38	Dodine as a Kosmo-Chaotropic Agent. *Journal of Physical Chemistry Letters*, **2019**, 10, 2600-2605	6.4	5
37	Pricing policy for declining demand using item preservation technology. *SpringerPlus*, **2016**, 5, 1957		5
36	Structural Consequences of Multisite Phosphorylation in the BAK1 Kinase Domain. *Biophysical Journal*, **2020**, 118, 698-707	2.9	5
35	Ancestral class-promiscuity as a driver of functional diversity in the BAHD acyltransferase family in plants		4
34	How do brassinosteroids activate their receptors?		4
33	Identification and analysis of sugar transporters capable of co-transporting glucose and xylose simultaneously. *Biotechnology Journal*, **2021**, 16, e2100238	5.6	4
32	When SWEETs Turn Tweens: Updates and Perspectives.. *Annual Review of Plant Biology*, **2021**,	30.7	4
31	Understanding the Conformational Diversity of Proton-Coupled Oligopeptide Transporter (POT) Family. *Biophysical Journal*, **2017**, 112, 16a-17a	2.9	3
30	Molecular basis of the activation and dissociation of dimeric PYL2 receptor in abscisic acid signaling.. *Physical Chemistry Chemical Physics*, **2021**,	3.6	3
29	Divalent cations promote TALE DNA-binding specificity. *Nucleic Acids Research*, **2020**, 48, 1406-1422	20.1	3
28	Inventory model for convertible item with deterioration. *Communications in Statistics - Theory and Methods*, **2016**, 45, 1137-1147	0.5	3
27	Maximizing Kinetic Information Gain of Markov State Models for Optimal Design of Spectroscopy Experiments. *Journal of Physical Chemistry B*, **2018**, 122, 10793-10805	3.4	3

26	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	5.2	3
25	Chiral emergence in multistep hierarchical assembly of achiral conjugated polymers.. *Nature Communications*, **2022**, 13, 2738	17.4	3
24	Machine Learning Guided Ligand-Protein Simulation Approach Elucidates the Binding Mechanism of Abscisic Acid. *Biophysical Journal*, **2017**, 112, 349a	2.9	2
23	Automatic Feature Selection in Markov State Models Using Genetic Algorithm. *Journal of Computational Science Education*, **2018**, 9, 14-22	1.5	2
22	The Substrate Import Mechanism of the Human Serotonin Transporter		2
21	Structural Basis for Negative Regulation of ABA Signaling by ROP11 GTPase		2
20	Role of substrate recognition in modulating strigolactone receptor selectivity in witchweed		2
19	Markov state modeling of membrane transport proteins. *Journal of Structural Biology*, **2021**, 213, 107800	3.4	2
18	Activation Mechanism of Strigolactone Receptors and Its Impact on Ligand Selectivity between Host and Parasitic Plants.. *Journal of Chemical Information and Modeling*, **2022**,	6.1	2
17	Inhibition of lung microbiota-derived proapoptotic peptides ameliorates acute exacerbation of pulmonary fibrosis.. *Nature Communications*, **2022**, 13, 1558	17.4	2
16	Understanding the Role of Arginine and Citrate as Eluents in Affinity Chromatography. *ACS Symposium Series*, **2013**, 67-86	0.4	1
15	Distinct Binding Mechanisms for Allosteric Sodium Ion in Cannabinoid Receptors.. *ACS Chemical Neuroscience*, **2022**,	5.7	1
14	TLmutation: predicting the effects of mutations using transfer learning		1
13	Molecular Basis of the Activation and Dissociation of Dimeric PYL2 Receptor in Abscisic Acid Signaling		1
12	Deep Mutagenesis of a Transporter for Uptake of a Non-Native Substrate Identifies Conformationally Dynamic Regions		1
11	Activation Mechanism of Strigolactone Receptors And Its Impact On Ligand Selectivity Between Host And Parasitic Plants		1
10	Impact of Increased Membrane Realism on Conformational Sampling of Proteins. *Journal of Chemical Theory and Computation*, **2021**, 17, 5342-5357	6.4	1
9	Investigation of gating in outer membrane porins provides new perspectives on antibiotic resistance mechanisms		1

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8	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,	11.5	1
7	Dual Role of Strigolactone Receptor Signaling Partner in Inhibiting Substrate Hydrolysis.. *Journal of Physical Chemistry B*, **2022**,	3.4	1
6	Engineered High-Affinity ACE2 Peptide Mitigates ARDS and Death Induced by Multiple SARS-CoV-2 Variants. **2021**,		1
5	Machine learning guided design of high affinity ACE2 decoys for SARS-CoV-2 neutralization. **2021**,		1
4	Mechanistic Origin of Partial Agonism of Tetrahydrocannabinol for Cannabinoid Receptors.. *Journal of Biological Chemistry*, **2022**, 101764	5.4	0
3	Integration of machine learning with computational structural biology of plants.. *Biochemical Journal*, **2022**, 479, 921-928	3.8	0
2	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	4.6	
1	Electrosorption: Structure and Potential-Dependent Selectivity in Redox-Metallopolymers: Electrochemically Mediated Multicomponent Metal Separations (Adv. Funct. Mater. 15/2021). *Advanced Functional Materials*, **2021**, 31, 2170103	15.6	