

# Diwakar Shukla

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Distinct Binding Mechanisms for Allosteric Sodium Ion in Cannabinoid Receptors.. <i>ACS Chemical Neuroscience</i> , <b>2022</b> ,	5.7	1
96	Engineered ACE2 decoy mitigates lung injury and death induced by SARS-CoV-2 variants.. <i>Nature Chemical Biology</i> , <b>2022</b> ,	11.7	10
95	Activation Mechanism of Strigolactone Receptors and Its Impact on Ligand Selectivity between Host and Parasitic Plants.. <i>Journal of Chemical Information and Modeling</i> , <b>2022</b> ,	6.1	2
94	Role of internal loop dynamics in antibiotic permeability of outer membrane porins.. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2022</b> , 119,	11.5	1
93	Inhibition of lung microbiota-derived proapoptotic peptides ameliorates acute exacerbation of pulmonary fibrosis.. <i>Nature Communications</i> , <b>2022</b> , 13, 1558	17.4	2
92	Dual Role of Strigolactone Receptor Signaling Partner in Inhibiting Substrate Hydrolysis.. <i>Journal of Physical Chemistry B</i> , <b>2022</b> ,	3.4	1
91	Mechanistic Origin of Partial Agonism of Tetrahydrocannabinol for Cannabinoid Receptors.. <i>Journal of Biological Chemistry</i> , <b>2022</b> , 101764	5.4	0
90	Integration of machine learning with computational structural biology of plants.. <i>Biochemical Journal</i> , <b>2022</b> , 479, 921-928	3.8	0
89	Chiral emergence in multistep hierarchical assembly of achiral conjugated polymers.. <i>Nature Communications</i> , <b>2022</b> , 13, 2738	17.4	3
88	Molecular basis of the activation and dissociation of dimeric PYL2 receptor in abscisic acid signaling.. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> ,	3.6	3
87	Electrosorption: Structure and Potential-Dependent Selectivity in Redox-Metallopolymers: Electrochemically Mediated Multicomponent Metal Separations (Adv. Funct. Mater. 15/2021). <i>Advanced Functional Materials</i> , <b>2021</b> , 31, 2170103	15.6	
86	Degradation of complex arabinoxylans by human colonic Bacteroidetes. <i>Nature Communications</i> , <b>2021</b> , 12, 459	17.4	15
85	Structure and Potential-Dependent Selectivity in Redox-Metallopolymers: Electrochemically Mediated Multicomponent Metal Separations. <i>Advanced Functional Materials</i> , <b>2021</b> , 31, 2009307	15.6	7
84	How do antiporters exchange substrates across the cell membrane? An atomic-level description of the complete exchange cycle in NarK. <i>Structure</i> , <b>2021</b> , 29, 922-933.e3	5.2	3
83	Impact of Increased Membrane Realism on Conformational Sampling of Proteins. <i>Journal of Chemical Theory and Computation</i> , <b>2021</b> , 17, 5342-5357	6.4	1
82	Identification and analysis of sugar transporters capable of co-transporting glucose and xylose simultaneously. <i>Biotechnology Journal</i> , <b>2021</b> , 16, e2100238	5.6	4
81	Markov state modeling of membrane transport proteins. <i>Journal of Structural Biology</i> , <b>2021</b> , 213, 107800	3.4	2

80	The shape of water in zeolites and its impact on epoxidation catalysis. <i>Nature Catalysis</i> , <b>2021</b> , 4, 797-808	36.5	14
79	Role of substrate recognition in modulating strigolactone receptor selectivity in witchweed. <i>Journal of Biological Chemistry</i> , <b>2021</b> , 297, 101092	5.4	7
78	When SWEETs Turn Tweens: Updates and Perspectives.. <i>Annual Review of Plant Biology</i> , <b>2021</b> ,	30.7	4
77	Engineered High-Affinity ACE2 Peptide Mitigates ARDS and Death Induced by Multiple SARS-CoV-2 Variants. <b>2021</b> ,		1
76	Machine learning guided design of high affinity ACE2 decoys for SARS-CoV-2 neutralization. <b>2021</b> ,		1
75	TLmutation: Predicting the Effects of Mutations Using Transfer Learning. <i>Journal of Physical Chemistry B</i> , <b>2020</b> , 124, 3845-3854	3.4	13
74	FingerprintContacts: Predicting Alternative Conformations of Proteins from Coevolution. <i>Journal of Physical Chemistry B</i> , <b>2020</b> , 124, 3605-3615	3.4	8
73	Structural Consequences of Multisite Phosphorylation in the BAK1 Kinase Domain. <i>Biophysical Journal</i> , <b>2020</b> , 118, 698-707	2.9	5
72	How does evolution design functional free energy landscapes of proteins? A case study on the emergence of regulation in the Cyclin Dependent Kinase family. <i>Molecular Systems Design and Engineering</i> , <b>2020</b> , 5, 392-400	4.6	
71	Molecular Mechanism of Brassinosteroid Perception by the Plant Growth Receptor BRI1. <i>Journal of Physical Chemistry B</i> , <b>2020</b> , 124, 355-365	3.4	8
70	Divalent cations promote TALE DNA-binding specificity. <i>Nucleic Acids Research</i> , <b>2020</b> , 48, 1406-1422	20.1	3
69	Distinct Substrate Transport Mechanism Identified in Homologous Sugar Transporters. <i>Journal of Physical Chemistry B</i> , <b>2019</b> , 123, 8411-8418	3.4	10
68	Dewetting Controls Plant Hormone Perception and Initiation of Drought Resistance Signaling. <i>Structure</i> , <b>2019</b> , 27, 692-702.e3	5.2	22
67	Ion Gel Dynamic Templates for Large Modulation of Morphology and Charge Transport Properties of Solution-Coated Conjugated Polymer Thin Films. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2019</b> , 11, 22561-22574	9.5	10
66	Molecular Basis of the Glucose Transport Mechanism in Plants. <i>ACS Central Science</i> , <b>2019</b> , 5, 1085-1096	16.8	23
65	Dodine as a Kosmo-Chaotropic Agent. <i>Journal of Physical Chemistry Letters</i> , <b>2019</b> , 10, 2600-2605	6.4	5
64	Structural architecture of a dimeric class C GPCR based on co-trafficking of sweet taste receptor subunits. <i>Journal of Biological Chemistry</i> , <b>2019</b> , 294, 4759-4774	5.4	30
63	Universality of the Sodium Ion Binding Mechanism in Class A G-Protein-Coupled Receptors. <i>Angewandte Chemie - International Edition</i> , <b>2018</b> , 57, 3048-3053	16.4	31

62	Universality of the Sodium Ion Binding Mechanism in Class A G-Protein-Coupled Receptors. <i>Angewandte Chemie</i> , <b>2018</b> , 130, 3102-3107	3.6	11
61	Characterizing Conformational Dynamics of Proteins Using Evolutionary Couplings. <i>Journal of Physical Chemistry B</i> , <b>2018</b> , 122, 1017-1025	3.4	11
60	Recruiting machine learning methods for molecular simulations of proteins. <i>Molecular Simulation</i> , <b>2018</b> , 44, 891-904	2	21
59	Using molecular simulation to explore the nanoscale dynamics of the plant kinome. <i>Biochemical Journal</i> , <b>2018</b> , 475, 905-921	3.8	18
58	Reinforcement Learning Based Adaptive Sampling: REAPing Rewards by Exploring Protein Conformational Landscapes. <i>Journal of Physical Chemistry B</i> , <b>2018</b> , 122, 8386-8395	3.4	48
57	Automatic Feature Selection in Markov State Models Using Genetic Algorithm. <i>Journal of Computational Science Education</i> , <b>2018</b> , 9, 14-22	1.5	2
56	SAXS-guided Enhanced Unbiased Sampling for Structure Determination of Proteins and Complexes. <i>Scientific Reports</i> , <b>2018</b> , 8, 17748	4.9	11
55	Maximizing Kinetic Information Gain of Markov State Models for Optimal Design of Spectroscopy Experiments. <i>Journal of Physical Chemistry B</i> , <b>2018</b> , 122, 10793-10805	3.4	3
54	Free Energy Landscape of the Complete Transport Cycle in a Key Bacterial Transporter. <i>ACS Central Science</i> , <b>2018</b> , 4, 1146-1154	16.8	25
53	Application of Hidden Markov Models in Biomolecular Simulations. <i>Methods in Molecular Biology</i> , <b>2017</b> , 1552, 29-41	1.4	6
52	Machine Learning Guided Ligand-Protein Simulation Approach Elucidates the Binding Mechanism of Abscisic Acid. <i>Biophysical Journal</i> , <b>2017</b> , 112, 349a	2.9	2
51	Molecular dynamics simulations reveal the conformational dynamics of BRI1 and BAK1 receptor-like kinases. <i>Journal of Biological Chemistry</i> , <b>2017</b> , 292, 12643-12652	5.4	33
50	Understanding the Conformational Diversity of Proton-Coupled Oligopeptide Transporter (POT) Family. <i>Biophysical Journal</i> , <b>2017</b> , 112, 16a-17a	2.9	3
49	Enhanced unbiased sampling of protein dynamics using evolutionary coupling information. <i>Scientific Reports</i> , <b>2017</b> , 7, 12700	4.9	31
48	Predicting Optimal DEER Label Positions to Study Protein Conformational Heterogeneity. <i>Journal of Physical Chemistry B</i> , <b>2017</b> , 121, 9761-9770	3.4	12
47	Allosteric Control of a Plant Receptor Kinase through S-Glutathionylation. <i>Biophysical Journal</i> , <b>2017</b> , 113, 2354-2363	2.9	28
46	Dynamic-template-directed multiscale assembly for large-area coating of highly-aligned conjugated polymer thin films. <i>Nature Communications</i> , <b>2017</b> , 8, 16070	17.4	66
45	Crops : Generating Virtual Crops Using an Integrative and Multi-scale Modeling Platform. <i>Frontiers in Plant Science</i> , <b>2017</b> , 8, 786	6.2	61

44	Pricing policy for declining demand using item preservation technology. <i>SpringerPlus</i> , <b>2016</b> , 5, 1957		5
43	Conformational heterogeneity of the calmodulin binding interface. <i>Nature Communications</i> , <b>2016</b> , 7, 10910	17.4	38
42	Inventory model for convertible item with deterioration. <i>Communications in Statistics - Theory and Methods</i> , <b>2016</b> , 45, 1137-1147	0.5	3
41	Markov State Models and tICA Reveal a Nonnative Folding Nucleus in Simulations of NuG2. <i>Biophysical Journal</i> , <b>2016</b> , 110, 1716-1719	2.9	25
40	Transition path theory analysis of c-Src kinase activation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2016</b> , 113, 9193-8	11.5	49
39	Heat dissipation guides activation in signaling proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2015</b> , 112, 10377-82	11.5	21
38	Cloud computing approaches for prediction of ligand binding poses and pathways. <i>Scientific Reports</i> , <b>2015</b> , 5, 7918	4.9	37
37	A network of molecular switches controls the activation of the two-component response regulator NtrC. <i>Nature Communications</i> , <b>2015</b> , 6, 7283	17.4	38
36	Elucidating Ligand-Modulated Conformational Landscape of GPCRs Using Cloud-Computing Approaches. <i>Methods in Enzymology</i> , <b>2015</b> , 557, 551-72	1.7	11
35	Markov state models provide insights into dynamic modulation of protein function. <i>Accounts of Chemical Research</i> , <b>2015</b> , 48, 414-22	24.3	172
34	Conserve Water: A Method for the Analysis of Solvent in Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , <b>2015</b> , 11, 1094-101	6.4	10
33	Activation pathway of Src kinase reveals intermediate states as targets for drug design. <i>Nature Communications</i> , <b>2014</b> , 5, 3397	17.4	244
32	Cloud-based simulations on Google Exacycle reveal ligand modulation of GPCR activation pathways. <i>Nature Chemistry</i> , <b>2014</b> , 6, 15-21	17.6	306
31	Complex pathways in folding of protein G explored by simulation and experiment. <i>Biophysical Journal</i> , <b>2014</b> , 107, 947-55	2.9	34
30	Automatic Selection of Order Parameters in the Analysis of Large Scale Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 5217-5223	6.4	15
29	To milliseconds and beyond: challenges in the simulation of protein folding. <i>Current Opinion in Structural Biology</i> , <b>2013</b> , 23, 58-65	8.1	281
28	OpenMM 4: A Reusable, Extensible, Hardware Independent Library for High Performance Molecular Simulation. <i>Journal of Chemical Theory and Computation</i> , <b>2013</b> , 9, 461-469	6.4	440
27	Understanding the Role of Arginine and Citrate as Eluents in Affinity Chromatography. <i>ACS Symposium Series</i> , <b>2013</b> , 67-86	0.4	1

26	Arginine and the Hofmeister Series: the role of ion-ion interactions in protein aggregation suppression. <i>Journal of Physical Chemistry B</i> , <b>2011</b> , 115, 7447-58	3-4	99
25	Understanding the synergistic effect of arginine and glutamic acid mixtures on protein solubility. <i>Journal of Physical Chemistry B</i> , <b>2011</b> , 115, 11831-9	3-4	53
24	Preferential interaction coefficients of proteins in aqueous arginine solutions and their molecular origins. <i>Journal of Physical Chemistry B</i> , <b>2011</b> , 115, 1243-53	3-4	45
23	Complex interactions between molecular ions in solution and their effect on protein stability. <i>Journal of the American Chemical Society</i> , <b>2011</b> , 133, 18713-8	16.4	31
22	Effects of PAMAM Dendrimer Salt Solutions on Protein Stability. <i>Journal of Physical Chemistry Letters</i> , <b>2011</b> , 2, 1782-1788	6.4	13
21	Understanding the role of arginine as an eluent in affinity chromatography via molecular computations. <i>Journal of Physical Chemistry B</i> , <b>2011</b> , 115, 2645-54	3-4	36
20	Effects of solute-solute interactions on protein stability studied using various counterions and dendrimers. <i>PLoS ONE</i> , <b>2011</b> , 6, e27665	3-7	15
19	Molecular level insight into intra-solvent interaction effects on protein stability and aggregation. <i>Advanced Drug Delivery Reviews</i> , <b>2011</b> , 63, 1074-85	18.5	69
18	Interaction of arginine with proteins and the mechanism by which it inhibits aggregation. <i>Journal of Physical Chemistry B</i> , <b>2010</b> , 114, 13426-38	3-4	153
17	Molecular computations of preferential interaction coefficients of proteins. <i>Journal of Physical Chemistry B</i> , <b>2009</b> , 113, 12546-54	3-4	70
16	Modeling of formation of nanoparticles in reverse micellar systems: Ostwald ripening of silver halide particles. <i>Langmuir</i> , <b>2009</b> , 25, 3786-93	4	12
15	CaCO <sub>3</sub> nanoparticle synthesis by carbonation of lime solution in microemulsion systems. <i>Nanotechnology</i> , <b>2007</b> , 18, 035607	3-4	13
14	A model for particle coagulation in reverse micelles with a size dependent coagulation rate. <i>Nanotechnology</i> , <b>2006</b> , 17, 261-267	3-4	8
13	A Monte Carlo Model for the Formation of Core-Shell Nanocrystals in Reverse Micellar Systems. <i>Industrial &amp; Engineering Chemistry Research</i> , <b>2006</b> , 45, 2249-2254	3-9	12
12	Modeling shell formation in core-shell nanocrystals in reverse micelle systems. <i>Langmuir</i> , <b>2006</b> , 22, 9500-6		21
11	Coagulation of nanoparticles in reverse micellar systems: a Monte Carlo model. <i>Langmuir</i> , <b>2005</b> , 21, 11528-33		18
10	The Substrate Import Mechanism of the Human Serotonin Transporter		2
9	Structural Basis for Negative Regulation of ABA Signaling by ROP11 GTPase		2

8	TLmutation: predicting the effects of mutations using transfer learning	1
7	Role of substrate recognition in modulating strigolactone receptor selectivity in witchweed	2
6	Ancestral class-promiscuity as a driver of functional diversity in the BAHD acyltransferase family in plants	4
5	How do brassinosteroids activate their receptors?	4
4	Molecular Basis of the Activation and Dissociation of Dimeric PYL2 Receptor in Abscisic Acid Signaling	1
3	Deep Mutagenesis of a Transporter for Uptake of a Non-Native Substrate Identifies Conformationally Dynamic Regions	1
2	Activation Mechanism of Strigolactone Receptors And Its Impact On Ligand Selectivity Between Host And Parasitic Plants	1
1	Investigation of gating in outer membrane porins provides new perspectives on antibiotic resistance mechanisms	1