Gregory Bowman

List of Publications by Year
in descending order

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Version: 2024-02-01

70	7,752	76326	91884
papers	citations	40 h-index	69 g-index

91	91	91	7197
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A cryptic pocket in Ebola VP35 allosterically controls RNA binding. Nature Communications, 2022, 13, 2269.	12.8	19
2	The intrinsically disordered protein TgIST from Toxoplasma gondii inhibits STAT1 signaling by blocking cofactor recruitment. Nature Communications, 2022, 13, .	12.8	15
3	The SARS-CoV-2 nucleocapsid protein is dynamic, disordered, and phase separates with RNA. Nature Communications, 2021, 12, 1936.	12.8	334
4	SARS-CoV-2 simulations go exascale to predict dramatic spike opening and cryptic pockets across the proteome. Nature Chemistry, 2021, 13, 651-659.	13.6	190
5	Deep learning the structural determinants of protein biochemical properties by comparing structural ensembles with DiffNets. Nature Communications, 2021, 12, 3023.	12.8	42
6	SARS-CoV-2 Nsp16 activation mechanism and a cryptic pocket with pan-coronavirus antiviral potential. Biophysical Journal, 2021, 120, 2880-2889.	0.5	52
7	Naturally Occurring Genetic Variants in the Oxytocin Receptor Alter Receptor Signaling Profiles. ACS Pharmacology and Translational Science, 2021, 4, 1543-1555.	4.9	6
8	Editorial: Experiments and Simulations: A Pas de Deux to Unravel Biological Function. Frontiers in Molecular Biosciences, 2021, 8, 799406.	3.5	0
9	Opening of a cryptic pocket in Î²-lactamase increases penicillinase activity. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	17
10	The Cap-Snatching SFTSV Endonuclease Domain Is an Antiviral Target. Cell Reports, 2020, 30, 153-163.e5.	6.4	31
11	Computing and optimizing over all fixed-points of discrete systems on large networks. Journal of the Royal Society Interface, 2020, 17, 20200126.	3.4	1
12	Investigating Cryptic Binding Sites by Molecular Dynamics Simulations. Accounts of Chemical Research, 2020, 53, 654-661.	15.6	106
13	Spatial and temporal alterations in protein structure by EGF regulate cryptic cysteine oxidation. Science Signaling, 2020, 13, .	3.6	43
14	Antagonism between substitutions in Î²-lactamase explains a path not taken in the evolution of bacterial drug resistance. Journal of Biological Chemistry, 2020, 295, 7376-7390.	3.4	14
15	Conformational distributions of isolated myosin motor domains encode their mechanochemical properties. ELife, 2020, 9, .	6.0	28
16	Cooperative Changes in Solvent Exposure Identify Cryptic Pockets, Switches, and Allosteric Coupling. Biophysical Journal, 2019, 116, 818-830.	0.5	42
17	Enspara: Modeling molecular ensembles with scalable data structures and parallel computing. Journal of Chemical Physics, 2019, 150, 044108.	3.0	45
18	Advanced Methods for Accessing Protein Shape-Shifting Present New Therapeutic Opportunities. Trends in Biochemical Sciences, 2019, 44, 351-364.	7.5	34

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19	Electron Cryo-microscopy Structure of Ebola Virus Nucleoprotein Reveals a Mechanism for Nucleocapsid-like Assembly. Cell, 2018, 172, 966-978.e12.	28.9	51
20	Mechanistic Basis for ATP-Dependent Inhibition of Glutamine Synthetase by Tabtoxinine-Î²-lactam. Biochemistry, 2018, 57, 117-135.	2.5	8
21	Choice of Adaptive Sampling Strategy Impacts State Discovery, Transition Probabilities, and the Apparent Mechanism of Conformational Changes. Journal of Chemical Theory and Computation, 2018, 14, 5459-5475.	5.3	55
22	Simulation of spontaneous G protein activation reveals a new intermediate driving GDP unbinding. ELife, 2018, 7, .	6.0	39
23	Quantifying Allosteric Communication via Both Concerted Structural Changes and Conformational Disorder with CARDS. Journal of Chemical Theory and Computation, 2017, 13, 1509-1517.	5.3	46
24	Propagation of the Allosteric Modulation Induced by Sodium in the Î´â€Opioid Receptor. Chemistry - A European Journal, 2017, 23, 4615-4624.	3.3	20
25	Warfarin traps human vitamin K epoxide reductase in an intermediate state during electron transfer. Nature Structural and Molecular Biology, 2017, 24, 69-76.	8.2	59
26	Endogenous retinoid X receptor ligands in mouse hematopoietic cells. Science Signaling, 2017, 10, .	3.6	18
27	Prediction of New Stabilizing Mutations Based on Mechanistic Insights from Markov State Models. ACS Central Science, 2017, 3, 1311-1321.	11.3	55
28	Bladder-cancer-associated mutations in RXRA activate peroxisome proliferator-activated receptors to drive urothelial proliferation. ELife, 2017, 6, .	6.0	55
29	Designing small molecules to target cryptic pockets yields both positive and negative allosteric modulators. PLoS ONE, 2017, 12, e0178678.	2.5	53
30	Accurately modeling nanosecond protein dynamics requires at least microseconds of simulation. Journal of Computational Chemistry, 2016, 37, 558-566.	3.3	51
31	Structure and Dynamics of PD-L1 and an Ultra-High-Affinity PD-1 Receptor Mutant. Structure, 2016, 24, 1719-1728.	3.3	86
32	How to Run FAST Simulations. Methods in Enzymology, 2016, 578, 213-225.	1.0	11
33	Modelling proteinsâ€™ hidden conformations to predict antibiotic resistance. Nature Communications, 2016, 7, 12965.	12.8	113
34	Defining NADH-Driven Allostery Regulating Apoptosis-Inducing Factor. Structure, 2016, 24, 2067-2079.	3.3	39
35	Tabtoxinine-Î²-lactam is a â€œstealthâ€•Î²-lactam antibiotic that evades Î²-lactamase-mediated antibiotic resistance. MedChemComm, 2016, 7, 118-127.	3.4	14
36	FAST Conformational Searches by Balancing Exploration/Exploitation Trade-Offs. Journal of Chemical Theory and Computation, 2015, 11, 5747-5757.	5.3	135

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37	Fluctuations within Folded Proteins: Implications for Thermodynamic and Allosteric Regulation. Accounts of Chemical Research, 2015, 48, 1098-1105.	15.6	48
38	Discovery of multiple hidden allosteric sites by combining Markov state models and experiments. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 2734-2739.	7.1	183
39	Cloud-based simulations on Google Exacycle reveal ligand modulation of GPCR activation pathways. Nature Chemistry, 2014, 6, 15-21.	13.6	388
40	Extensive Conformational Heterogeneity within Protein Cores. Journal of Physical Chemistry B, 2014, 118, 6417-6423.	2.6	34
41	A Tutorial on Building Markov State Models with MSMBuilder and Coarse-Graining Them with BACE. Methods in Molecular Biology, 2014, 1084, 141-158.	0.9	13
42	Introduction and Overview of This Book. Advances in Experimental Medicine and Biology, 2014, 797, 1-6.	1.6	8
43	Software for Building Markov State Models. Advances in Experimental Medicine and Biology, 2014, 797, 139-139.	1.6	18
44	An Overview and Practical Guide to Building Markov State Models. Advances in Experimental Medicine and Biology, 2014, 797, 7-22.	1.6	23
45	Quantitative comparison of alternative methods for coarse-graining biological networks. Journal of Chemical Physics, 2013, 139, 121905.	3.0	49
46	Dynamics of an Intrinsically Disordered Protein Reveal Metastable Conformations That Potentially Seed Aggregation. Journal of the American Chemical Society, 2013, 135, 16092-16101.	13.7	160
47	Hierarchical NystrÃ¶m methods for constructing Markov state models for conformational dynamics. Journal of Chemical Physics, 2013, 138, 174106.	3.0	51
48	Improved coarse-graining of Markov state models via explicit consideration of statistical uncertainty. Journal of Chemical Physics, 2012, 137, 134111.	3.0	74
49	Mechanistic and structural insight into the functional dichotomy between IL-2 and IL-15. Nature Immunology, 2012, 13, 1187-1195.	14.5	206
50	Equilibrium fluctuations of a single folded protein reveal a multitude of potential cryptic allosteric sites. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 11681-11686.	7.1	234
51	Exploiting a natural conformational switch to engineer an interleukin-2 â€˜superkineâ€™. Nature, 2012, 484, 529-533.	27.8	438
52	Investigating How Peptide Length and a Pathogenic Mutation Modify the Structural Ensemble of Amyloid Beta Monomer. Biophysical Journal, 2012, 102, 315-324.	0.5	114
53	Slow Unfolded-State Structuring in Acyl-CoA Binding Protein Folding Revealed by Simulation and Experiment. Journal of the American Chemical Society, 2012, 134, 12565-12577.	13.7	132
54	Atomistic Folding Simulations of the Five-Helix Bundle Protein Î»_{6â˜85}. Journal of the American Chemical Society, 2011, 133, 664-667.	13.7	137

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55	Markov State Model Reveals Folding and Functional Dynamics in Ultra-Long MD Trajectories. Journal of the American Chemical Society, 2011, 133, 18413-18419.	13.7	150
56	MSMBuilder2: Modeling Conformational Dynamics on the Picosecond to Millisecond Scale. Journal of Chemical Theory and Computation, 2011, 7, 3412-3419.	5.3	381
57	Taming the complexity of protein folding. Current Opinion in Structural Biology, 2011, 21, 4-11.	5.7	156
58	A Role for Both Conformational Selection and Induced Fit in Ligand Binding by the LAO Protein. PLoS Computational Biology, 2011, 7, e1002054.	3.2	201
59	Molecular Simulation of ab Initio Protein Folding for a Millisecond Folder NTL9(1â˜39). Journal of the American Chemical Society, 2010, 132, 1526-1528.	13.7	473
60	Protein folded states are kinetic hubs. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 10890-10895.	7.1	207
61	Network models for molecular kinetics and their initial applications to human health. Cell Research, 2010, 20, 622-630.	12.0	55
62	Everything you wanted to know about Markov State Models but were afraid to ask. Methods, 2010, 52, 99-105.	3.8	591
63	Enhanced Modeling via Network Theory: Adaptive Sampling of Markov State Models. Journal of Chemical Theory and Computation, 2010, 6, 787-794.	5.3	208
64	CONSTRUCTING MULTI-RESOLUTION MARKOV STATE MODELS (MSMS) TO ELUCIDATE RNA HAIRPIN FOLDING MECHANISMS. , 2009, , 228-239.		38
65	Progress and challenges in the automated construction of Markov state models for full protein systems. Journal of Chemical Physics, 2009, 131, 124101.	3.0	346
66	Simulated tempering yields insight into the lowâ€resolution Rosetta scoring functions. Proteins: Structure, Function and Bioinformatics, 2009, 74, 777-788.	2.6	25
67	Using generalized ensemble simulations and Markov state models to identify conformational states. Methods, 2009, 49, 197-201.	3.8	272
68	Rapid equilibrium sampling initiated from nonequilibrium data. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 19765-19769.	7.1	148
69	The Roles of Entropy and Kinetics in Structure Prediction. PLoS ONE, 2009, 4, e5840.	2.5	8
70	Structural Insight into RNA Hairpin Folding Intermediates. Journal of the American Chemical Society, 2008, 130, 9676-9678.	13.7	94