

Gregory Bowman

List of Publications by Year in descending order

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Version: 2024-02-01

70
papers

7,752
citations

76326

40
h-index

91884

69
g-index

91
all docs

91
docs citations

91
times ranked

7197
citing authors

#	ARTICLE	IF	CITATIONS
1	Everything you wanted to know about Markov State Models but were afraid to ask. <i>Methods</i> , 2010, 52, 99-105.	3.8	591
2	Molecular Simulation of <i>ab Initio</i> Protein Folding for a Millisecond Folder NTL9(1 ^{âˆ’39}). <i>Journal of the American Chemical Society</i> , 2010, 132, 1526-1528.	13.7	473
3	Exploiting a natural conformational switch to engineer an interleukin-2 <i>â€</i> superkine ^{â€} ™. <i>Nature</i> , 2012, 484, 529-533.	27.8	438
4	Cloud-based simulations on Google Exacycle reveal ligand modulation of GPCR activation pathways. <i>Nature Chemistry</i> , 2014, 6, 15-21.	13.6	388
5	MSMBuilder2: Modeling Conformational Dynamics on the Picosecond to Millisecond Scale. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3412-3419.	5.3	381
6	Progress and challenges in the automated construction of Markov state models for full protein systems. <i>Journal of Chemical Physics</i> , 2009, 131, 124101.	3.0	346
7	The SARS-CoV-2 nucleocapsid protein is dynamic, disordered, and phase separates with RNA. <i>Nature Communications</i> , 2021, 12, 1936.	12.8	334
8	Using generalized ensemble simulations and Markov state models to identify conformational states. <i>Methods</i> , 2009, 49, 197-201.	3.8	272
9	Equilibrium fluctuations of a single folded protein reveal a multitude of potential cryptic allosteric sites. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2012, 109, 11681-11686.	7.1	234
10	Enhanced Modeling via Network Theory: Adaptive Sampling of Markov State Models. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 787-794.	5.3	208
11	Protein folded states are kinetic hubs. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 10890-10895.	7.1	207
12	Mechanistic and structural insight into the functional dichotomy between IL-2 and IL-15. <i>Nature Immunology</i> , 2012, 13, 1187-1195.	14.5	206
13	A Role for Both Conformational Selection and Induced Fit in Ligand Binding by the LAO Protein. <i>PLoS Computational Biology</i> , 2011, 7, e1002054.	3.2	201
14	SARS-CoV-2 simulations go exascale to predict dramatic spike opening and cryptic pockets across the proteome. <i>Nature Chemistry</i> , 2021, 13, 651-659.	13.6	190
15	Discovery of multiple hidden allosteric sites by combining Markov state models and experiments. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 2734-2739.	7.1	183
16	Dynamics of an Intrinsically Disordered Protein Reveal Metastable Conformations That Potentially Seed Aggregation. <i>Journal of the American Chemical Society</i> , 2013, 135, 16092-16101.	13.7	160
17	Taming the complexity of protein folding. <i>Current Opinion in Structural Biology</i> , 2011, 21, 4-11.	5.7	156
18	Markov State Model Reveals Folding and Functional Dynamics in Ultra-Long MD Trajectories. <i>Journal of the American Chemical Society</i> , 2011, 133, 18413-18419.	13.7	150

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19	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
20	Atomistic Folding Simulations of the Five-Helix Bundle Protein $\hat{\nu}$ 85. Journal of the American Chemical Society, 2011, 133, 664-667.	13.7	137
21	FAST Conformational Searches by Balancing Exploration/Exploitation Trade-Offs. Journal of Chemical Theory and Computation, 2015, 11, 5747-5757.	5.3	135
22	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
23	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
24	Modelling proteins' hidden conformations to predict antibiotic resistance. Nature Communications, 2016, 7, 12965.	12.8	113
25	Investigating Cryptic Binding Sites by Molecular Dynamics Simulations. Accounts of Chemical Research, 2020, 53, 654-661.	15.6	106
26	Structural Insight into RNA Hairpin Folding Intermediates. Journal of the American Chemical Society, 2008, 130, 9676-9678.	13.7	94
27	Structure and Dynamics of PD-L1 and an Ultra-High-Affinity PD-1 Receptor Mutant. Structure, 2016, 24, 1719-1728.	3.3	86
28	Improved coarse-graining of Markov state models via explicit consideration of statistical uncertainty. Journal of Chemical Physics, 2012, 137, 134111.	3.0	74
29	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
30	Network models for molecular kinetics and their initial applications to human health. Cell Research, 2010, 20, 622-630.	12.0	55
31	Prediction of New Stabilizing Mutations Based on Mechanistic Insights from Markov State Models. ACS Central Science, 2017, 3, 1311-1321.	11.3	55
32	Bladder-cancer-associated mutations in RXRA activate peroxisome proliferator-activated receptors to drive urothelial proliferation. ELife, 2017, 6, .	6.0	55
33	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
34	Designing small molecules to target cryptic pockets yields both positive and negative allosteric modulators. PLoS ONE, 2017, 12, e0178678.	2.5	53
35	SARS-CoV-2 Nsp16 activation mechanism and a cryptic pocket with pan-coronavirus antiviral potential. Biophysical Journal, 2021, 120, 2880-2889.	0.5	52
36	Hierarchical Nyström methods for constructing Markov state models for conformational dynamics. Journal of Chemical Physics, 2013, 138, 174106.	3.0	51

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37	Accurately modeling nanosecond protein dynamics requires at least microseconds of simulation. <i>Journal of Computational Chemistry</i> , 2016, 37, 558-566.	3.3	51
38	Electron Cryo-microscopy Structure of Ebola Virus Nucleoprotein Reveals a Mechanism for Nucleocapsid-like Assembly. <i>Cell</i> , 2018, 172, 966-978.e12.	28.9	51
39	Quantitative comparison of alternative methods for coarse-graining biological networks. <i>Journal of Chemical Physics</i> , 2013, 139, 121905.	3.0	49
40	Fluctuations within Folded Proteins: Implications for Thermodynamic and Allosteric Regulation. <i>Accounts of Chemical Research</i> , 2015, 48, 1098-1105.	15.6	48
41	Quantifying Allosteric Communication via Both Concerted Structural Changes and Conformational Disorder with CARDS. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1509-1517.	5.3	46
42	Enspara: Modeling molecular ensembles with scalable data structures and parallel computing. <i>Journal of Chemical Physics</i> , 2019, 150, 044108.	3.0	45
43	Spatial and temporal alterations in protein structure by EGF regulate cryptic cysteine oxidation. <i>Science Signaling</i> , 2020, 13, .	3.6	43
44	Cooperative Changes in Solvent Exposure Identify Cryptic Pockets, Switches, and Allosteric Coupling. <i>Biophysical Journal</i> , 2019, 116, 818-830.	0.5	42
45	Deep learning the structural determinants of protein biochemical properties by comparing structural ensembles with DiffNets. <i>Nature Communications</i> , 2021, 12, 3023.	12.8	42
46	Defining NADH-Driven Allostery Regulating Apoptosis-Inducing Factor. <i>Structure</i> , 2016, 24, 2067-2079.	3.3	39
47	Simulation of spontaneous G protein activation reveals a new intermediate driving GDP unbinding. <i>ELife</i> , 2018, 7, .	6.0	39
48	CONSTRUCTING MULTI-RESOLUTION MARKOV STATE MODELS (MSMS) TO ELUCIDATE RNA HAIRPIN FOLDING MECHANISMS. , 2009, , 228-239.		38
49	Extensive Conformational Heterogeneity within Protein Cores. <i>Journal of Physical Chemistry B</i> , 2014, 118, 6417-6423.	2.6	34
50	Advanced Methods for Accessing Protein Shape-Shifting Present New Therapeutic Opportunities. <i>Trends in Biochemical Sciences</i> , 2019, 44, 351-364.	7.5	34
51	The Cap-Snatching SFTSV Endonuclease Domain Is an Antiviral Target. <i>Cell Reports</i> , 2020, 30, 153-163.e5.	6.4	31
52	Conformational distributions of isolated myosin motor domains encode their mechanochemical properties. <i>ELife</i> , 2020, 9, .	6.0	28
53	Simulated tempering yields insight into the low-resolution Rosetta scoring functions. <i>Proteins: Structure, Function and Bioinformatics</i> , 2009, 74, 777-788.	2.6	25
54	An Overview and Practical Guide to Building Markov State Models. <i>Advances in Experimental Medicine and Biology</i> , 2014, 797, 7-22.	1.6	23

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55	Propagation of the Allosteric Modulation Induced by Sodium in the μ -Opioid Receptor. <i>Chemistry - A European Journal</i> , 2017, 23, 4615-4624.	3.3	20
56	A cryptic pocket in Ebola VP35 allosterically controls RNA binding. <i>Nature Communications</i> , 2022, 13, 2269.	12.8	19
57	Endogenous retinoid X receptor ligands in mouse hematopoietic cells. <i>Science Signaling</i> , 2017, 10, .	3.6	18
58	Software for Building Markov State Models. <i>Advances in Experimental Medicine and Biology</i> , 2014, 797, 139-139.	1.6	18
59	Opening of a cryptic pocket in β -lactamase increases penicillinase activity. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	7.1	17
60	The intrinsically disordered protein TgIST from <i>Toxoplasma gondii</i> inhibits STAT1 signaling by blocking cofactor recruitment. <i>Nature Communications</i> , 2022, 13, .	12.8	15
61	Tabtoxinine- β -lactam is a "stealth" β -lactam antibiotic that evades β -lactamase-mediated antibiotic resistance. <i>MedChemComm</i> , 2016, 7, 118-127.	3.4	14
62	Antagonism between substitutions in β -lactamase explains a path not taken in the evolution of bacterial drug resistance. <i>Journal of Biological Chemistry</i> , 2020, 295, 7376-7390.	3.4	14
63	A Tutorial on Building Markov State Models with MSMBuilder and Coarse-Graining Them with BACE. <i>Methods in Molecular Biology</i> , 2014, 1084, 141-158.	0.9	13
64	How to Run FAST Simulations. <i>Methods in Enzymology</i> , 2016, 578, 213-225.	1.0	11
65	Mechanistic Basis for ATP-Dependent Inhibition of Glutamine Synthetase by Tabtoxinine- β -lactam. <i>Biochemistry</i> , 2018, 57, 117-135.	2.5	8
66	Introduction and Overview of This Book. <i>Advances in Experimental Medicine and Biology</i> , 2014, 797, 1-6.	1.6	8
67	The Roles of Entropy and Kinetics in Structure Prediction. <i>PLoS ONE</i> , 2009, 4, e5840.	2.5	8
68	Naturally Occurring Genetic Variants in the Oxytocin Receptor Alter Receptor Signaling Profiles. <i>ACS Pharmacology and Translational Science</i> , 2021, 4, 1543-1555.	4.9	6
69	Computing and optimizing over all fixed-points of discrete systems on large networks. <i>Journal of the Royal Society Interface</i> , 2020, 17, 20200126.	3.4	1
70	Editorial: Experiments and Simulations: A Pas de Deux to Unravel Biological Function. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 799406.	3.5	0