

James C Gumbart

List of Publications by Year in descending order

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111
papers

21,616
citations

76326

40
h-index

25787

108
g-index

125
all docs

125
docs citations

125
times ranked

25597
citing authors

#	ARTICLE	IF	CITATIONS
1	Scalable molecular dynamics with NAMD. <i>Journal of Computational Chemistry</i> , 2005, 26, 1781-1802.	3.3	15,208
2	Rapid parameterization of small molecules using the force field toolkit. <i>Journal of Computational Chemistry</i> , 2013, 34, 2757-2770.	3.3	403
3	Structural insight into the biogenesis of β -barrel membrane proteins. <i>Nature</i> , 2013, 501, 385-390.	27.8	368
4	The Adaptive Biasing Force Method: Everything You Always Wanted To Know but Were Afraid To Ask. <i>Journal of Physical Chemistry B</i> , 2015, 119, 1129-1151.	2.6	351
5	Standard Binding Free Energies from Computer Simulations: What Is the Best Strategy?. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 794-802.	5.3	298
6	Cryo-EM structure of the ribosomeâ€‘SecYE complex in the membrane environment. <i>Nature Structural and Molecular Biology</i> , 2011, 18, 614-621.	8.2	264
7	Structure of Monomeric Yeast and Mammalian Sec61 Complexes Interacting with the Translating Ribosome. <i>Science</i> , 2009, 326, 1369-1373.	12.6	263
8	Structural basis for iron piracy by pathogenic <i>Neisseria</i> . <i>Nature</i> , 2012, 483, 53-58.	27.8	239
9	Efficient Determination of Proteinâ€‘Protein Standard Binding Free Energies from First Principles. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3789-3798.	5.3	188
10	Simulation-Based Approaches for Determining Membrane Permeability of Small Compounds. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 721-733.	5.4	174
11	The β -barrel assembly machinery in motion. <i>Nature Reviews Microbiology</i> , 2017, 15, 197-204.	28.6	174
12	Lateral Opening and Exit Pore Formation Are Required for BamA Function. <i>Structure</i> , 2014, 22, 1055-1062.	3.3	166
13	Structure of the SecY channel during initiation of protein translocation. <i>Nature</i> , 2014, 506, 102-106.	27.8	138
14	Supercomputer-Based Ensemble Docking Drug Discovery Pipeline with Application to Covid-19. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 5832-5852.	5.4	134
15	Architecture and assembly of the σ^70 -positive cell wall. <i>Molecular Microbiology</i> , 2013, 88, 664-672.	2.5	116
16	Generalized scalable multiple copy algorithms for molecular dynamics simulations in NAMD. <i>Computer Physics Communications</i> , 2014, 185, 908-916.	7.5	115
17	Structural and Functional Characterization of the LPS Transporter LptDE from Gram-Negative Pathogens. <i>Structure</i> , 2016, 24, 965-976.	3.3	110
18	Regulation of the Protein-Conducting Channel by a Bound Ribosome. <i>Structure</i> , 2009, 17, 1453-1464.	3.3	107

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19	Mechanics of Force Propagation in TonB-Dependent Outer Membrane Transport. <i>Biophysical Journal</i> , 2007, 93, 496-504.	0.5	98
20	Escherichia coli Peptidoglycan Structure and Mechanics as Predicted by Atomic-Scale Simulations. <i>PLoS Computational Biology</i> , 2014, 10, e1003475.	3.2	92
21	Comprehensive structure and functional adaptations of the yeast nuclear pore complex. <i>Cell</i> , 2022, 185, 361-378.e25.	28.9	87
22	Accelerating Membrane Simulations with Hydrogen Mass Repartitioning. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4673-4686.	5.3	85
23	Mechanisms of SecM-Mediated Stalling in the Ribosome. <i>Biophysical Journal</i> , 2012, 103, 331-341.	0.5	82
24	Molecular Dynamics Studies of the Archaeal Translocon. <i>Biophysical Journal</i> , 2006, 90, 2356-2367.	0.5	78
25	Free-energy cost for translocon-assisted insertion of membrane proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 3596-3601.	7.1	74
26	Intrinsic Curvature Properties of Photosynthetic Proteins in Chromatophores. <i>Biophysical Journal</i> , 2008, 95, 2822-2836.	0.5	73
27	Protein-Induced Membrane Curvature Investigated through Molecular Dynamics Flexible Fitting. <i>Biophysical Journal</i> , 2009, 97, 321-329.	0.5	68
28	Symmetry-Restrained Flexible Fitting for Symmetric EM Maps. <i>Structure</i> , 2011, 19, 1211-1218.	3.3	66
29	Distribution of mechanical stress in the Escherichia coli cell envelope. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2018, 1860, 2566-2575.	2.6	66
30	A novel human <i>IL2RB</i> mutation results in T and NK cell-driven immune dysregulation. <i>Journal of Experimental Medicine</i> , 2019, 216, 1255-1267.	8.5	64
31	Structural Determinants of Lateral Gate Opening in the Protein Translocon. <i>Biochemistry</i> , 2007, 46, 11147-11157.	2.5	59
32	The mobility of two kinase domains in the <i>Escherichia coli</i> chemoreceptor array varies with signalling state. <i>Molecular Microbiology</i> , 2013, 89, 831-841.	2.5	59
33	Accurate determination of protein:ligand standard binding free energies from molecular dynamics simulations. <i>Nature Protocols</i> , 2022, 17, 1114-1141.	12.0	56
34	Molecular dynamics simulations of membrane proteins under asymmetric ionic concentrations. <i>Journal of General Physiology</i> , 2013, 142, 465-475.	1.9	51
35	BFE: A User-Friendly Graphical Interface Facilitating Absolute Binding Free-Energy Calculations. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 556-560.	5.4	51
36	Coarse-grained simulations of bacterial cell wall growth reveal that local coordination alone can be sufficient to maintain rod shape. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, E3689-98.	7.1	50

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37	Determination of Membrane-Insertion Free Energies by Molecular Dynamics Simulations. Biophysical Journal, 2012, 102, 795-801.	0.5	49
38	Outer membrane protein size and LPS O-antigen define protective antibody targeting to the Salmonella surface. Nature Communications, 2020, 11, 851.	12.8	49
39	Role of the Native Outer-Membrane Environment on the Transporter BtuB. Biophysical Journal, 2016, 111, 1409-1417.	0.5	48
40	Inhibitor binding influences the protonation states of histidines in SARS-CoV-2 main protease. Chemical Science, 2021, 12, 1513-1527.	7.4	47
41	β^2 -Barrel proteins tether the outer membrane in many Gram-negative bacteria. Nature Microbiology, 2021, 6, 19-26.	13.3	46
42	Applications of the molecular dynamics flexible fitting method. Journal of Structural Biology, 2011, 173, 420-427.	2.8	44
43	Thermodynamics of Deca-alanine Folding in Water. Journal of Chemical Theory and Computation, 2014, 10, 2836-2844.	5.3	44
44	Machine Learning Reveals the Critical Interactions for SARS-CoV-2 Spike Protein Binding to ACE2. Journal of Physical Chemistry Letters, 2021, 12, 5494-5502.	4.6	44
45	Stepwise gating of the Sec61 protein-conducting channel by Sec63 and Sec62. Nature Structural and Molecular Biology, 2021, 28, 162-172.	8.2	43
46	C-terminal kink formation is required for lateral gating in BamA. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E7942-E7949.	7.1	42
47	Reconciling the Roles of Kinetic and Thermodynamic Factors in Membrane Protein Insertion. Journal of the American Chemical Society, 2013, 135, 2291-2297.	13.7	41
48	Molecular Basis for the Activation of a Catalytic Asparagine Residue in a Self-Cleaving Bacterial Autotransporter. Journal of Molecular Biology, 2012, 415, 128-142.	4.2	40
49	Transitions of Double-Stranded DNA Between the A- and B-Forms. Journal of Physical Chemistry B, 2016, 120, 8449-8456.	2.6	38
50	Living on the edge: Simulations of bacterial outer-membrane proteins. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1753-1759.	2.6	37
51	The Roles of Pore Ring and Plug in the SecY Protein-conducting Channel. Journal of General Physiology, 2008, 132, 709-719.	1.9	36
52	Free Energy of Nascent-Chain Folding in the Translocon. Journal of the American Chemical Society, 2011, 133, 7602-7607.	13.7	36
53	Transmembrane but not soluble helices fold inside the ribosome tunnel. Nature Communications, 2018, 9, 5246.	12.8	36
54	Plasticity within the barrel domain of BamA mediates a hybrid-barrel mechanism by BAM. Nature Communications, 2021, 12, 7131.	12.8	34

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55	Coupling of Calcium and Substrate Binding through Loop Alignment in the Outer-Membrane Transporter BtuB. <i>Journal of Molecular Biology</i> , 2009, 393, 1129-1142.	4.2	30
56	Structural basis for substrate selection by the translocation and assembly module of the β -barrel assembly machinery. <i>Molecular Microbiology</i> , 2017, 106, 142-156.	2.5	29
57	Membrane Curvature Induced by Aggregates of LH2s and Monomeric LH1s. <i>Biophysical Journal</i> , 2009, 97, 2978-2984.	0.5	28
58	Folding free energy landscapes of α -sheets with non-polarizable and polarizable CHARMM force fields. <i>Journal of Chemical Physics</i> , 2018, 149, 072317.	3.0	28
59	Identification of Binding Sites for Efflux Pump Inhibitors of the AcrAB-TolC Component AcrA. <i>Biophysical Journal</i> , 2019, 116, 648-658.	0.5	27
60	Conformational Changes of the Clamp of the Protein Translocation ATPase SecA. <i>Journal of Molecular Biology</i> , 2015, 427, 2348-2359.	4.2	26
61	Structure and Misfolding of the Flexible Tripartite Coiled-Coil Domain of Glaucoma-Associated Myocilin. <i>Structure</i> , 2017, 25, 1697-1707.e5.	3.3	26
62	ACE2 glycans preferentially interact with SARS-CoV-2 over SARS-CoV. <i>Chemical Communications</i> , 2021, 57, 5949-5952.	4.1	26
63	Fatal arrhythmias: Another reason why doctors remain cautious about chloroquine/hydroxychloroquine for treating COVID-19. <i>Heart Rhythm</i> , 2020, 17, 1445-1451.	0.7	25
64	Bifunctional Janus Particles as Multivalent Synthetic Nanoparticle Antibodies (SNABs) for Selective Depletion of Target Cells. <i>Nano Letters</i> , 2021, 21, 875-886.	9.1	24
65	Self-Assembly of Photosynthetic Membranes. <i>ChemPhysChem</i> , 2010, 11, 1154-1159.	2.1	23
66	Computed Free Energies of Peptide Insertion into Bilayers are Independent of Computational Method. <i>Journal of Membrane Biology</i> , 2018, 251, 345-356.	2.1	22
67	Exploring adsorption of neutral aromatic pollutants onto graphene nanomaterials via molecular dynamics simulations and theoretical linear solvation energy relationships. <i>Environmental Science: Nano</i> , 2018, 5, 2117-2128.	4.3	22
68	Membrane thinning and lateral gating are consistent features of BamA across multiple species. <i>PLoS Computational Biology</i> , 2020, 16, e1008355.	3.2	22
69	Conformational Dynamics of AcrA Govern Multidrug Efflux Pump Assembly. <i>ACS Infectious Diseases</i> , 2019, 5, 1926-1935.	3.8	21
70	Development of CHARMM-Compatible Force-Field Parameters for Cobalamin and Related Cofactors from Quantum Mechanical Calculations. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 784-798.	5.3	20
71	Non-detergent isolation of a cyanobacterial photosystem I using styrene maleic acid alternating copolymers. <i>RSC Advances</i> , 2019, 9, 31781-31796.	3.6	19
72	Tuning Proton Transfer Thermodynamics in SARS-CoV-2 Main Protease: Implications for Catalysis and Inhibitor Design. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 4195-4202.	4.6	19

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73	The Effect of (â²)-Epigallocatechin-3-Gallate on the Amyloid-Î² Secondary Structure. Biophysical Journal, 2020, 119, 349-359.	0.5	18
74	Presence of substrate aids lateral gate separation in LptD. Biochimica Et Biophysica Acta - Biomembranes, 2020, 1862, 183025.	2.6	17
75	Adaptation of the periplasm to maintain spatial constraints essential for cell envelope processes and cell viability. ELife, 2022, 11, .	6.0	17
76	Quantifying arrhythmic long QT effects of hydroxychloroquine and azithromycin with whole-heart optical mapping and simulations. Heart Rhythm O2, 2021, 2, 394-404.	1.7	16
77	Parametrization of macrolide antibiotics using the force field toolkit. Journal of Computational Chemistry, 2015, 36, 2052-2063.	3.3	15
78	Decrypting protein insertion through the translocon with free-energy calculations. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1663-1671.	2.6	15
79	Redox-Driven Conformational Dynamics in a Photosystem-II-Inspired Î²-Hairpin Maquette Determined through Spectroscopy and Simulation. Journal of Physical Chemistry B, 2017, 121, 3536-3545.	2.6	15
80	Structural insight into toxin secretion by contact-dependent growth inhibition transporters. ELife, 2020, 9, .	6.0	14
81	Structural and biophysical characterization of an epitope-specific engineered Fab fragment and complexation with membrane proteins: implications for co-crystallization. Acta Crystallographica Section D: Biological Crystallography, 2015, 71, 896-906.	2.5	13
82	Stable calcium-free myocilin olfactomedin domain variants reveal challenges in differentiating between benign and glaucoma-causing mutations. Journal of Biological Chemistry, 2019, 294, 12717-12728.	3.4	13
83	Lpp positions peptidoglycan at the AcrA-TolC interface in the AcrAB-TolC multidrug efflux pump. Biophysical Journal, 2021, 120, 3973-3982.	0.5	13
84	Parameterization of a drug molecule with a halogen ïf-hole particle using ffTK: Implementation, testing, and comparison. Journal of Chemical Physics, 2020, 153, 164104.	3.0	11
85	DNA Scrunching in the Packaging of Viral Genomes. Journal of Physical Chemistry B, 2016, 120, 6200-6207.	2.6	10
86	Toward the rational design of macrolide antibiotics to combat resistance. Chemical Biology and Drug Design, 2017, 90, 641-652.	3.2	10
87	BamA is required for autotransporter secretion. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129581.	2.4	10
88	Gatekeeping Ketosynthases Dictate Initiation of Assembly Line Biosynthesis of Pyrrolic Polyketides. Journal of the American Chemical Society, 2021, 143, 7617-7622.	13.7	10
89	Restoring and Enhancing the Potency of Existing Antibiotics against Drug-Resistant Gram-Negative Bacteria through the Development of Potent Small-Molecule Adjuvants. ACS Infectious Diseases, 2022, 8, 1491-1508.	3.8	10
90	Tyrosine, cysteine, and proton coupled electron transfer in a ribonucleotide reductase-inspired beta hairpin maquette. Chemical Communications, 2019, 55, 9399-9402.	4.1	9

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91	Synergistic Biophysical Techniques Reveal Structural Mechanisms of Engineered Cationic Antimicrobial Peptides in Lipid Model Membranes. <i>Chemistry - A European Journal</i> , 2020, 26, 6247-6256.	3.3	9
92	Preparing Membrane Proteins for Simulation Using CHARMM-GUI. <i>Methods in Molecular Biology</i> , 2021, 2302, 237-251.	0.9	9
93	The Mechanism of Action of Hepatitis B Virus Capsid Assembly Modulators Can Be Predicted from Binding to Early Assembly Intermediates. <i>Journal of Medicinal Chemistry</i> , 2022, 65, 4854-4864.	6.4	8
94	Inward-facing glycine residues create sharp turns in β^2 -barrel membrane proteins. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2021, 1863, 183662.	2.6	7
95	IcmQ in the Type 4b Secretion System Contains an NAD ⁺ Binding Domain. <i>Structure</i> , 2013, 21, 1361-1373.	3.3	6
96	Structure and Function of Tryptophan-Tyrosine Dyads in Biomimetic β^2 Hairpins. <i>Journal of Physical Chemistry B</i> , 2019, 123, 2780-2791.	2.6	6
97	Molecular Machinery Responsible for Graphene Oxide's Distinct Inhibitory Effects toward <i>Pseudomonas aeruginosa</i> and <i>Staphylococcus aureus</i> Pathogens. <i>ACS Applied Bio Materials</i> , 2021, 4, 660-668.	4.6	6
98	Accelerating the use of molecular modeling in the high school classroom with VMD Lite. <i>Biochemistry and Molecular Biology Education</i> , 2016, 44, 124-129.	1.2	5
99	A Minimal Membrane Metal Transport System: Dynamics and Energetics of <i>mer</i> Proteins. <i>Journal of Computational Chemistry</i> , 2020, 41, 528-537.	3.3	5
100	Coarse-Grained Simulations of DNA Reveal Angular Dependence of Sticky-End Binding. <i>Journal of Physical Chemistry B</i> , 2021, 125, 4016-4024.	2.6	5
101	Folding and Insertion of Transmembrane Helices at the ER. <i>International Journal of Molecular Sciences</i> , 2021, 22, 12778.	4.1	5
102	Resolving the Hydride Transfer Pathway in Oxidative Conversion of Proline to Pyrrole. <i>Biochemistry</i> , 2022, 61, 206-215.	2.5	5
103	ATP-Dependent Signaling in Simulations of a Revised Model of Cystic Fibrosis Transmembrane Conductance Regulator (CFTR). <i>Journal of Physical Chemistry B</i> , 2019, 123, 3177-3188.	2.6	4
104	Combinatorial phosphorylation modulates the structure and function of the G protein β^3 subunit in yeast. <i>Science Signaling</i> , 2021, 14, .	3.6	4
105	Membrane proteins: Where theory meets experiment. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2016, 1858, 1553-1555.	2.6	3
106	Coarse-Grained Molecular Dynamics Simulations of the Bacterial Cell Wall. <i>Methods in Molecular Biology</i> , 2016, 1440, 247-270.	0.9	3
107	Joint neutron/molecular dynamics vibrational spectroscopy reveals softening of HIV-1 protease upon binding of a tight inhibitor. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 3586-3597.	2.8	3
108	The Role of Extracellular Loops in the Folding of Outer Membrane Protein X (OmpX) of <i>Escherichia coli</i> . <i>Frontiers in Molecular Biosciences</i> , 0, 9, .	3.5	3

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109	Producing membrane proteins one simulation at a time. Journal of Biological Chemistry, 2017, 292, 19546-19547.	3.4	1
110	Diverse Protein-Folding Pathways and Functions of β^2 -Hairpins and β^2 -Sheets. , 2018, , 1-20.		0
111	A Novel Approach to Simulating the Gating Transitions of Mechanosensitive Channels. Biophysical Journal, 2021, 120, 185-186.	0.5	0