James C Gumbart

List of Publications by Year in Descending Order

107 papers	17,252 citations	35 h-index	125 g-index
125 ext. papers	19,966 ext. citations	7.7 avg, IF	6.27 L-index

#	Paper	IF	Citations
107	Accurate determination of protein:ligand standard binding free energies from molecular dynamics simulations.. *Nature Protocols*, **2022**,	18.8	5
106	Comprehensive structure and functional adaptations of the yeast nuclear pore complex.. *Cell*, **2021**,	56.2	18
105	Folding and Insertion of Transmembrane Helices at the ER. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	1
104	Coarse-Grained Simulations of DNA Reveal Angular Dependence of Sticky-End Binding. *Journal of Physical Chemistry B*, **2021**, 125, 4016-4024	3.4	1
103	Tuning Proton Transfer Thermodynamics in SARS-CoV-2 Main Protease: Implications for Catalysis and Inhibitor Design. *Journal of Physical Chemistry Letters*, **2021**, 12, 4195-4202	6.4	11
102	Gatekeeping Ketosynthases Dictate Initiation of Assembly Line Biosynthesis of Pyrrolic Polyketides. *Journal of the American Chemical Society*, **2021**, 143, 7617-7622	16.4	2
101	Machine Learning Reveals the Critical Interactions for SARS-CoV-2 Spike Protein Binding to ACE2. *Journal of Physical Chemistry Letters*, **2021**, 12, 5494-5502	6.4	14
100	Barrel proteins tether the outer membrane in many Gram-negative bacteria. *Nature Microbiology*, **2021**, 6, 19-26	26.6	23
99	A Novel Approach to Simulating the Gating Transitions of Mechanosensitive Channels. *Biophysical Journal*, **2021**, 120, 185-186	2.9	
98	Molecular Machinery Responsible for Graphene Oxide's Distinct Inhibitory Effects toward Pseudomonas aeruginosa and Staphylococcus aureus Pathogens. *ACS Applied Bio Materials*, **2021**, 4, 660-668	4.1	2
97	Preparing Membrane Proteins for Simulation Using CHARMM-GUI. *Methods in Molecular Biology*, **2021**, 2302, 237-251	1.4	2
96	Stepwise gating of the Sec61 protein-conducting channel by Sec63 and Sec62. *Nature Structural and Molecular Biology*, **2021**, 28, 162-172	17.6	14
95	Bifunctional Janus Particles as Multivalent Synthetic Nanoparticle Antibodies (SNAbs) for Selective Depletion of Target Cells. *Nano Letters*, **2021**, 21, 875-886	11.5	6
94	Quantifying arrhythmic long QT effects of hydroxychloroquine and azithromycin with whole-heart optical mapping and simulations. *Heart Rhythm O2*, **2021**, 2, 394-404	1.5	6
93	Lpp positions peptidoglycan at the AcrA-TolC interface in the AcrAB-TolC multidrug efflux pump. *Biophysical Journal*, **2021**, 120, 3973-3982	2.9	2
92	Inward-facing glycine residues create sharp turns in barrel membrane proteins. *Biochimica Et Biophysica Acta - Biomembranes*, **2021**, 1863, 183662	3.8	0
91	ACE2 glycans preferentially interact with SARS-CoV-2 over SARS-CoV. *Chemical Communications*, **2021**, 57, 5949-5952	5.8	6

90	Inhibitor binding influences the protonation states of histidines in SARS-CoV-2 main protease.. *Chemical Science*, **2021**, 12, 1513-1527	9.4	29
89	Plasticity within the barrel domain of BamA mediates a hybrid-barrel mechanism by BAM. *Nature Communications*, **2021**, 12, 7131	17.4	4
88	Supercomputer-Based Ensemble Docking Drug Discovery Pipeline with Application to Covid-19. *Journal of Chemical Information and Modeling*, **2020**, 60, 5832-5852	6.1	71
87	Fatal arrhythmias: Another reason why doctors remain cautious about chloroquine/hydroxychloroquine for treating COVID-19. *Heart Rhythm*, **2020**, 17, 1445-1451	6.7	17
86	The Effect of (-)-Epigallocatechin-3-Gallate on the Amyloid-β Secondary Structure. *Biophysical Journal*, **2020**, 119, 349-359	2.9	9
85	Synergistic Biophysical Techniques Reveal Structural Mechanisms of Engineered Cationic Antimicrobial Peptides in Lipid Model Membranes. *Chemistry - A European Journal*, **2020**, 26, 6247-6256	4.8	2
84	BamA is required for autotransporter secretion. *Biochimica Et Biophysica Acta - General Subjects*, **2020**, 1864, 129581	4	4
83	Outer membrane protein size and LPS O-antigen define protective antibody targeting to the Salmonella surface. *Nature Communications*, **2020**, 11, 851	17.4	23
82	Membrane thinning and lateral gating are consistent features of BamA across multiple species. *PLoS Computational Biology*, **2020**, 16, e1008355	5	7
81	Supercomputer-Based Ensemble Docking Drug Discovery Pipeline with Application to Covid-19. *ChemRxiv*, **2020**,	4.4	7
80	Structural insight into toxin secretion by contact-dependent growth inhibition transporters. *ELife*, **2020**, 9,	8.9	6
79	A Minimal Membrane Metal Transport System: Dynamics and Energetics of mer Proteins. *Journal of Computational Chemistry*, **2020**, 41, 528-537	3.5	2
78	Parameterization of a drug molecule with a halogen σhole particle using ffTK: Implementation, testing, and comparison. *Journal of Chemical Physics*, **2020**, 153, 164104	3.9	1
77	Presence of substrate aids lateral gate separation in LptD. *Biochimica Et Biophysica Acta - Biomembranes*, **2020**, 1862, 183025	3.8	7
76	Tuning Proton Transfer Thermodynamics in SARS-Cov-2 Main Protease: Implications for Catalysis and Inhibitor Design. *ChemRxiv*, **2020**,	4.4	2
75	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	5.4	7
74	Conformational Dynamics of AcrA Govern Multidrug Efflux Pump Assembly. *ACS Infectious Diseases*, **2019**, 5, 1926-1935	5.5	10
73	Identification of Binding Sites for Efflux Pump Inhibitors of the AcrAB-TolC Component AcrA. *Biophysical Journal*, **2019**, 116, 648-658	2.9	13

72	A novel human mutation results in T and NK cell-driven immune dysregulation. *Journal of Experimental Medicine*, **2019**, 216, 1255-1267	16.6	38
71	Structure and Function of Tryptophan-Tyrosine Dyads in Biomimetic Hairpins. *Journal of Physical Chemistry B*, **2019**, 123, 2780-2791	3.4	1
70	ATP-Dependent Signaling in Simulations of a Revised Model of Cystic Fibrosis Transmembrane Conductance Regulator (CFTR). *Journal of Physical Chemistry B*, **2019**, 123, 3177-3188	3.4	1
69	Tyrosine, cysteine, and proton coupled electron transfer in a ribonucleotide reductase-inspired beta hairpin maquette. *Chemical Communications*, **2019**, 55, 9399-9402	5.8	6
68	Accelerating Membrane Simulations with Hydrogen Mass Repartitioning. *Journal of Chemical Theory and Computation*, **2019**, 15, 4673-4686	6.4	33
67	Non-detergent isolation of a cyanobacterial photosystem I using styrene maleic acid alternating copolymers.. *RSC Advances*, **2019**, 9, 31781-31796	3.7	11
66	Computed Free Energies of Peptide Insertion into Bilayers are Independent of Computational Method. *Journal of Membrane Biology*, **2018**, 251, 345-356	2.3	15
65	Diverse Protein-Folding Pathways and Functions of Hairpins and Sheets **2018**, 1-20		
64	BFEE: A User-Friendly Graphical Interface Facilitating Absolute Binding Free-Energy Calculations. *Journal of Chemical Information and Modeling*, **2018**, 58, 556-560	6.1	34
63	Development of CHARMM-Compatible Force-Field Parameters for Cobalamin and Related Cofactors from Quantum Mechanical Calculations. *Journal of Chemical Theory and Computation*, **2018**, 14, 784-798	6.4	14
62	Exploring adsorption of neutral aromatic pollutants onto graphene nanomaterials via molecular dynamics simulations and theoretical linear solvation energy relationships. *Environmental Science: Nano*, **2018**, 5, 2117-2128	7.1	15
61	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	11.5	29
60	Folding free energy landscapes of -sheets with non-polarizable and polarizable CHARMM force fields. *Journal of Chemical Physics*, **2018**, 149, 072317	3.9	20
59	Transmembrane but not soluble helices fold inside the ribosome tunnel. *Nature Communications*, **2018**, 9, 5246	17.4	18
58	Distribution of mechanical stress in the Escherichia coli cell envelope. *Biochimica Et Biophysica Acta - Biomembranes*, **2018**, 1860, 2566-2575	3.8	48
57	The barrel assembly machinery in motion. *Nature Reviews Microbiology*, **2017**, 15, 197-204	22.2	119
56	Redox-Driven Conformational Dynamics in a Photosystem-II-Inspired Hairpin Maquette Determined through Spectroscopy and Simulation. *Journal of Physical Chemistry B*, **2017**, 121, 3536-3545	3.4	9
55	Toward the rational design of macrolide antibiotics to combat resistance. *Chemical Biology and Drug Design*, **2017**, 90, 641-652	2.9	6

54	Structural basis for substrate selection by the translocation and assembly module of the β-barrel assembly machinery. *Molecular Microbiology*, **2017**, 106, 142-156	4.1	24
53	Producing membrane proteins one simulation at a time. *Journal of Biological Chemistry*, **2017**, 292, 19546-19547	3.4	
52	Structure and Misfolding of the Flexible Tripartite Coiled-Coil Domain of Glaucoma-Associated Myocilin. *Structure*, **2017**, 25, 1697-1707.e5	5.2	16
51	Accelerating the use of molecular modeling in the high school classroom with VMD Lite. *Biochemistry and Molecular Biology Education*, **2016**, 44, 124-9	1.3	5
50	DNA Scrunching in the Packaging of Viral Genomes. *Journal of Physical Chemistry B*, **2016**, 120, 6200-7	3.4	8
49	Coarse-Grained Molecular Dynamics Simulations of the Bacterial Cell Wall. *Methods in Molecular Biology*, **2016**, 1440, 247-70	1.4	2
48	Living on the edge: Simulations of bacterial outer-membrane proteins. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 1753-9	3.8	25
47	Simulation-Based Approaches for Determining Membrane Permeability of Small Compounds. *Journal of Chemical Information and Modeling*, **2016**, 56, 721-33	6.1	127
46	Structural and Functional Characterization of the LPS Transporter LptDE from Gram-Negative Pathogens. *Structure*, **2016**, 24, 965-976	5.2	77
45	Decrypting protein insertion through the translocon with free-energy calculations. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 1663-71	3.8	12
44	Transitions of Double-Stranded DNA Between the A- and B-Forms. *Journal of Physical Chemistry B*, **2016**, 120, 8449-56	3.4	27
43	Role of the Native Outer-Membrane Environment on the Transporter BtuB. *Biophysical Journal*, **2016**, 111, 1409-1417	2.9	34
42	Coarse-grained simulations of bacterial cell wall growth reveal that local coordination alone can be sufficient to maintain rod shape. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, E3689-98	11.5	35
41	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		9
40	The adaptive biasing force method: everything you always wanted to know but were afraid to ask. *Journal of Physical Chemistry B*, **2015**, 119, 1129-51	3.4	240
39	Parametrization of macrolide antibiotics using the force field toolkit. *Journal of Computational Chemistry*, **2015**, 36, 2052-63	3.5	9
38	Conformational Changes of the Clamp of the Protein Translocation ATPase SecA. *Journal of Molecular Biology*, **2015**, 427, 2348-59	6.5	20
37	Thermodynamics of Deca-alanine Folding in Water. *Journal of Chemical Theory and Computation*, **2014**, 10, 2836-2844	6.4	37

36	Structure of the SecY channel during initiation of protein translocation. *Nature*, **2014**, 506, 102-6	50.4	119
35	Lateral opening and exit pore formation are required for BamA function. *Structure*, **2014**, 22, 1055-62	5.2	142
34	Generalized Scalable Multiple Copy Algorithms for Molecular Dynamics Simulations in NAMD. *Computer Physics Communications*, **2014**, 185, 908-916	4.2	88
33	Escherichia coli peptidoglycan structure and mechanics as predicted by atomic-scale simulations. *PLoS Computational Biology*, **2014**, 10, e1003475	5	66
32	Efficient determination of protein-protein standard binding free energies from first principles. *Journal of Chemical Theory and Computation*, **2013**, 9,	6.4	133
31	Structural insight into the biogenesis of β-barrel membrane proteins. *Nature*, **2013**, 501, 385-90	50.4	309
30	IcmQ in the Type 4b secretion system contains an NAD+ binding domain. *Structure*, **2013**, 21, 1361-73	5.2	5
29	Reconciling the roles of kinetic and thermodynamic factors in membrane-protein insertion. *Journal of the American Chemical Society*, **2013**, 135, 2291-7	16.4	37
28	Rapid parameterization of small molecules using the Force Field Toolkit. *Journal of Computational Chemistry*, **2013**, 34, 2757-70	3.5	313
27	The mobility of two kinase domains in the Escherichia coli chemoreceptor array varies with signalling state. *Molecular Microbiology*, **2013**, 89, 831-41	4.1	45
26	Architecture and assembly of the Gram-positive cell wall. *Molecular Microbiology*, **2013**, 88, 664-72	4.1	85
25	Standard binding free energies from computer simulations: What is the best strategy?. *Journal of Chemical Theory and Computation*, **2013**, 9, 794-802	6.4	224
24	Molecular dynamics simulations of membrane proteins under asymmetric ionic concentrations. *Journal of General Physiology*, **2013**, 142, 465-75	3.4	38
23	Molecular basis for the activation of a catalytic asparagine residue in a self-cleaving bacterial autotransporter. *Journal of Molecular Biology*, **2012**, 415, 128-42	6.5	34
22	Determination of membrane-insertion free energies by molecular dynamics simulations. *Biophysical Journal*, **2012**, 102, 795-801	2.9	43
21	Mechanisms of SecM-mediated stalling in the ribosome. *Biophysical Journal*, **2012**, 103, 331-41	2.9	67
20	Structural basis for iron piracy by pathogenic Neisseria. *Nature*, **2012**, 483, 53-8	50.4	199
19	Applications of the molecular dynamics flexible fitting method. *Journal of Structural Biology*, **2011**, 173, 420-7	3.4	38

18	Cryo-EM structure of the ribosome-SecYE complex in the membrane environment. *Nature Structural and Molecular Biology*, **2011**, 18, 614-21	17.6	232
17	Symmetry-restrained flexible fitting for symmetric EM maps. *Structure*, **2011**, 19, 1211-8	5.2	57
16	Free energy of nascent-chain folding in the translocon. *Journal of the American Chemical Society*, **2011**, 133, 7602-7	16.4	25
15	Free-energy cost for translocon-assisted insertion of membrane proteins. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 3596-601	11.5	54
14	Self-assembly of photosynthetic membranes. *ChemPhysChem*, **2010**, 11, 1154-9	3.2	19
13	Regulation of the protein-conducting channel by a bound ribosome. *Structure*, **2009**, 17, 1453-64	5.2	95
12	Coupling of calcium and substrate binding through loop alignment in the outer-membrane transporter BtuB. *Journal of Molecular Biology*, **2009**, 393, 1129-42	6.5	27
11	Protein-induced membrane curvature investigated through molecular dynamics flexible fitting. *Biophysical Journal*, **2009**, 97, 321-9	2.9	64
10	Membrane curvature induced by aggregates of LH2s and monomeric LH1s. *Biophysical Journal*, **2009**, 97, 2978-84	2.9	28
9	Structure of monomeric yeast and mammalian Sec61 complexes interacting with the translating ribosome. *Science*, **2009**, 326, 1369-73	33.3	236
8	Intrinsic curvature properties of photosynthetic proteins in chromatophores. *Biophysical Journal*, **2008**, 95, 2822-36	2.9	69
7	The roles of pore ring and plug in the SecY protein-conducting channel. *Journal of General Physiology*, **2008**, 132, 709-19	3.4	31
6	Structural determinants of lateral gate opening in the protein translocon. *Biochemistry*, **2007**, 46, 11147-57	3.1	55
5	Mechanics of force propagation in TonB-dependent outer membrane transport. *Biophysical Journal*, **2007**, 93, 496-504	2.9	88
4	Molecular dynamics studies of the archaeal translocon. *Biophysical Journal*, **2006**, 90, 2356-67	2.9	72
3	Scalable molecular dynamics with NAMD. *Journal of Computational Chemistry*, **2005**, 26, 1781-802	3.5	12650
2	Critical interactions for SARS-CoV-2 spike protein binding to ACE2 identified by machine learning		1
1	SARS-CoV-2 spike opening dynamics and energetics reveal the individual roles of glycans and their collective impact		2