Huan-Xiang Zhou

List of Publications by Year in Descending Order

277 papers	16,626 citations	69 h-index	118 g-index
345 ext. papers	18,365 ext. citations	6.1 avg, IF	7.42 L-index

#	Paper	IF	Citations
277	Preferential Interactions of a Crowder Protein with the Specific Binding Site of a Native Protein Complex.. *Journal of Physical Chemistry Letters*, **2022**, 792-800	6.4	0
276	Binding free energy decomposition and multiple unbinding paths of buried ligands in a PreQ1 riboswitch. *PLoS Computational Biology*, **2021**, 17, e1009603	5	0
275	Shape recovery of deformed biomolecular droplets: Dependence on condensate viscoelasticity. *Journal of Chemical Physics*, **2021**, 155, 145102	3.9	0
274	Shear relaxation governs fusion dynamics of biomolecular condensates. *Nature Communications*, **2021**, 12, 5995	17.4	9
273	Macromolecular regulators have matching effects on the phase equilibrium and interfacial tension of biomolecular condensates. *Protein Science*, **2021**, 30, 1360-1370	6.3	5
272	Effects of Cholesterol on the Partitioning of a Drug Molecule in Lipid Bilayers. *Journal of Physical Chemistry B*, **2021**, 125, 5338-5345	3.4	1
271	Characterizing protein kinase A (PKA) subunits as macromolecular regulators of PKA RI□ liquid-liquid phase separation. *Journal of Chemical Physics*, **2021**, 154, 221101	3.9	2
270	Fuzzy Association of an Intrinsically Disordered Protein with Acidic Membranes. *Jacs Au*, **2021**, 1, 66-78		3
269	Viscoelasticity of biomolecular condensates conforms to the Jeffreys model. *Journal of Chemical Physics*, **2021**, 154, 041103	3.9	9
268	Machine Learning-Enabled Pipeline for Large-Scale Virtual Drug Screening. *Journal of Chemical Information and Modeling*, **2021**, 61, 4236-4244	6.1	4
267	Removing Thermostat Distortions of Protein Dynamics in Constant-Temperature Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2021**, 17, 5920-5932	6.4	1
266	Functional stability of water wire-carbonyl interactions in an ion channel. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 11908-11915	11.5	18
265	Out-of-Register Parallel □Sheets and Antiparallel □Sheets Coexist in 150-kDa Oligomers Formed by Amyloid-□(1-42). *Journal of Molecular Biology*, **2020**, 432, 4388-4407	6.5	15
264	Sequence-Dependent Correlated Segments in the Intrinsically Disordered Region of ChiZ. *Biomolecules*, **2020**, 10,	5.9	4
263	Tug of War between Condensate Phases in a Minimal Macromolecular System. *Journal of the American Chemical Society*, **2020**, 142, 8848-8861	16.4	15
262	Membrane Association and Functional Mechanism of Synaptotagmin-1 in Triggering Vesicle Fusion. *Biophysical Journal*, **2020**, 119, 1255-1265	2.9	3
261	Determinants for Fusion Speed of Biomolecular Droplets. *Angewandte Chemie - International Edition*, **2020**, 59, 20837-20840	16.4	19

260	Profiling SARS-CoV-2 Main Protease (M) Binding to Repurposed Drugs Using Molecular Dynamics Simulations in Classical and Neural Network-Trained Force Fields. *ACS Combinatorial Science*, **2020**, 22, 826-832	3.9	21
259	Determination of Condensate Material Properties from Droplet Deformation. *Journal of Physical Chemistry B*, **2020**, 124, 8372-8379	3.4	10
258	Determinants for Fusion Speed of Biomolecular Droplets. *Angewandte Chemie*, **2020**, 132, 21023-21026	3.6	0
257	Calculation of Second Virial Coefficients of Atomistic Proteins Using Fast Fourier Transform. *Journal of Physical Chemistry B*, **2019**, 123, 8203-8215	3.4	8
256	Three archetypical classes of macromolecular regulators of protein liquid-liquid phase separation. *Proceedings of the National Academy of Sciences of the United States of America*, **2019**, 116, 19474-19483	11.5	47
255	Transfer Free Energies of Test Proteins Into Crowded Protein Solutions Have Simple Dependence on Crowder Concentration. *Frontiers in Molecular Biosciences*, **2019**, 6, 39	5.6	4
254	Designed Mutations Alter the Binding Pathways of an Intrinsically Disordered Protein. *Scientific Reports*, **2019**, 9, 6172	4.9	11
253	Influenza A M2 Channel Clustering at High Protein/Lipid Ratios: Viral Budding Implications. *Biophysical Journal*, **2019**, 116, 1075-1084	2.9	21
252	Both Ligands and Macromolecular Crowders Preferentially Bind to Closed Conformations of Maltose Binding Protein. *Biochemistry*, **2019**, 58, 2208-2217	3.2	3
251	Fatty Acids Compete with A□n Binding to Serum Albumin by Quenching Its Conformational Flexibility. *Biophysical Journal*, **2019**, 116, 248-257	2.9	11
250	Hinge-Shift Mechanism Modulates Allosteric Regulations in Human Pin1. *Journal of Physical Chemistry B*, **2018**, 122, 5623-5629	3.4	20
249	Using the fast fourier transform in binding free energy calculations. *Journal of Computational Chemistry*, **2018**, 39, 621-636	3.5	14
248	Electrostatic Interactions in Protein Structure, Folding, Binding, and Condensation. *Chemical Reviews*, **2018**, 118, 1691-1741	68.1	290
247	Liquid-Liquid Phase Separation of Patchy Particles Illuminates Diverse Effects of Regulatory Components on Protein Droplet Formation. *Scientific Reports*, **2018**, 8, 6728	4.9	65
246	Why Do Disordered and Structured Proteins Behave Differently in Phase Separation?. *Trends in Biochemical Sciences*, **2018**, 43, 499-516	10.3	62
245	Intrinsically Disordered Protein Exhibits Both Compaction and Expansion under Macromolecular Crowding. *Biophysical Journal*, **2018**, 114, 1067-1079	2.9	40
244	Atomistic Modeling of Intrinsically Disordered Proteins Under Polyethylene Glycol Crowding: Quantitative Comparison with Experimental Data and Implication of Protein-Crowder Attraction. *Journal of Physical Chemistry B*, **2018**, 122, 11262-11270	3.4	11
243	A conserved glycine harboring disease-associated mutations permits NMDA receptor slow deactivation and high Ca permeability. *Nature Communications*, **2018**, 9, 3748	17.4	22

242	Temperature-induced collapse of a disordered peptide observed by three sampling methods in molecular dynamics simulations. *Journal of Chemical Physics*, **2018**, 149, 072313	3.9	12
241	Gating Motions and Stationary Gating Properties of Ionotropic Glutamate Receptors: Computation Meets Electrophysiology. *Accounts of Chemical Research*, **2017**, 50, 814-822	24.3	3
240	Advancing NMDA Receptor Physiology by Integrating Multiple Approaches. *Trends in Neurosciences*, **2017**, 40, 129-137	13.3	16
239	Divergent roles of a peripheral transmembrane segment in AMPA and NMDA receptors. *Journal of General Physiology*, **2017**, 149, 661-680	3.4	23
238	Rate Constants and Mechanisms of Protein-Ligand Binding. *Annual Review of Biophysics*, **2017**, 46, 105-130	21.1	39
237	Structural modeling for the open state of an NMDA receptor. *Journal of Structural Biology*, **2017**, 200, 369-375	3.4	11
236	Protein folding, binding, and droplet formation in cell-like conditions. *Current Opinion in Structural Biology*, **2017**, 43, 28-37	8.1	34
235	Unidirectional allostery in the regulatory subunit RIfacilitates efficient deactivation of protein kinase A. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, E6776-E6785	11.5	12
234	Mechanism and rate constants of the Cdc42 GTPase binding with intrinsically disordered effectors. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84, 674-85	4.2	13
233	Fast Method for Computing Chemical Potentials and Liquid-Liquid Phase Equilibria of Macromolecular Solutions. *Journal of Physical Chemistry B*, **2016**, 120, 8164-74	3.4	29
232	Challenges in structural approaches to cell modeling. *Journal of Molecular Biology*, **2016**, 428, 2943-64	6.5	36
231	The Transmembrane Domain Mediates Tetramerization of Amino-3-hydroxy-5-methyl-4-isoxazolepropionic Acid (AMPA) Receptors. *Journal of Biological Chemistry*, **2016**, 291, 6595-606	5.4	17
230	Protein Allostery and Conformational Dynamics. *Chemical Reviews*, **2016**, 116, 6503-15	68.1	209
229	Differential Binding of Rimantadine Enantiomers to Influenza A M2 Proton Channel. *Journal of the American Chemical Society*, **2016**, 138, 1506-9	16.4	24
228	Allosteric activation of SENP1 by SUMO1 grasp domain involves a dock-and-coalesce mechanism. *ELife*, **2016**, 5,	8.9	7
227	Prediction of homoprotein and heteroprotein complexes by protein docking and template-based modeling: A CASP-CAPRI experiment. *Proteins: Structure, Function and Bioinformatics*, **2016**, 84 Suppl 1, 323-48	4.2	111
226	A Fast Method for Computing Chemical Potentials and Phase Equilibria of Macromolecular Mixtures. *Biophysical Journal*, **2016**, 110, 386a-387a	2.9	
225	Semiclosed Conformations of the Ligand-Binding Domains of NMDA Receptors during Stationary Gating. *Biophysical Journal*, **2016**, 111, 1418-1428	2.9	17

224	Electrostatic effects on the folding stability of FKBP12. *Protein Engineering, Design and Selection*, **2016**, 29, 301-308	1.9	5
223	Dynamically Driven Protein Allostery Exhibits Disparate Responses for Fast and Slow Motions. *Biophysical Journal*, **2015**, 108, 2771-4	2.9	20
222	Dynamic Short Hydrogen Bonds in Histidine Tetrad of Full-Length M2 Proton Channel Reveal Tetrameric Structural Heterogeneity and Functional Mechanism. *Structure*, **2015**, 23, 2300-2308	5.2	40
221	Disorder-to-Order Transition of an Active-Site Loop Mediates the Allosteric Activation of Sortase A. *Biophysical Journal*, **2015**, 109, 1706-15	2.9	24
220	Mechanism-Based Mathematical Model for Gating of Ionotropic Glutamate Receptors. *Journal of Physical Chemistry B*, **2015**, 119, 10934-40	3.4	12
219	Reduced curvature of ligand-binding domain free-energy surface underlies partial agonism at NMDA receptors. *Structure*, **2015**, 23, 228-236	5.2	27
218	Structure of CrgA, a cell division structural and regulatory protein from Mycobacterium tuberculosis, in lipid bilayers. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, E119-26	11.5	39
217	Two pathways mediate interdomain allosteric regulation in pin1. *Structure*, **2015**, 23, 237-247	5.2	56
216	Theoretical frameworks for multiscale modeling and simulation. *Current Opinion in Structural Biology*, **2014**, 25, 67-76	8.1	28
215	Blind prediction of interfacial water positions in CAPRI. *Proteins: Structure, Function and Bioinformatics*, **2014**, 82, 620-32	4.2	43
214	General rules for the arrangements and gating motions of pore-lining helices in homomeric ion channels. *Nature Communications*, **2014**, 5, 4641	17.4	12
213	Further Development of the FFT-based Method for Atomistic Modeling of Protein Folding and Binding under Crowding: Optimization of Accuracy and Speed. *Journal of Chemical Theory and Computation*, **2014**, 10, 2824-2835	6.4	21
212	SAXS/SANS probe of intermolecular interactions in concentrated protein solutions. *Biophysical Journal*, **2014**, 106, 771-3	2.9	6
211	Both protein dynamics and ligand concentration can shift the binding mechanism between conformational selection and induced fit. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 10197-202	11.5	61
210	Mechanical coupling maintains the fidelity of NMDA receptor-mediated currents. *Nature Neuroscience*, **2014**, 17, 914-22	25.5	75
209	Distinct mechanisms of a phosphotyrosyl peptide binding to two SH2 domains. *Journal of Theoretical and Computational Chemistry*, **2014**, 13, 1440003	1.8	2
208	Multidimensional reaction rate theory with anisotropic diffusion. *Journal of Chemical Physics*, **2014**, 141, 204106	3.9	16
207	Binding of MgtR, a Salmonella transmembrane regulatory peptide, to MgtC, a Mycobacterium tuberculosis virulence factor: a structural study. *Journal of Molecular Biology*, **2014**, 426, 436-46	6.5	14

206	Design rules for selective binding of nuclear localization signals to minor site of importin-β. *PLoS ONE*, **2014**, 9, e91025	3.7	11
205	Simulation and Modeling of Crowding Effects on the Thermodynamic and Kinetic Properties of Proteins with Atomic Details. *Biophysical Reviews*, **2013**, 5, 207-215	3.7	23
204	Molecular structure of RADA16-I designer self-assembling peptide nanofibers. *ACS Nano*, **2013**, 7, 7562-72	12.7	101
203	An FFT-based method for modeling protein folding and binding under crowding: benchmarking on ellipsoidal and all-atom crowders. *Journal of Chemical Theory and Computation*, **2013**, 9,	6.4	25
202	Modeling protein association mechanisms and kinetics. *Current Opinion in Structural Biology*, **2013**, 23, 887-93	8.1	70
201	Effects of Macromolecular Crowding on the Conformational Ensembles of Disordered Proteins. *Journal of Physical Chemistry Letters*, **2013**, 4,	6.4	44
200	Solid-state NMR evidence for β-hairpin structure within MAX8 designer peptide nanofibers. *Biophysical Journal*, **2013**, 105, 222-30	2.9	21
199	An NMDA receptor gating mechanism developed from MD simulations reveals molecular details underlying subunit-specific contributions. *Biophysical Journal*, **2013**, 104, 2170-81	2.9	36
198	Influence of crowded cellular environments on protein folding, binding, and oligomerization: biological consequences and potentials of atomistic modeling. *FEBS Letters*, **2013**, 587, 1053-61	3.8	127
197	Influences of membrane mimetic environments on membrane protein structures. *Annual Review of Biophysics*, **2013**, 42, 361-92	21.1	199
196	Polymer crowders and protein crowders act similarly on protein folding stability. *FEBS Letters*, **2013**, 587, 394-7	3.8	56
195	PIPE: A Suite of Web Servers for Predictions Ranging From Protein Structure to Binding Kinetics. *Biophysical Reviews*, **2013**, 5, 41-46	3.7	1
194	Modeling the membrane environment has implications for membrane protein structure and function: influenza A M2 protein. *Protein Science*, **2013**, 22, 381-94	6.3	41
193	calculations and validation of the pH-dependent structures of the His37-Trp41 quartet, the heart of acid activation and proton conductance in the M2 protein of Influenza A virus. *Chemical Science*, **2013**, 4, 2776-2787	9.4	18
192	Folding free energy surfaces of three small proteins under crowding: validation of the postprocessing method by direct simulation. *Physical Biology*, **2013**, 10, 045001	3	11
191	Inter- and intrasubunit interactions between transmembrane helices in the open state of P2X receptor channels. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, E4045-54	11.5	41
190	Using the concept of transient complex for affinity predictions in CAPRI rounds 20-27 and beyond. *Proteins: Structure, Function and Bioinformatics*, **2013**, 81, 2229-36	4.2	7
189	Poisson-Boltzmann Calculations: van der Waals or Molecular Surface?. *Communications in Computational Physics*, **2013**, 13, 1-12	2.4	38

188	Competitive interactions of ligands and macromolecular crowders with maltose binding protein. *PLoS ONE*, **2013**, 8, e74969	3.7	22
187	Community-wide evaluation of methods for predicting the effect of mutations on protein-protein interactions. *Proteins: Structure, Function and Bioinformatics*, **2013**, 81, 1980-7	4.2	78
186	Intrinsic disorder: signaling via highly specific but short-lived association. *Trends in Biochemical Sciences*, **2012**, 37, 43-8	10.3	109
185	Familial hypertrophic cardiomyopathy related E180G mutation increases flexibility of human cardiac □-tropomyosin. *FEBS Letters*, **2012**, 586, 3503-7	3.8	22
184	M2 protein from influenza A: from multiple structures to biophysical and functional insights. *Current Opinion in Virology*, **2012**, 2, 128-33	7.5	51
183	A method for computing association rate constants of atomistically represented proteins under macromolecular crowding. *Physical Biology*, **2012**, 9, 066008	3	23
182	Glycines: role in □-helical membrane protein structures and a potential indicator of native conformation. *Biochemistry*, **2012**, 51, 4779-89	3.2	54
181	Contrasting factors on the kinetic path to protein complex formation diminish the effects of crowding agents. *Biophysical Journal*, **2012**, 103, 1011-9	2.9	35
180	Recent progress in structure-based anti-influenza drug design. *Drug Discovery Today*, **2012**, 17, 1111-20	8.8	58
179	Size matters in activation/inhibition of ligand-gated ion channels. *Trends in Pharmacological Sciences*, **2012**, 33, 482-93	13.2	13
178	Persistence length of human cardiac □-tropomyosin measured by single molecule direct probe microscopy. *PLoS ONE*, **2012**, 7, e39676	3.7	24
177	Rate constants and mechanisms of intrinsically disordered proteins binding to structured targets. *Physical Chemistry Chemical Physics*, **2012**, 14, 10466-76	3.6	64
176	A common model for cytokine receptor activation: combined scissor-like rotation and self-rotation of receptor dimer induced by class I cytokine. *PLoS Computational Biology*, **2012**, 8, e1002427	5	20
175	Prediction and dissection of widely-varying association rate constants of actin-binding proteins. *PLoS Computational Biology*, **2012**, 8, e1002696	5	9
174	Gating mechanism of a P2X4 receptor developed from normal mode analysis and molecular dynamics simulations. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 4140-5	11.5	47
173	BDflex: a method for efficient treatment of molecular flexibility in calculating protein-ligand binding rate constants from brownian dynamics simulations. *Journal of Chemical Physics*, **2012**, 137, 135105	3.9	15
172	Role of diffusion in the kinetics of reversible enzyme-catalyzed reactions. *Bulletin of the Korean Chemical Society*, **2012**, 33, 925-928	1.2	14
171	Rationalizing 5000-fold differences in receptor-binding rate constants of four cytokines. *Biophysical Journal*, **2011**, 101, 1175-83	2.9	17

170	Atomistic mechanism for the activation and desensitization of an AMPA-subtype glutamate receptor. *Nature Communications*, **2011**, 2, 354	17.4	42
169	Drug sensitivity, drug-resistant mutations, and structures of three conductance domains of viral porins. *Biochimica Et Biophysica Acta - Biomembranes*, **2011**, 1808, 538-46	3.8	15
168	Community-wide assessment of protein-interface modeling suggests improvements to design methodology. *Journal of Molecular Biology*, **2011**, 414, 289-302	6.5	114
167	Structural models of protein-DNA complexes based on interface prediction and docking. *Current Protein and Peptide Science*, **2011**, 12, 531-9	2.8	4
166	Automated prediction of protein association rate constants. *Structure*, **2011**, 19, 1744-51	5.2	91
165	Influence of solubilizing environments on membrane protein structures. *Trends in Biochemical Sciences*, **2011**, 36, 117-25	10.3	169
164	A theory for the proton transport of the influenza virus M2 protein: extensive test against conductance data. *Biophysical Journal*, **2011**, 100, 912-21	2.9	31
163	Diffusion-influenced ligand binding to buried sites in macromolecules and transmembrane channels. *Journal of Chemical Physics*, **2011**, 135, 075103	3.9	27
162	Mechanistic insight into the h(2)o/d (2)o isotope effect in the proton transport of the influenza virus m2 protein. *Journal of Membrane Biology*, **2011**, 244, 93-6	2.3	10
161	Q&A: What is biophysics?. *BMC Biology*, **2011**, 9, 13	7.3	4
160	A solvable model for the diffusion and reaction of neurotransmitters in a synaptic junction. *BMC Biophysics*, **2011**, 4, 5	0	4
159	Equivalence of two approaches for modeling ion permeation through a transmembrane channel with an internal binding site. *Journal of Chemical Physics*, **2011**, 134, 135101	3.9	3
158	Theory and simulation of diffusion-influenced, stochastically gated ligand binding to buried sites. *Journal of Chemical Physics*, **2011**, 135, 145101	3.9	8
157	Full reconstruction of a vectorial protein folding pathway by atomic force microscopy and molecular dynamics simulations.. *Journal of Biological Chemistry*, **2011**, 286, 8708	5.4	78
156	Rapid search for specific sites on DNA through conformational switch of nonspecifically bound proteins. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 8651-6	11.5	72
155	Theory and simulation on the kinetics of protein-ligand binding coupled to conformational change. *Journal of Chemical Physics*, **2011**, 134, 105101	3.9	30
154	Full reconstruction of a vectorial protein folding pathway by atomic force microscopy and molecular dynamics simulations. *Journal of Biological Chemistry*, **2010**, 285, 38167-72	5.4	34
153	Effects of macromolecular crowding on protein conformational changes. *PLoS Computational Biology*, **2010**, 6, e1000833	5	70

152	Insight into the mechanism of the influenza A proton channel from a structure in a lipid bilayer. *Science*, **2010**, 330, 509-12	33.3	375
151	Equilibrium sampling for biomolecules under mechanical tension. *Biophysical Journal*, **2010**, 98, 733-40	2.9	5
150	From induced fit to conformational selection: a continuum of binding mechanism controlled by the timescale of conformational transitions. *Biophysical Journal*, **2010**, 98, L15-7	2.9	140
149	The folding transition-state ensemble of a four-helix bundle protein: helix propensity as a determinant and macromolecular crowding as a probe. *Biophysical Journal*, **2010**, 98, 2273-80	2.9	22
148	Diffusion-Influenced Transport of Ions across a Transmembrane Channel with an Internal Binding Site. *Journal of Physical Chemistry Letters*, **2010**, 1, 1973-1976	6.4	16
147	Method to Predict Crowding Effects by Postprocessing Molecular Dynamics Trajectories: Application to the Flap Dynamics of HIV-1 Protease. *Journal of Physical Chemistry Letters*, **2010**, 1, 107-110	6.4	39
146	Rate theories for biologists. *Quarterly Reviews of Biophysics*, **2010**, 43, 219-93	7	107
145	Generalized fundamental measure theory for atomistic modeling of macromolecular crowding. *Physical Review E*, **2010**, 81, 031919	2.4	26
144	A Less Invasive Approach to Rheology Measurements. *Physics Magazine*, **2010**, 3,	1.1	4
143	The gates of ion channels and enzymes. *Trends in Biochemical Sciences*, **2010**, 35, 179-85	10.3	71
142	Application of Biased Metropolis Algorithms: From protons to proteins. *Mathematics and Computers in Simulation*, **2010**, 80, 1056-1067	3.3	6
141	Selection of near-native poses in CAPRI rounds 13-19. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 3166-73	4.2	9
140	Speeding by a crowd. *Physics Magazine*, **2010**, 3,	1.1	2
139	Dissection of the high rate constant for the binding of a ribotoxin to the ribosome. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 6974-9	11.5	25
138	Correction for Qin and Zhou, Dissection of the high rate constant for the binding of a ribotoxin to the ribosome. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 12208-12208	11.5	78
137	Blocking effect of an immuno-suppressive agent, cynarin, on CD28 of T-cell receptor. *Pharmaceutical Research*, **2009**, 26, 375-81	4.5	23
136	Nonadditive effects of mixed crowding on protein stability. *Proteins: Structure, Function and Bioinformatics*, **2009**, 77, 133-8	4.2	81
135	Inverse tuning of metal binding affinity and protein stability by altering charged coordination residues in designed calcium binding proteins. *PMC Biophysics*, **2009**, 2, 11		8

134	Crowding effects of membrane proteins. *Journal of Physical Chemistry B*, **2009**, 113, 7995-8005	3.4	47
133	Atomistic modeling of macromolecular crowding predicts modest increases in protein folding and binding stability. *Biophysical Journal*, **2009**, 97, 12-9	2.9	93
132	Effect of macromolecular crowding on protein binding stability: modest stabilization and significant biological consequences. *Biophysical Journal*, **2009**, 97, 906-11	2.9	87
131	Theory of free energy and entropy in noncovalent binding. *Chemical Reviews*, **2009**, 109, 4092-107	68.1	291
130	Conformational heterogeneity of the M2 proton channel and a structural model for channel activation. *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 13311-6	11.5	99
129	Fundamental aspects of protein-protein association kinetics. *Chemical Reviews*, **2009**, 109, 839-60	68.1	528
128	Solid-state NMR and MD simulations of the antiviral drug amantadine solubilized in DMPC bilayers. *Biophysical Journal*, **2008**, 94, 1295-302	2.9	44
127	A method to determine dielectric constants in nonhomogeneous systems: application to biological membranes. *Biophysical Journal*, **2008**, 94, 1185-93	2.9	78
126	Prediction of protein solubility from calculation of transfer free energy. *Biophysical Journal*, **2008**, 95, 2601-9	2.9	40
125	The effects of macromolecular crowding on the mechanical stability of protein molecules. *Protein Science*, **2008**, 17, 2156-66	6.3	56
124	A secondary gate as a mechanism for inhibition of the M2 proton channel by amantadine. *Journal of Physical Chemistry B*, **2008**, 112, 7977-9	3.4	95
123	Protein folding in confined and crowded environments. *Archives of Biochemistry and Biophysics*, **2008**, 469, 76-82	4.1	124
122	Prediction of salt and mutational effects on the association rate of U1A protein and U1 small nuclear RNA stem/loop II. *Journal of Physical Chemistry B*, **2008**, 112, 5955-60	3.4	22
121	On the Dielectric Boundary in Poisson-Boltzmann Calculations. *Journal of Chemical Theory and Computation*, **2008**, 4, 507-514	6.4	26
120	Accurate Calculations of Binding, Folding, and Transfer Free Energies by a Scaled Generalized Born Method. *Journal of Chemical Theory and Computation*, **2008**, 4, 1733-1744	6.4	9
119	Modeling Protein–Protein and Protein–Nucleic Acid Interactions: Structure, Thermodynamics, and Kinetics. *Annual Reports in Computational Chemistry*, **2008**, 67-87	1.8	3
118	Spontaneous conformational change and toxin binding in alpha7 acetylcholine receptor: insight into channel activation and inhibition. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 8280-5	11.5	41
117	Calculation of free-energy differences and potentials of mean force by a multi-energy gap method. *Journal of Chemical Physics*, **2008**, 128, 114104	3.9	4

116	Protein association with circular DNA: rate enhancement by nonspecific binding. *Journal of Chemical Physics*, **2008**, 128, 115108	3.9	10
115	Test of the Gouy-Chapman theory for a charged lipid membrane against explicit-solvent molecular dynamics simulations. *Physical Review Letters*, **2008**, 101, 038103	7.4	40
114	A minimum-reaction-flux solution to master-equation models of protein folding. *Journal of Chemical Physics*, **2008**, 128, 195104	3.9	6
113	The debut of PMC Biophysics. *PMC Biophysics*, **2008**, 1, 1		2
112	Electrostatic rate enhancement and transient complex of protein-protein association. *Proteins: Structure, Function and Bioinformatics*, **2008**, 71, 320-35	4.2	123
111	Effect of mixed macromolecular crowding agents on protein folding. *Proteins: Structure, Function and Bioinformatics*, **2008**, 72, 1109-13	4.2	57
110	Macromolecular crowding and confinement: biochemical, biophysical, and potential physiological consequences. *Annual Review of Biophysics*, **2008**, 37, 375-97	21.1	1553
109	Rational design of a conformation-switchable Ca2+- and Tb3+-binding protein without the use of multiple coupled metal-binding sites. *FEBS Journal*, **2008**, 275, 5048-61	5.7	9
108	GBr(6): a parameterization-free, accurate, analytical generalized born method. *Journal of Physical Chemistry B*, **2007**, 111, 3055-61	3.4	74
107	Energy landscape and transition state of protein-protein association. *Biophysical Journal*, **2007**, 92, 1486-502	2.9	55
106	Do electrostatic interactions destabilize protein-nucleic acid binding?. *Biopolymers*, **2007**, 86, 112-8	2.2	40
105	A holistic approach to protein docking. *Proteins: Structure, Function and Bioinformatics*, **2007**, 69, 743-9	4.2	18
104	Prediction of protein-protein association rates from a transition-state theory. *Structure*, **2007**, 15, 215-24	5.2	55
103	Calculation of protein-ligand binding affinities. *Annual Review of Biophysics and Biomolecular Structure*, **2007**, 36, 21-42		712
102	meta-PPISP: a meta web server for protein-protein interaction site prediction. *Bioinformatics*, **2007**, 23, 3386-7	7.2	136
101	Helix formation inside a nanotube: possible influence of backbone-water hydrogen bonding by the confining surface through modulation of water activity. *Journal of Chemical Physics*, **2007**, 127, 245101	3.9	24
100	GBr6NL: a generalized Born method for accurately reproducing solvation energy of the nonlinear Poisson-Boltzmann equation. *Journal of Chemical Physics*, **2007**, 126, 195102	3.9	38
99	DISPLAR: an accurate method for predicting DNA-binding sites on protein surfaces. *Nucleic Acids Research*, **2007**, 35, 1465-77	20.1	121

98	PI2PE: protein interface/interior prediction engine. *Nucleic Acids Research*, **2007**, 35, W357-62	20.1	29
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