Huan-Xiang Zhou

List of Publications by Citations

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	Macromolecular crowding and confinement: biochemical, biophysical, and potential physiological consequences. *Annual Review of Biophysics*, **2008**, 37, 375-97	21.1	1553
276	Calculation of protein-ligand binding affinities. *Annual Review of Biophysics and Biomolecular Structure*, **2007**, 36, 21-42		712
275	Fundamental aspects of protein-protein association kinetics. *Chemical Reviews*, **2009**, 109, 839-60	68.1	528
274	Protein design: a hierarchic approach. *Science*, **1995**, 270, 935-41	33.3	509
273	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
272	Stabilization of proteins in confined spaces. *Biochemistry*, **2001**, 40, 11289-93	3.2	345
271	Theory of free energy and entropy in noncovalent binding. *Chemical Reviews*, **2009**, 109, 4092-107	68.1	291
270	Electrostatic Interactions in Protein Structure, Folding, Binding, and Condensation. *Chemical Reviews*, **2018**, 118, 1691-1741	68.1	290
269	Prediction of protein interaction sites from sequence profile and residue neighbor list. *Proteins: Structure, Function and Bioinformatics*, **2001**, 44, 336-43	4.2	259
268	Demonstration of positionally disordered water within a protein hydrophobic cavity by NMR. *Science*, **1995**, 267, 1813-7	33.3	225
267	Histidines, heart of the hydrogen ion channel from influenza A virus: toward an understanding of conductance and proton selectivity. *Proceedings of the National Academy of Sciences of the United States of America*, **2006**, 103, 6865-70	11.5	213
266	Prediction of interface residues in protein-protein complexes by a consensus neural network method: test against NMR data. *Proteins: Structure, Function and Bioinformatics*, **2005**, 61, 21-35	4.2	213
265	Protein Allostery and Conformational Dynamics. *Chemical Reviews*, **2016**, 116, 6503-15	68.1	209
264	Conformation gating as a mechanism for enzyme specificity. *Proceedings of the National Academy of Sciences of the United States of America*, **1998**, 95, 9280-3	11.5	201
263	Influences of membrane mimetic environments on membrane protein structures. *Annual Review of Biophysics*, **2013**, 42, 361-92	21.1	199
262	Electrostatic enhancement of diffusion-controlled protein-protein association: comparison of theory and experiment on barnase and barstar. *Journal of Molecular Biology*, **1998**, 278, 1015-24	6.5	186
261	Influence of solubilizing environments on membrane protein structures. *Trends in Biochemical Sciences*, **2011**, 36, 117-25	10.3	169

260	Protein folding and binding in confined spaces and in crowded solutions. *Journal of Molecular Recognition*, **2004**, 17, 368-75	2.6	155
259	Interaction-site prediction for protein complexes: a critical assessment. *Bioinformatics*, **2007**, 23, 2203-9	7.2	143
258	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
257	meta-PPISP: a meta web server for protein-protein interaction site prediction. *Bioinformatics*, **2007**, 23, 3386-7	7.2	136
256	Brownian dynamics study of the influences of electrostatic interaction and diffusion on protein-protein association kinetics. *Biophysical Journal*, **1993**, 64, 1711-26	2.9	134
255	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
254	Fast Boundary Element Method for the Linear Poisson−Boltzmann Equation. *Journal of Physical Chemistry B*, **2002**, 106, 2741-2754	3.4	127
253	Loops, linkages, rings, catenanes, cages, and crowders: entropy-based strategies for stabilizing proteins. *Accounts of Chemical Research*, **2004**, 37, 123-30	24.3	126
252	Protein folding in confined and crowded environments. *Archives of Biochemistry and Biophysics*, **2008**, 469, 76-82	4.1	124
251	Electrostatic rate enhancement and transient complex of protein-protein association. *Proteins: Structure, Function and Bioinformatics*, **2008**, 71, 320-35	4.2	123
250	Prediction of solvent accessibility and sites of deleterious mutations from protein sequence. *Nucleic Acids Research*, **2005**, 33, 3193-9	20.1	123
249	DISPLAR: an accurate method for predicting DNA-binding sites on protein surfaces. *Nucleic Acids Research*, **2007**, 35, 1465-77	20.1	121
248	Comparison of calculation and experiment implicates significant electrostatic contributions to the binding stability of barnase and barstar. *Biophysical Journal*, **2003**, 85, 49-60	2.9	119
247	Polymer models of protein stability, folding, and interactions. *Biochemistry*, **2004**, 43, 2141-54	3.2	117
246	Community-wide assessment of protein-interface modeling suggests improvements to design methodology. *Journal of Molecular Biology*, **2011**, 414, 289-302	6.5	114
245	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
244	Boundary element solution of macromolecular electrostatics: interaction energy between two proteins. *Biophysical Journal*, **1993**, 65, 955-63	2.9	110
243	Intrinsic disorder: signaling via highly specific but short-lived association. *Trends in Biochemical Sciences*, **2012**, 37, 43-8	10.3	109

242	Rate theories for biologists. *Quarterly Reviews of Biophysics*, **2010**, 43, 219-93	7	107
241	Molecular structure of RADA16-I designer self-assembling peptide nanofibers. *ACS Nano*, **2013**, 7, 7562-72	12.7	101
240	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
239	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
238	Atomistic modeling of macromolecular crowding predicts modest increases in protein folding and binding stability. *Biophysical Journal*, **2009**, 97, 12-9	2.9	93
237	Automated prediction of protein association rate constants. *Structure*, **2011**, 19, 1744-51	5.2	91
236	Macromolecular electrostatic energy within the nonlinear Poisson□Boltzmann equation. *Journal of Chemical Physics*, **1994**, 100, 3152-3162	3.9	89
235	Effect of macromolecular crowding on protein binding stability: modest stabilization and significant biological consequences. *Biophysical Journal*, **2009**, 97, 906-11	2.9	87
234	Modeling of protein conformational fluctuations in pKa predictions. *Journal of Molecular Biology*, **1997**, 267, 1002-11	6.5	86
233	Microscopic formulation of Marcus□theory of electron transfer. *Journal of Chemical Physics*, **1995**, 103, 3481-3494	3.9	85
232	Hydrodynamic friction and the capacitance of arbitrarily shaped objects. *Physical Review E*, **1994**, 49, 5319-5331	2.4	85
231	A rate process with an entropy barrier. *Journal of Chemical Physics*, **1991**, 94, 6147-6152	3.9	83
230	The affinity-enhancing roles of flexible linkers in two-domain DNA-binding proteins. *Biochemistry*, **2001**, 40, 15069-73	3.2	82
229	Nonadditive effects of mixed crowding on protein stability. *Proteins: Structure, Function and Bioinformatics*, **2009**, 77, 133-8	4.2	81
228	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
227	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
226	A method to determine dielectric constants in nonhomogeneous systems: application to biological membranes. *Biophysical Journal*, **2008**, 94, 1185-93	2.9	78
225	Theory and simulation of the time-dependent rate coefficients of diffusion-influenced reactions. *Biophysical Journal*, **1996**, 71, 2440-57	2.9	78

224	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
223	A Brownian dynamics algorithm for calculating the hydrodynamic friction and the electrostatic capacitance of an arbitrarily shaped object. *Journal of Chemical Physics*, **1994**, 100, 3821-3826	3.9	76
222	Mechanical coupling maintains the fidelity of NMDA receptor-mediated currents. *Nature Neuroscience*, **2014**, 17, 914-22	25.5	75
221	A Gaussian-chain model for treating residual charge-charge interactions in the unfolded state of proteins. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 3569-74	11.5	75
220	GBr(6): a parameterization-free, accurate, analytical generalized born method. *Journal of Physical Chemistry B*, **2007**, 111, 3055-61	3.4	74
219	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
218	Disparate ionic-strength dependencies of on and off rates in protein-protein association. *Biopolymers*, **2001**, 59, 427-33	2.2	72
217	Electrostatic contributions to T4 lysozyme stability: solvent-exposed charges versus semi-buried salt bridges. *Biophysical Journal*, **2002**, 83, 1341-7	2.9	72
216	The gates of ion channels and enzymes. *Trends in Biochemical Sciences*, **2010**, 35, 179-85	10.3	71
215	Quantitative account of the enhanced affinity of two linked scFvs specific for different epitopes on the same antigen. *Journal of Molecular Biology*, **2003**, 329, 1-8	6.5	71
214	Loops in Proteins Can Be Modeled as Worm-Like Chains. *Journal of Physical Chemistry B*, **2001**, 105, 6763-6766	3.4	71
213	Position-dependent stabilizing effects in .alpha.-helices: N-terminal capping in synthetic model peptides. *Journal of the American Chemical Society*, **1992**, 114, 6560-6562	16.4	71
212	Modeling protein association mechanisms and kinetics. *Current Opinion in Structural Biology*, **2013**, 23, 887-93	8.1	70
211	Effects of macromolecular crowding on protein conformational changes. *PLoS Computational Biology*, **2010**, 6, e1000833	5	70
210	Data-driven docking: HADDOCK's adventures in CAPRI. *Proteins: Structure, Function and Bioinformatics*, **2005**, 60, 232-8	4.2	70
209	Chemically Driven Motility of Brownian Particles. *Physical Review Letters*, **1996**, 77, 194-197	7.4	69
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205	Rate constants and mechanisms of intrinsically disordered proteins binding to structured targets. *Physical Chemistry Chemical Physics*, **2012**, 14, 10466-76	3.6	64
204	Effects of pH, salt, and macromolecular crowding on the stability of FK506-binding protein: an integrated experimental and theoretical study. *Journal of Molecular Biology*, **2005**, 351, 219-32	6.5	64
203	Electrostatic contribution to the binding stability of protein-protein complexes. *Proteins: Structure, Function and Bioinformatics*, **2006**, 65, 87-102	4.2	64
202	Comparison between molecular dynamics simulations and the Smoluchowski theory of reactions in a hard-sphere liquid. *Journal of Chemical Physics*, **1991**, 95, 5948-5952	3.9	63
201	Why Do Disordered and Structured Proteins Behave Differently in Phase Separation?. *Trends in Biochemical Sciences*, **2018**, 43, 499-516	10.3	62
200	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
199	Theory and Simulation of Stochastically-Gated Diffusion-Influenced Reactions. *The Journal of Physical Chemistry*, **1996**, 100, 2597-2604		61
198	Effects of Mutations and Complex Formation on the Reduction Potentials of Cytochrome c and Cytochrome c Peroxidase. *Journal of the American Chemical Society*, **1994**, 116, 10362-10375	16.4	61
197	Enhancement of association rates by nonspecific binding to DNA and cell membranes. *Physical Review Letters*, **2004**, 93, 178101	7.4	60
196	Diffusive reaction rates from Brownian dynamics simulations: Replacing the outer cutoff surface by an analytical treatment. *Journal of Chemical Physics*, **1992**, 97, 5682-5686	3.9	60
195	Recent progress in structure-based anti-influenza drug design. *Drug Discovery Today*, **2012**, 17, 1111-20	8.8	58
194	Effect of mixed macromolecular crowding agents on protein folding. *Proteins: Structure, Function and Bioinformatics*, **2008**, 72, 1109-13	4.2	57
193	Two pathways mediate interdomain allosteric regulation in pin1. *Structure*, **2015**, 23, 237-247	5.2	56
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191	The effects of macromolecular crowding on the mechanical stability of protein molecules. *Protein Science*, **2008**, 17, 2156-66	6.3	56
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187	Salt Bridges Stabilize the Folded Structure of Barnase. *Journal of Physical Chemistry B*, **2001**, 105, 7334-7340	3.4	54
186	Toward the physical basis of thermophilic proteins: linking of enriched polar interactions and reduced heat capacity of unfolding. *Biophysical Journal*, **2002**, 83, 3126-33	2.9	52
185	Hydrogen bonds between short polar side chains and peptide backbone: Prevalence in proteins and effects on helix-forming propensities **1999**, 34, 497-507		52
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	Enhancement of protein-protein association rate by interaction potential: accuracy of prediction based on local Boltzmann factor. *Biophysical Journal*, **1997**, 73, 2441-5	2.9	51
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180	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
179	Crowding effects of membrane proteins. *Journal of Physical Chemistry B*, **2009**, 113, 7995-8005	3.4	47
178	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
177	Interactions of macromolecules with salt ions: an electrostatic theory for the Hofmeister effect. *Proteins: Structure, Function and Bioinformatics*, **2005**, 61, 69-78	4.2	46
176	Effects of Macromolecular Crowding on the Conformational Ensembles of Disordered Proteins. *Journal of Physical Chemistry Letters*, **2013**, 4,	6.4	44
175	Solid-state NMR and MD simulations of the antiviral drug amantadine solubilized in DMPC bilayers. *Biophysical Journal*, **2008**, 94, 1295-302	2.9	44
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170	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
169	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
168	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
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164	Intrinsically Disordered Protein Exhibits Both Compaction and Expansion under Macromolecular Crowding. *Biophysical Journal*, **2018**, 114, 1067-1079	2.9	40
163	Prediction of protein solubility from calculation of transfer free energy. *Biophysical Journal*, **2008**, 95, 2601-9	2.9	40
162	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
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159	Calculation of translational friction and intrinsic viscosity. I. General formulation for arbitrarily shaped particles. *Biophysical Journal*, **1995**, 69, 2286-97	2.9	40
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157	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
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151	Challenges in structural approaches to cell modeling. *Journal of Molecular Biology*, **2016**, 428, 2943-64	6.5	36
150	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
149	Control of reduction potential by protein matrix: lesson from a spherical protein model. *Journal of Biological Inorganic Chemistry*, **1997**, 2, 109-113	3.7	36
148	Similarity and difference in the unfolding of thermophilic and mesophilic cold shock proteins studied by molecular dynamics simulations. *Biophysical Journal*, **2006**, 91, 2451-63	2.9	36
147	A 240-Fold Electrostatic Rate-Enhancement for AcetylcholinesteraseSubstrate Binding Can Be Predicted by the Potential within the Active Site. *Journal of the American Chemical Society*, **1996**, 118, 13069-13070	16.4	36
146	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
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143	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
142	Dielectric and orientational relaxation in a Brownian dipolar lattice. *Journal of Chemical Physics*, **1992**, 97, 3610-3620	3.9	34
141	Quantitative relation between intermolecular and intramolecular binding of pro-rich peptides to SH3 domains. *Biophysical Journal*, **2006**, 91, 3170-81	2.9	32
140	Fold recognition and accurate query-template alignment by a combination of PSI-BLAST and threading. *Proteins: Structure, Function and Bioinformatics*, **2001**, 42, 23-37	4.2	32
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135	PI2PE: protein interface/interior prediction engine. *Nucleic Acids Research*, **2007**, 35, W357-62	20.1	29

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126	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
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121	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
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114	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
113	A method for computing association rate constants of atomistically represented proteins under macromolecular crowding. *Physical Biology*, **2012**, 9, 066008	3	23
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110	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
109	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
108	Effect of backbone cyclization on protein folding stability: chain entropies of both the unfolded and the folded states are restricted. *Journal of Molecular Biology*, **2003**, 332, 257-64	6.5	22
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105	Influenza A M2 Channel Clustering at High Protein/Lipid Ratios: Viral Budding Implications. *Biophysical Journal*, **2019**, 116, 1075-1084	2.9	21
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103	Solid-state NMR evidence for □hairpin structure within MAX8 designer peptide nanofibers. *Biophysical Journal*, **2013**, 105, 222-30	2.9	21
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