Charles L Brooks

List of Publications by Year
in descending order

257 papers	37,994 citations	8181 76 h-index	3182 186 g-index
261 all docs	261 docs citations	261 times ranked	29440 citing authors

#	Article	IF	Citations
1	CHARMM: The biomolecular simulation program. Journal of Computational Chemistry, 2009, 30, 1545-1614.	3.3	7,077
2	Extending the treatment of backbone energetics in protein force fields: Limitations of gas-phase quantum mechanics in reproducing protein conformational distributions in molecular dynamics simulations. Journal of Computational Chemistry, 2004, 25, 1400-1415.	3.3	3,145
3	CHARMM-GUI Input Generator for NAMD, GROMACS, AMBER, OpenMM, and CHARMM/OpenMM Simulations Using the CHARMM36 Additive Force Field. Journal of Chemical Theory and Computation, 2016, 12, 405-413.	5.3	2,567
4	Detailed analysis of grid-based molecular docking: A case study of CDOCKER?A CHARMm-based MD docking algorithm. Journal of Computational Chemistry, 2003, 24, 1549-1562.	3.3	1,299
5	A modified TIP3P water potential for simulation with Ewald summation. Journal of Chemical Physics, 2004, 121, 10096-10103.	3.0	1,063
6	Improved Treatment of the Protein Backbone in Empirical Force Fields. Journal of the American Chemical Society, 2004, 126, 698-699.	13.7	912
7	MMTSB Tool Set: enhanced sampling and multiscale modeling methods for applications in structural biology. Journal of Molecular Graphics and Modelling, 2004, 22, 377-395.	2.4	807
8	Generalized born model with a simple smoothing function. Journal of Computational Chemistry, 2003, 24, 1691-1702.	3.3	642
9	Stochastic boundary conditions for molecular dynamics simulations of ST2 water. Chemical Physics Letters, 1984, 105, 495-500.	2.6	548
10	Performance comparison of generalized born and Poisson methods in the calculation of electrostatic solvation energies for protein structures. Journal of Computational Chemistry, 2004, 25, 265-284.	3.3	523
11	Recent advances in the development and application of implicit solvent models in biomolecule simulations. Current Opinion in Structural Biology, 2004, 14, 217-224.	5.7	521
12	FROMFOLDINGTHEORIES TOFOLDINGPROTEINS: A Review and Assessment of Simulation Studies of Protein Folding and Unfolding. Annual Review of Physical Chemistry, 2001, 52, 499-535.	10.8	483
13	New analytic approximation to the standard molecular volume definition and its application to generalized Born calculations. Journal of Computational Chemistry, 2003, 24, 1348-1356.	3.3	474
14	Assessing Scoring Functions for Proteinâ^'Ligand Interactions. Journal of Medicinal Chemistry, 2004, 47, 3032-3047.	6.4	464
15	CHARMM fluctuating charge force field for proteins: I parameterization and application to bulk organic liquid simulations. Journal of Computational Chemistry, 2004, 25, 1-16.	3.3	457
16	Novel generalized Born methods. Journal of Chemical Physics, 2002, 116, 10606-10614.	3.0	416
17	CHARMM fluctuating charge force field for proteins: II Protein/solvent properties from molecular dynamics simulations using a nonadditive electrostatic model. Journal of Computational Chemistry, 2004, 25, 1504-1514.	3.3	410
18	An Implicit Membrane Generalized Born Theory for the Study of Structure, Stability, and Interactions of Membrane Proteins. Biophysical Journal, 2003, 85, 2900-2918.	0.5	384

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19	Development of a Generalized Born Model Parametrization for Proteins and Nucleic Acids. Journal of Physical Chemistry B, 1999, 103, 3765-3773.	2.6	366
20	The origins of asymmetry in the folding transition states of protein L and protein G. Protein Science, 2009, 11, 2351-2361.	7.6	352
21	Charge Screening and the Dielectric Constant of Proteins:â€‰ Insights from Molecular Dynamics. Journal of the American Chemical Society, 1996, 118, 8452-8458.	13.7	348
22	VIPERdb2: an enhanced and web API enabled relational database for structural virology. Nucleic Acids Research, 2009, 37, D436-D442.	14.5	348
23	Balancing Solvation and Intramolecular Interactions:Â Toward a Consistent Generalized Born Force Field. Journal of the American Chemical Society, 2006, 128, 3728-3736.	13.7	327
24	Î»â€dynamics: A new approach to free energy calculations. Journal of Chemical Physics, 1996, 105, 2414-2423.	3.0	324
25	Constant-pH molecular dynamics using continuous titration coordinates. Proteins: Structure, Function and Bioinformatics, 2004, 56, 738-752.	2.6	316
26	CHARMM-GUI ligand reader and modeler for CHARMM force field generation of small molecules. Journal of Computational Chemistry, 2017, 38, 1879-1886.	3.3	311
27	Comparative study of several algorithms for flexible ligand docking. Journal of Computer-Aided Molecular Design, 2003, 17, 755-763.	2.9	297
28	Recent advances in implicit solvent-based methods for biomolecular simulations. Current Opinion in Structural Biology, 2008, 18, 140-148.	5.7	294
29	Protein Dynamics in Enzymatic Catalysis:Â Exploration of Dihydrofolate Reductase. Journal of the American Chemical Society, 2000, 122, 225-231.	13.7	289
30	Constant pH Molecular Dynamics with Proton Tautomerism. Biophysical Journal, 2005, 89, 141-157.	0.5	269
31	Community-wide assessment of GPCR structure modelling and ligand docking: GPCR Dock 2008. Nature Reviews Drug Discovery, 2009, 8, 455-463.	46.4	260
32	SYMMETRY, FORM, AND SHAPE: Guiding Principles for Robustness in Macromolecular Machines. Annual Review of Biophysics and Biomolecular Structure, 2006, 35, 115-133.	18.3	251
33	Large-scale allosteric conformational transitions of adenylate kinase appear to involve a population-shift mechanism. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 18496-18501.	7.1	240
34	Insights from Coarse-Grained GÅ•Models for Protein Folding and Dynamics. International Journal of Molecular Sciences, 2009, 10, 889-905.	4.1	228
35	Statistical clustering techniques for the analysis of long molecular dynamics trajectories: analysis of 2.2-ns trajectories of YPGDV. Biochemistry, 1993, 32, 412-420.	2.5	215
36	Correlated motion and the effect of distal mutations in dihydrofolate reductase. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 6980-6985.	7.1	209

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37	Force Field Influence on the Observation of Ï€-Helical Protein Structures in Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2003, 107, 2831-2836.	2.6	204
38	Improved GÅ•like Models Demonstrate the Robustness of Protein Folding Mechanisms Towards Non-native Interactions. Journal of Molecular Biology, 2003, 334, 309-325.	4.2	200
39	Calculations on folding of segment B1 of streptococcal protein G 1 1Edited by F. Cohen. Journal of Molecular Biology, 1998, 278, 439-456.	4.2	196
40	Diversity and Identity of Mechanical Properties of Icosahedral Viral Capsids Studied with Elastic Network Normal Mode Analysis. Journal of Molecular Biology, 2005, 345, 299-314.	4.2	177
41	Virus Particle Explorer (VIPER), a Website for Virus Capsid Structures and Their Computational Analyses. Journal of Virology, 2001, 75, 11943-11947.	3.4	174
42	Toward the Accurate First-Principles Prediction of Ionization Equilibria in Proteinsâ€. Biochemistry, 2006, 45, 9363-9373.	2.5	170
43	Parametrization of halogen bonds in the CHARMM general force field: Improved treatment of ligandâ€“protein interactions. Bioorganic and Medicinal Chemistry, 2016, 24, 4812-4825.	3.0	168
44	Î»â€Dynamics free energy simulation methods. Journal of Computational Chemistry, 2009, 30, 1692-1700.	3.3	164
45	Hierarchy of RNA Functional Dynamics. Annual Review of Biochemistry, 2014, 83, 441-466.	11.1	162
46	Constant-temperature free energy surfaces for physical and chemical processes. The Journal of Physical Chemistry, 1993, 97, 4509-4513.	2.9	156
47	STATISTICAL THERMODYNAMICS: Taking a Walk on a Landscape. Science, 2001, 293, 612-613.	12.6	156
48	Linking folding with aggregation in Alzheimer's Î²-amyloid peptides. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 16880-16885.	7.1	145
49	Assessing energy functions for flexible docking. Journal of Computational Chemistry, 1998, 19, 1612-1622.	3.3	144
50	MATCH: An atomâ€typing toolset for molecular mechanics force fields. Journal of Computational Chemistry, 2012, 33, 189-202.	3.3	140
51	Implicit solvation based on generalized Born theory in different dielectric environments. Journal of Chemical Physics, 2004, 120, 903-911.	3.0	136
52	Protein and Peptide Folding Explored with Molecular Simulations. Accounts of Chemical Research, 2002, 35, 447-454.	15.6	131
53	Implicit modeling of nonpolar solvation for simulating protein folding and conformational transitions. Physical Chemistry Chemical Physics, 2008, 10, 471-481.	2.8	130
54	Thermodynamics of aqueous solvation: Solution properties of alcohols and alkanes. Journal of Chemical Physics, 1987, 87, 3029-3037.	3.0	127

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55	Ligandâ^'Protein DataBase:Â Linking Proteinâ^'Ligand Complex Structures to Binding Data. Journal of Medicinal Chemistry, 2001, 44, 3592-3598.	6.4	126
56	The structural basis for biphasic kinetics in the folding of the WW domain from a formin-binding protein: Lessons for protein design?. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 3954-3959.	7.1	126
57	Can molecular dynamics simulations provide high-resolution refinement of protein structure?. Proteins: Structure, Function and Bioinformatics, 2007, 67, 922-930.	2.6	124
58	An electrostatic basis for the stability of thermophilic proteins. Proteins: Structure, Function and Bioinformatics, 2004, 57, 128-141.	2.6	122
59	Antibody evolution constrains conformational heterogeneity by tailoring protein dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 13722-13727.	7.1	118
60	Fluctuating charge force fields: recent developments and applications from small molecules to macromolecular biological systems. Molecular Simulation, 2006, 32, 231-249.	2.0	116
61	Assessing search strategies for flexible docking. Journal of Computational Chemistry, 1998, 19, 1623-1631.	3.3	112
62	Thermodynamics of protein folding: A statistical mechanical study of a small all-Î² protein. , 1997, 42, 745-757.		106
63	Mechanics of bacteriophage maturation. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 2342-2347.	7.1	106
64	Invariant Polymorphism in Virus Capsid Assembly. Journal of the American Chemical Society, 2009, 131, 2606-2614.	13.7	105
65	Modern protein force fields behave comparably in molecular dynamics simulations. Journal of Computational Chemistry, 2002, 23, 1045-1057.	3.3	99
66	Constant pH molecular dynamics of proteins in explicit solvent with proton tautomerism. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1319-1331.	2.6	99
67	Molecular Interactions between Graphene and Biological Molecules. Journal of the American Chemical Society, 2017, 139, 1928-1936.	13.7	96
68	Do active site conformations of small ligands correspond to low free-energy solution structures?. Journal of Computer-Aided Molecular Design, 1998, 12, 563-572.	2.9	94
69	Exploring the space of protein folding Hamiltonians: The balance of forces in a minimalist Î²-barrel model. Journal of Chemical Physics, 1998, 109, 2895-2903.	3.0	92
70	WExplore: Hierarchical Exploration of High-Dimensional Spaces Using the Weighted Ensemble Algorithm. Journal of Physical Chemistry B, 2014, 118, 3532-3542.	2.6	91
71	Constant pH Molecular Dynamics Simulations of Nucleic Acids in Explicit Solvent. Journal of Chemical Theory and Computation, 2012, 8, 36-46.	5.3	89
72	Flexible <scp>CDOCKER</scp>: Development and application of a pseudoâ€explicit structureâ€based docking method within <scp>CHARMM</scp>. Journal of Computational Chemistry, 2016, 37, 753-762.	3.3	88

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73	Accurate reconstruction of all-atom protein representations from side-chain-based low-resolution models. Proteins: Structure, Function and Bioinformatics, 2000, 41, 86-97.	2.6	85
74	Exploring atomistic details of pH-dependent peptide folding. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 18546-18550.	7.1	85
75	Energetic frustration and the nature of the transition state in protein folding. Journal of Chemical Physics, 2000, 113, 7663-7671.	3.0	84
76	Multisite Î» Dynamics for Simulated Structureâ€“Activity Relationship Studies. Journal of Chemical Theory and Computation, 2011, 7, 2728-2739.	5.3	82
77	Single transcriptional and translational preQ1 riboswitches adopt similar pre-folded ensembles that follow distinct folding pathways into the same ligand-bound structure. Nucleic Acids Research, 2013, 41, 10462-10475.	14.5	81
78	A method for predicting protein structure from sequence. Current Biology, 1993, 3, 414-423.	3.9	80
79	Evaluating CASP4 predictions with physical energy functions. Proteins: Structure, Function and Bioinformatics, 2002, 49, 232-245.	2.6	78
80	Membrane Assembly of Simple Helix Homo-Oligomers Studied via Molecular Dynamics Simulations. Biophysical Journal, 2007, 92, 854-863.	0.5	75
81	Ordering a Dynamic Protein Via a Small-Molecule Stabilizer. Journal of the American Chemical Society, 2013, 135, 3363-3366.	13.7	74
82	Periodic Table of Virus Capsids: Implications for Natural Selection and Design. PLoS ONE, 2010, 5, e9423.	2.5	69
83	Application of torsion angle molecular dynamics for efficient sampling of protein conformations. Journal of Computational Chemistry, 2005, 26, 1565-1578.	3.3	67
84	Chaperone activation by unfolding. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, E1254-62.	7.1	67
85	Molecular Mechanism for Isoform-Selective Inhibition of Acyl Protein Thioesterases 1 and 2 (APT1 and) Tj ETQq1 1 0.784314 rgBT /Over	3.4	67
86	A nonadditive methanol force field: Bulk liquid and liquid-vapor interfacial properties via molecular dynamics simulations using a fluctuating charge model. Journal of Chemical Physics, 2005, 122, 024508.	3.0	66
87	A reexamination of the hydrophobic effect: Exploring the role of the solvent model in computing the methaneâ€“methane potential of mean force. Journal of Chemical Physics, 1997, 106, 9265-9269.	3.0	65
88	Integrating folding kinetics and protein function: Biphasic kinetics and dual binding specificity in a WW domain. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 3432-3437.	7.1	65
89	Are Many-Body Effects Important in Protein Folding?. Journal of Physical Chemistry B, 2000, 104, 9554-9563.	2.6	64
90	Deciphering protein evolution and fitness landscapes with latent space models. Nature Communications, 2019, 10, 5644.	12.8	64

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91	Multireference Configuration Interaction Calculations of Electronic States ofN-Methylformamide, Acetamide, andN-Methylacetamide. Journal of Physical Chemistry A, 1997, 101, 4821-4827.	2.5	63
92	Surveying implicit solvent models for estimating small molecule absolute hydration free energies. Journal of Computational Chemistry, 2011, 32, 2909-2923.	3.3	63
93	Refinement of NMR Structures Using Implicit Solvent and Advanced Sampling Techniques. Journal of the American Chemical Society, 2004, 126, 16038-16047.	13.7	60
94	Electrostatic properties of cowpea chlorotic mottle virus and cucumber mosaic virus capsids. Biopolymers, 2006, 82, 106-120.	2.4	59
95	Curious structure in â€œcanonicalâ€•alanine-based peptides. , 1997, 28, 59-71.		58
96	Barriers to Hydride Transfer in Wild Type and Mutant Dihydrofolate Reductase from E. coli. Journal of Physical Chemistry B, 2003, 107, 14042-14051.	2.6	58
97	Topological constraints: using RNA secondary structure to model 3D conformation, folding pathways, and dynamic adaptation. Current Opinion in Structural Biology, 2011, 21, 296-305.	5.7	58
98	Mechanism of Vps4 hexamer function revealed by cryo-EM. Science Advances, 2017, 3, e1700325.	10.3	58
99	Sekikaic Acid and Lobaric Acid Target a Dynamic Interface of the Coactivator CBP/p300. Angewandte Chemie - International Edition, 2012, 51, 11258-11262.	13.8	57
100	Functionally Important Conformations of the Met20 Loop in Dihydrofolate Reductase are Populated by Rapid Thermal Fluctuations. Journal of the American Chemical Society, 2009, 131, 5642-5647.	13.7	56
101	Membrane Environment Modulates the pK_a Values of Transmembrane Helices. Journal of Physical Chemistry B, 2015, 119, 4601-4607.	2.6	56
102	Prepaying the entropic cost for allosteric regulation in KIX. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 12067-12072.	7.1	55
103	Effects of Peptide Immobilization Sites on the Structure and Activity of Surface-Tethered Antimicrobial Peptides. Journal of Physical Chemistry C, 2015, 119, 7146-7155.	3.1	55
104	Adaptive Landscape Flattening Accelerates Sampling of Alchemical Space in Multisite Î» Dynamics. Journal of Physical Chemistry B, 2017, 121, 3626-3635.	2.6	54
105	Coarse Grained Models Reveal Essential Contributions of Topological Constraints to the Conformational Free Energy of RNA Bulges. Journal of Physical Chemistry B, 2014, 118, 2615-2627.	2.6	53
106	Cooperative and Directional Folding of the preQ₁ Riboswitch Aptamer Domain. Journal of the American Chemical Society, 2011, 133, 4196-4199.	13.7	52
107	Unraveling the structural complexity in a single-stranded RNA tail: implications for efficient ligand binding in the prequeuosine riboswitch. Nucleic Acids Research, 2012, 40, 1345-1355.	14.5	52
108	Visualizing chaperone-assisted protein folding. Nature Structural and Molecular Biology, 2016, 23, 691-697.	8.2	52

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109	Subdomain Competition, Cooperativity, and Topological Frustration in the Folding of CheY. Journal of Molecular Biology, 2008, 382, 485-495.	4.2	51
110	Probing Site-Specific Structural Information of Peptides at Model Membrane Interface In Situ. Journal of the American Chemical Society, 2015, 137, 10190-10198.	13.7	51
111	Investigating the Effect of Two-Point Surface Attachment on Enzyme Stability and Activity. Journal of the American Chemical Society, 2018, 140, 16560-16569.	13.7	51
112	The coupling of structural fluctuations to hydride transfer in dihydrofolate reductase. Proteins: Structure, Function and Bioinformatics, 2004, 57, 444-457.	2.6	50
113	pH-Dependent Dynamics of Complex RNA Macromolecules. Journal of Chemical Theory and Computation, 2013, 9, 935-943.	5.3	48
114	Ligand Modulates Cross-Coupling between Riboswitch Folding and Transcriptional Pausing. Molecular Cell, 2018, 72, 541-552.e6.	9.7	48
115	Viral Capsid Proteins Are Segregated in Structural Fold Space. PLoS Computational Biology, 2013, 9, e1002905.	3.2	47
116	3D maps of RNA interhelical junctions. Nature Protocols, 2011, 6, 1536-1545.	12.0	46
117	Native States of Fast-Folding Proteins Are Kinetic Traps. Journal of the American Chemical Society, 2013, 135, 4729-4734.	13.7	46
118	Modeling of the metallo-?-lactamase fromB. fragilis: Structural and dynamic effects of inhibitor binding. Proteins: Structure, Function and Bioinformatics, 2001, 44, 448-459.	2.6	44
119	How Dihydrofolate Reductase Facilitates Protonation of Dihydrofolate. Journal of the American Chemical Society, 2003, 125, 8718-8719.	13.7	44
120	Ribosome motions modulate electrostatic properties. Biopolymers, 2004, 74, 423-431.	2.4	44
121	Predicting extreme pK_a shifts in staphylococcal nuclease mutants with constant pH molecular dynamics. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3276-3286.	2.6	43
122	Determination of Viral Capsid Elastic Properties from Equilibrium Thermal Fluctuations. Physical Review Letters, 2011, 106, 188101.	7.8	43
123	Molecular-Level Insights into Orientation-Dependent Changes in the Thermal Stability of Enzymes Covalently Immobilized on Surfaces. Langmuir, 2015, 31, 6145-6153.	3.5	43
124	Effect of immobilization site on the orientation and activity of surface-tethered enzymes. Physical Chemistry Chemical Physics, 2018, 20, 1021-1029.	2.8	43
125	Automated, Accurate, and Scalable Relative Proteinâ€“Ligand Binding Free-Energy Calculations Using Lambda Dynamics. Journal of Chemical Theory and Computation, 2020, 16, 7895-7914.	5.3	43
126	Harmonic Fourier beads method for studying rare events on rugged energy surfaces. Journal of Chemical Physics, 2006, 125, 174108.	3.0	42

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127	Probing pH-Dependent Dissociation of HdeA Dimers. Journal of the American Chemical Society, 2011, 133, 19393-19398.	13.7	42
128	Frequent side chain methyl carbon-oxygen hydrogen bonding in proteins revealed by computational and stereochemical analysis of neutron structures. Proteins: Structure, Function and Bioinformatics, 2015, 83, 403-410.	2.6	42
129	Rapid Screening of Binding Affinities:Â Application of the Î»-Dynamics Method to a Trypsin-Inhibitor System. Journal of the American Chemical Society, 1998, 120, 1920-1921.	13.7	41
130	A molecular dynamics simulation study of segment B1 of protein G. , 1997, 29, 193-202.		40
131	Deprotonation by Dehydration: The Origin of Ammonium Sensing in the AmtB Channel. PLoS Computational Biology, 2007, 3, e22.	3.2	40
132	Prediction of protein loop conformations using multiscale modeling methods with physical energy scoring functions. Journal of Computational Chemistry, 2008, 29, 820-831.	3.3	40
133	Applying efficient implicit nongeometric constraints in alchemical free energy simulations. Journal of Computational Chemistry, 2011, 32, 3423-3432.	3.3	39
134	Efficient Sampling of Ligand Orientations and Conformations in Free Energy Calculations Using the Î»-Dynamics Method. Journal of Physical Chemistry B, 2000, 104, 6903-6910.	2.6	38
135	On the Morphology of Viral Capsids: Elastic Properties and Buckling Transitions. Journal of Physical Chemistry B, 2012, 116, 8604-8609.	2.6	38
136	Uncovering pH-Dependent Transient States of Proteins with Buried Ionizable Residues. Journal of the American Chemical Society, 2014, 136, 8496-8499.	13.7	38
137	Folding Intermediate in the Villin Headpiece Domain Arises from Disruption of a N-Terminal Hydrogen-Bonded Network. Journal of the American Chemical Society, 2007, 129, 3056-3057.	13.7	37
138	Exploring the Symmetry and Mechanism of Virus Capsid Maturation Via an Ensemble of Pathways. Biophysical Journal, 2012, 102, 606-612.	0.5	37
139	Generation of native-like protein structures from limited NMR data, modern force fields and advanced conformational sampling. Journal of Biomolecular NMR, 2005, 31, 59-64.	2.8	36
140	Accelerated CDOCKER with GPUs, Parallel Simulated Annealing, and Fast Fourier Transforms. Journal of Chemical Theory and Computation, 2020, 16, 3910-3919.	5.3	36
141	VIPERdb v3.0: a structure-based data analytics platform for viral capsids. Nucleic Acids Research, 2021, 49, D809-D816.	14.5	35
142	Conformational change of the methionine 20 loop ofEscherichia colidihydrofolate reductase modulates pKaof the bound dihydrofolate. Protein Science, 2007, 16, 1087-1100.	7.6	34
143	New insights into the fundamental role of topological constraints as a determinant of two-way junction conformation. Nucleic Acids Research, 2012, 40, 892-904.	14.5	34
144	Fast Solver for Large Scale Multistate Bennett Acceptance Ratio Equations. Journal of Chemical Theory and Computation, 2019, 15, 799-802.	5.3	34

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145	The importance of explicit chain representation in protein folding models: An examination of ising-like models. Proteins: Structure, Function and Bioinformatics, 2003, 53, 740-747.	2.6	33
146	FoldGPCR: Structure prediction protocol for the transmembrane domain of G proteinâ€coupled receptors from class A. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2189-2201.	2.6	33
147	Viral Capsid Equilibrium Dynamics Reveals Nonuniform Elastic Properties. Biophysical Journal, 2011, 100, L59-L61.	0.5	33
148	Conformational Dynamics of a Regulator of G-Protein Signaling Protein Reveals a Mechanism of Allosteric Inhibition by a Small Molecule. ACS Chemical Biology, 2013, 8, 2778-2784.	3.4	33
149	Gibbs Sampler-Based Î»-Dynamics and Raoâ€“Blackwell Estimator for Alchemical Free Energy Calculation. Journal of Chemical Theory and Computation, 2017, 13, 2501-2510.	5.3	33
150	Assessing the quality of absolute hydration free energies among CHARMMâ€compatible ligand parameterization schemes. Journal of Computational Chemistry, 2013, 34, 893-903.	3.3	32
151	Biasing Potential Replica Exchange Multisite Î»-Dynamics for Efficient Free Energy Calculations. Journal of Chemical Theory and Computation, 2015, 11, 1267-1277.	5.3	32
152	Molecular interactions between single layered MoS₂ and biological molecules. Chemical Science, 2018, 9, 1769-1773.	7.4	32
153	VIPERdb: A Tool for Virus Research. Annual Review of Virology, 2018, 5, 477-488.	6.7	32
154	Flipping of the Ribosomal A-Site Adenines Provides a Basis for tRNA Selection. Journal of Molecular Biology, 2014, 426, 3201-3213.	4.2	31
155	Correlation between knowledge-based and detailed atomic potentials: Application to the unfolding of the GCN4 leucine zipper. Proteins: Structure, Function and Bioinformatics, 1999, 35, 447-452.	2.6	30
156	Detailed considerations for a balanced and broadly applicable force field: A study of substituted benzenes modeled with OPLS-AA. Journal of Computational Chemistry, 2005, 26, 1529-1541.	3.3	30
157	Geometric considerations in virus capsid size specificity, auxiliary requirements, and buckling. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 8531-8536.	7.1	30
158	Tilable nature of virus capsids and the role of topological constraints in natural capsid design. Physical Review E, 2008, 77, 051902.	2.1	29
159	Topological Frustration in Î²Î±-Repeat Proteins: Sequence Diversity Modulates the Conserved Folding Mechanisms of Î±/Î²/Î± Sandwich Proteins. Journal of Molecular Biology, 2010, 398, 332-350.	4.2	29
160	Exploring Proteinâ€“Nanoparticle Interactions with Coarseâ€Grained Protein Folding Models. Small, 2017, 13, 1603748.	10.0	29
161	Conformational flexibility in free energy simulations. Chemical Physics Letters, 1989, 156, 256-260.	2.6	28
162	Improved model building and assessment of the Calciumâ€sensing receptor transmembrane domain. Proteins: Structure, Function and Bioinformatics, 2008, 71, 215-226.	2.6	28

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163	Toward Accurate Prediction of the Protonation Equilibrium of Nucleic Acids. Journal of Physical Chemistry Letters, 2013, 4, 760-766.	4.6	28
164	A Simple and Fast Approach for Predicting ¹H and ¹³C Chemical Shifts: Toward Chemical Shift-Guided Simulations of RNA. Journal of Physical Chemistry B, 2014, 118, 12168-12175.	2.6	28
165	PCASSO: A fast and efficient Cî±â€based method for accurately assigning protein secondary structure elements. Journal of Computational Chemistry, 2014, 35, 1757-1761.	3.3	28
166	Predicting Binding Free Energies in a Large Combinatorial Chemical Space Using Multisite Î» Dynamics. Journal of Physical Chemistry Letters, 2018, 9, 3328-3332.	4.6	28
167	Molecular Mechanisms of Interactions between Monolayered Transition Metal Dichalcogenides and Biological Molecules. Journal of the American Chemical Society, 2019, 141, 9980-9988.	13.7	28
168	Structural Basis for Selectivity in Flavin-Dependent Monooxygenase-Catalyzed Oxidative Dearomatization. ACS Catalysis, 2019, 9, 3633-3640.	11.2	28
169	Classical molecular dynamics. Journal of Chemical Physics, 2021, 154, 100401.	3.0	28
170	Application of Multiple Topology Î»-Dynamics to a Hostâ"Guest System:â€‰ Î²-Cyclodextrin with Substituted Benzenes. Journal of Physical Chemistry B, 2001, 105, 9316-9322.	2.6	27
171	Role of the essential light chain in the activation of smooth muscle myosin by regulatory light chain phosphorylation. Journal of Structural Biology, 2014, 185, 375-382.	2.8	27
172	Residue-level resolution of alphavirus envelope protein interactions in pH-dependent fusion. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 2034-2039.	7.1	27
173	Multiscale Modeling of a Conditionally Disordered pH-Sensing Chaperone. Journal of Molecular Biology, 2015, 427, 1670-1680.	4.2	27
174	Approaching protein design with multisite Î» dynamics: Accurate and scalable mutational folding free energies in T4 lysozyme. Protein Science, 2018, 27, 1910-1922.	7.6	26
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