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	Addressing Intersite Coupling Unlocks Large Combinatorial Chemical Spaces for Alchemical Free Energy Methods. Journal of Chemical Theory and Computation, 2022, 18, 2114-2123.	5.3	7
2	Optimizing Multisite Î»-Dynamics Throughput with Charge Renormalization. Journal of Chemical Information and Modeling, 2022, 62, 1479-1488.	5.4	8
3	Alchemical Free Energy Methods Applied to Complexes of the First Bromodomain of BRD4. Journal of Chemical Information and Modeling, 2022, 62, 1458-1470.	5.4	8
4	Allostery in the dynamic coactivator domain KIX occurs through minor conformational micro-states. PLoS Computational Biology, 2022, 18, e1009977.	3.2	3
5	A fine balance of hydrophobic-electrostatic communication pathways in a pH-switching protein. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	3
6	VIPERdb v3.0: a structure-based data analytics platform for viral capsids. Nucleic Acids Research, 2021, 49, D809-D816.	14.5	35
7	Classical molecular dynamics. Journal of Chemical Physics, 2021, 154, 100401.	3.0	28
8	Capturing the Catalytic Proton of Dihydrofolate Reductase: Implications for General Acidâ€“Base Catalysis. ACS Catalysis, 2021, 11, 5873-5884.	11.2	8
9	A strategy for proline and glycine mutations to proteins with alchemical free energy calculations. Journal of Computational Chemistry, 2021, 42, 1088-1094.	3.3	12
10	Norstictic Acid Is a Selective Allosteric Transcriptional Regulator. Journal of the American Chemical Society, 2021, 143, 9297-9302.	13.7	13
11	Generalizing the Discrete Gibbs Sampler-Based Î»-Dynamics Approach for Multisite Sampling of Many Ligands. Journal of Chemical Theory and Computation, 2021, 17, 3895-3907.	5.3	7
12	Flexible CDOCKER: Hybrid Searching Algorithm and Scoring Function with Side Chain Conformational Entropy. Journal of Chemical Information and Modeling, 2021, 61, 5535-5549.	5.4	13
13	BLaDE: A Basic Lambda Dynamics Engine for GPU-Accelerated Molecular Dynamics Free Energy Calculations. Journal of Chemical Theory and Computation, 2021, 17, 6799-6807.	5.3	23
14	Accelerating the Generalized Born with Molecular Volume and Solvent Accessible Surface Area Implicit Solvent Model Using Graphics Processing Units. Journal of Computational Chemistry, 2020, 41, 830-838.	3.3	9
15	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
16	Accelerated CDOCKER with GPUs, Parallel Simulated Annealing, and Fast Fourier Transforms. Journal of Chemical Theory and Computation, 2020, 16, 3910-3919.	5.3	36
17	Exploring pH Dependent Host/Guest Binding Affinities. Journal of Physical Chemistry B, 2020, 124, 6520-6528.	2.6	6
18	Electrostatic Forces Control the Negative Allosteric Regulation in a Disordered Protein Switch. Journal of Physical Chemistry Letters, 2020, 11, 864-868.	4.6	13

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19	M2 amphipathic helices facilitate pH-dependent conformational transition in influenza A virus. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 3583-3591.	7.1	24
20	Overcoming Challenging Substituent Perturbations with Multisite Î»-Dynamics: A Case Study Targeting Î²-Secretase 1. Journal of Physical Chemistry Letters, 2019, 10, 4875-4880.	4.6	17
21	Frustration and folding of a TIM barrel protein. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 16378-16383.	7.1	18
22	Modeling pH-Dependent NMR Chemical Shift Perturbations in Peptides. Biophysical Journal, 2019, 117, 258-268.	0.5	2
23	Computational Studies of Catalytic Loop Dynamics in Yersinia Protein Tyrosine Phosphatase Using Pathway Optimization Methods. Journal of Physical Chemistry B, 2019, 123, 7840-7851.	2.6	4
24	Hydroxyl Radical-Coupled Electron-Transfer Mechanism of Flavin-Dependent Hydroxylases. Journal of Physical Chemistry B, 2019, 123, 8065-8073.	2.6	12
25	Enhanced Sampling Applied to Modeling Allosteric Regulation in Transcription. Journal of Physical Chemistry Letters, 2019, 10, 5963-5968.	4.6	9
26	Fast Solver for Large Scale Multistate Bennett Acceptance Ratio Equations. Journal of Chemical Theory and Computation, 2019, 15, 799-802.	5.3	34
27	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
28	Positioning-Group-Enabled Biocatalytic Oxidative Dearomatization. ACS Central Science, 2019, 5, 1010-1016.	11.3	14
29	Structural Basis for Selectivity in Flavin-Dependent Monooxygenase-Catalyzed Oxidative Dearomatization. ACS Catalysis, 2019, 9, 3633-3640.	11.2	28
30	Deciphering protein evolution and fitness landscapes with latent space models. Nature Communications, 2019, 10, 5644.	12.8	64
31	CDOCKER and $$lambda$$-dynamics for prospective prediction in D3R Grand Challenge 2. Journal of Computer-Aided Molecular Design, 2018, 32, 89-102.	2.9	9
32	Molecular interactions between single layered MoS₂ and biological molecules. Chemical Science, 2018, 9, 1769-1773.	7.4	32
33	Effect of immobilization site on the orientation and activity of surface-tethered enzymes. Physical Chemistry Chemical Physics, 2018, 20, 1021-1029.	2.8	43
34	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
35	Reply to â€˜Misreading chaperoneâ€“substrate complexes from random noiseâ€™. Nature Structural and Molecular Biology, 2018, 25, 990-991.	8.2	2
36	VIPERdb: A Tool for Virus Research. Annual Review of Virology, 2018, 5, 477-488.	6.7	32

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37	Ligand Modulates Cross-Coupling between Riboswitch Folding and Transcriptional Pausing. Molecular Cell, 2018, 72, 541-552.e6.	9.7	48
38	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
39	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
40	Conservation of coactivator engagement mechanism enables small-molecule allosteric modulators. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 8960-8965.	7.1	23
41	Molecular Interactions between Graphene and Biological Molecules. Journal of the American Chemical Society, 2017, 139, 1928-1936.	13.7	96
42	Exploring Proteinâ€“Nanoparticle Interactions with Coarseâ€Grained Protein Folding Models. Small, 2017, 13, 1603748.	10.0	29
43	Adaptive Landscape Flattening Accelerates Sampling of Alchemical Space in Multisite Î» Dynamics. Journal of Physical Chemistry B, 2017, 121, 3626-3635.	2.6	54
44	A rapid solvent accessible surface area estimator for coarse grained molecular simulations. Journal of Computational Chemistry, 2017, 38, 1270-1274.	3.3	15
45	Mechanism of Vps4 hexamer function revealed by cryo-EM. Science Advances, 2017, 3, e1700325.	10.3	58
46	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
47	Gibbs Sampler-Based λ-Dynamics and Raoâ€“Blackwell Estimator for Alchemical Free Energy Calculation. Journal of Chemical Theory and Computation, 2017, 13, 2501-2510.	5.3	33
48	Growth-incompetent monomers of human calcitonin lead to a noncanonical direct relationship between peptide concentration and aggregation lag time. Journal of Biological Chemistry, 2017, 292, 14963-14976.	3.4	16
49	Tuning RNA folding and function through rational design of junction topology. Nucleic Acids Research, 2017, 45, 9706-9715.	14.5	7
50	Secondary structure encodes a cooperative tertiary folding funnel in theAzoarcusribozyme. Nucleic Acids Research, 2016, 44, 402-412.	14.5	3
51	Orientation Determination of a Hybrid Peptide Immobilized on CVD-Based Reactive Polymer Surfaces. Journal of Physical Chemistry C, 2016, 120, 19078-19086.	3.1	12
52	Nonuniform elastic properties of macromolecules and effect of prestrain on their continuum nature. Physical Review E, 2016, 93, 012417.	2.1	11
53	Capturing a Dynamic Chaperoneâ€“Substrate Interaction Using NMR-Informed Molecular Modeling. Journal of the American Chemical Society, 2016, 138, 9826-9839.	13.7	25
54	Efficient implementation of constant pH molecular dynamics on modern graphics processors. Journal of Computational Chemistry, 2016, 37, 2171-2180.	3.3	22

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55	A Synthetic Loop Replacement Peptide That Blocks Canonical NFâ€ºB Signaling. Angewandte Chemie, 2016, 128, 15221-15225.	2.0	4
56	A Synthetic Loop Replacement Peptide That Blocks Canonical NFâ€ºB Signaling. Angewandte Chemie - International Edition, 2016, 55, 14997-15001.	13.8	11
57	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
58	Parallelization and improvements of the generalized born model with a simple s<scp>W</scp>itching function for modern graphics processors. Journal of Computational Chemistry, 2016, 37, 927-939.	3.3	23
59	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
60	Visualizing chaperone-assisted protein folding. Nature Structural and Molecular Biology, 2016, 23, 691-697.	8.2	52
61	Coupled folding and binding with 2D Windowâ€Exchange Umbrella Sampling. Journal of Computational Chemistry, 2016, 37, 587-594.	3.3	21
62	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
63	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
64	Editorial. Protein Science, 2016, 25, 5-8.	7.6	0
65	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
66	PCalign: a method to quantify physicochemical similarity of protein-protein interfaces. BMC Bioinformatics, 2015, 16, 33.	2.6	16
67	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
68	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
69	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
70	pH-Dependent Transient Conformational States Control Optical Properties in Cyan Fluorescent Protein. Journal of the American Chemical Society, 2015, 137, 2892-2900.	13.7	17
71	Multiscale Modeling of a Conditionally Disordered pH-Sensing Chaperone. Journal of Molecular Biology, 2015, 427, 1670-1680.	4.2	27
72	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

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73	Noncanonical Secondary Structure Stabilizes Mitochondrial tRNA^{Ser(UCN)} by Reducing the Entropic Cost of Tertiary Folding. Journal of the American Chemical Society, 2015, 137, 3592-3599.	13.7	15
74	CapsidMaps: Proteinâ€“protein interaction pattern discovery platform for the structural analysis of virus capsids using Google Maps. Journal of Structural Biology, 2015, 190, 47-55.	2.8	9
75	Stability and orientation of cecropin P1 on maleimide self-assembled monolayer (SAM) surfaces and suggested functional mutations. Chinese Chemical Letters, 2015, 26, 485-490.	9.0	9
76	Accurate Modeling of Ionic Surfactants at High Concentration. Journal of Physical Chemistry B, 2015, 119, 6217-6224.	2.6	15
77	Membrane Environment Modulates the pK_a Values of Transmembrane Helices. Journal of Physical Chemistry B, 2015, 119, 4601-4607.	2.6	56
78	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
79	Regulation of calreticulinâ€“major histocompatibility complex (MHC) class I interactions by ATP. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E5608-17.	7.1	16
80	Proteinâ€“Protein Interfaces in Viral Capsids Are Structurally Unique. Journal of Molecular Biology, 2015, 427, 3613-3624.	4.2	5
81	Interfacial Behaviors of Antimicrobial Peptide Cecropin P1 Immobilized on Different Self-Assembled Monolayers. Journal of Physical Chemistry C, 2015, 119, 22542-22551.	3.1	20
82	Predicting Protein Backbone Chemical Shifts From CÎ± Coordinates: Extracting High Resolution Experimental Observables from Low Resolution Models. Journal of Chemical Theory and Computation, 2015, 11, 325-331.	5.3	13
83	Efficient in silico exploration of RNA interhelical conformations using Euler angles and WExplore. Nucleic Acids Research, 2014, 42, 12126-12137.	14.5	25
84	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
85	Flipping of the Ribosomal A-Site Adenines Provides a Basis for tRNA Selection. Journal of Molecular Biology, 2014, 426, 3201-3213.	4.2	31
86	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
87	Topological constraints are major determinants of tRNA tertiary structure and dynamics and provide basis for tertiary folding cooperativity. Nucleic Acids Research, 2014, 42, 11792-11804.	14.5	22
88	Hamiltonian Mapping Revisited: Calibrating Minimalist Models to Capture Molecular Recognition by Intrinsically Disordered Proteins. Journal of Physical Chemistry Letters, 2014, 5, 3441-3444.	4.6	11
89	WExplore: Hierarchical Exploration of High-Dimensional Spaces Using the Weighted Ensemble Algorithm. Journal of Physical Chemistry B, 2014, 118, 3532-3542.	2.6	91
90	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

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91	Constant pH molecular dynamics of proteins in explicit solvent with proton tautomerism. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1319-1331.	2.6	99
92	pH-Induced Stability Switching of the Bacteriophage HK97 Maturation Pathway. Journal of the American Chemical Society, 2014, 136, 3097-3107.	13.7	21
93	Hierarchy of RNA Functional Dynamics. Annual Review of Biochemistry, 2014, 83, 441-466.	11.1	162
94	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
95	Modulation of frustration in folding by sequence permutation. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 10562-10567.	7.1	24
96	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
97	Uncovering pH-Dependent Transient States of Proteins with Buried Ionizable Residues. Journal of the American Chemical Society, 2014, 136, 8496-8499.	13.7	38
98	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
99	Native States of Fast-Folding Proteins Are Kinetic Traps. Journal of the American Chemical Society, 2013, 135, 4729-4734.	13.7	46
100	Toward Accurate Prediction of the Protonation Equilibrium of Nucleic Acids. Journal of Physical Chemistry Letters, 2013, 4, 760-766.	4.6	28
101	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
102	Ordering a Dynamic Protein Via a Small-Molecule Stabilizer. Journal of the American Chemical Society, 2013, 135, 3363-3366.	13.7	74
103	Deconstructing Activation Events in Rhodopsin. Journal of the American Chemical Society, 2013, 135, 10906-10909.	13.7	15
104	Binding and Folding of the Small Bacterial Chaperone HdeA. Journal of Physical Chemistry B, 2013, 117, 13219-13225.	2.6	16
105	pH-Dependent Dynamics of Complex RNA Macromolecules. Journal of Chemical Theory and Computation, 2013, 9, 935-943.	5.3	48
106	Quantifying Chaperone-Mediated Transitions in the Proteostasis Network of E. coli. PLoS Computational Biology, 2013, 9, e1003324.	3.2	5
107	Viral Capsid Proteins Are Segregated in Structural Fold Space. PLoS Computational Biology, 2013, 9, e1002905.	3.2	47
108	Chaperone activation by unfolding. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, E1254-62.	7.1	67

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109	pHâ€sensitive residues in the p19 RNA silencing suppressor protein from carnation Italian ringspot virus affect siRNA binding stability. Protein Science, 2013, 22, 595-604.	7.6	18
110	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
111	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
112	Mechanics of bacteriophage maturation. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 2342-2347.	7.1	106
113	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
114	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
115	Constant pH Molecular Dynamics Simulations of Nucleic Acids in Explicit Solvent. Journal of Chemical Theory and Computation, 2012, 8, 36-46.	5.3	89
116	FROM MOLECULAR PHYLOGENETICS TO QUANTUM CHEMISTRY: DISCOVERING ENZYME DESIGN PRINCIPLES THROUGH COMPUTATION. Computational and Structural Biotechnology Journal, 2012, 2, e201209018.	4.1	2
117	On the Morphology of Viral Capsids: Elastic Properties and Buckling Transitions. Journal of Physical Chemistry B, 2012, 116, 8604-8609.	2.6	38
118	Quantifying Hub-like Behavior in Protein Folding Networks. Journal of Chemical Theory and Computation, 2012, 8, 3044-3052.	5.3	22
119	Exploring the Symmetry and Mechanism of Virus Capsid Maturation Via an Ensemble of Pathways. Biophysical Journal, 2012, 102, 606-612.	0.5	37
120	MATCH: An atomâ€typing toolset for molecular mechanics force fields. Journal of Computational Chemistry, 2012, 33, 189-202.	3.3	140
121	Multiscale Modeling of Virus Structure, Assembly, and Dynamics. Biological and Medical Physics Series, 2012, , 167-189.	0.4	0
122	Cooperative and Directional Folding of the preQ₁ Riboswitch Aptamer Domain. Journal of the American Chemical Society, 2011, 133, 4196-4199.	13.7	52
123	Viral Capsid Equilibrium Dynamics Reveals Nonuniform Elastic Properties. Biophysical Journal, 2011, 100, L59-L61.	0.5	33
124	Probing pH-Dependent Dissociation of HdeA Dimers. Journal of the American Chemical Society, 2011, 133, 19393-19398.	13.7	42
125	Multisite Î» Dynamics for Simulated Structureâ€“Activity Relationship Studies. Journal of Chemical Theory and Computation, 2011, 7, 2728-2739.	5.3	82
126	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

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127	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
128	A Mechanism for Evolving Novel Plant Sesquiterpene Synthase Function. Molecular Informatics, 2011, 30, 896-906.	2.5	19
129	Surveying implicit solvent models for estimating small molecule absolute hydration free energies. Journal of Computational Chemistry, 2011, 32, 2909-2923.	3.3	63
130	Applying efficient implicit nongeometric constraints in alchemical free energy simulations. Journal of Computational Chemistry, 2011, 32, 3423-3432.	3.3	39
131	Determination of Viral Capsid Elastic Properties from Equilibrium Thermal Fluctuations. Physical Review Letters, 2011, 106, 188101.	7.8	43
132	3D maps of RNA interhelical junctions. Nature Protocols, 2011, 6, 1536-1545.	12.0	46
133	Steric and thermodynamic limits of design for the incorporation of large unnatural amino acids in aminoacylâ€tRNA synthetase enzymes. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1926-1938.	2.6	4
134	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
135	The flexible Câ€terminal arm of the Lassa arenavirus Zâ€protein mediates interactions with multiple binding partners. Proteins: Structure, Function and Bioinformatics, 2010, 78, 2251-2264.	2.6	11
136	Periodic Table of Virus Capsids: Implications for Natural Selection and Design. PLoS ONE, 2010, 5, e9423.	2.5	69
137	Hexameric Helicase Deconstructed: Interplay of Conformational Changes and Substrate Coupling. Biophysical Journal, 2010, 98, 1449-1457.	0.5	15
138	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
139	VIPERdb2: an enhanced and web API enabled relational database for structural virology. Nucleic Acids Research, 2009, 37, D436-D442.	14.5	348
140	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
141	CHARMM: The biomolecular simulation program. Journal of Computational Chemistry, 2009, 30, 1545-1614.	3.3	7,077
142	Î»â€Dynamics free energy simulation methods. Journal of Computational Chemistry, 2009, 30, 1692-1700.	3.3	164
143	Predicting structurally conserved contacts for homologous proteins using sequence conservation filters. Proteins: Structure, Function and Bioinformatics, 2009, 77, 448-453.	2.6	11
144	Community-wide assessment of GPCR structure modelling and ligand docking: GPCR Dock 2008. Nature Reviews Drug Discovery, 2009, 8, 455-463.	46.4	260

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145	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
146	Invariant Polymorphism in Virus Capsid Assembly. Journal of the American Chemical Society, 2009, 131, 2606-2614.	13.7	105
147	Insights from Coarse-Grained GÅ•Models for Protein Folding and Dynamics. International Journal of Molecular Sciences, 2009, 10, 889-905.	4.1	228
148	The origins of asymmetry in the folding transition states of protein L and protein G. Protein Science, 2009, 11, 2351-2361.	7.6	352
149	Validating CHARMM Parameters and Exploring Charge Distribution Rules in Structure-Based Drug Design. Journal of Chemical Theory and Computation, 2009, 5, 1680-1691.	5.3	13
150	De novo modeling of GPCR class A structures. , 2009, , .		0
151	Improved model building and assessment of the Calciumâ€sensing receptor transmembrane domain. Proteins: Structure, Function and Bioinformatics, 2008, 71, 215-226.	2.6	28
152	A novel method to map and compare proteinâ€“protein interactions in spherical viral capsids. Proteins: Structure, Function and Bioinformatics, 2008, 73, 644-655.	2.6	13
153	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
154	Implicit modeling of nonpolar solvation for simulating protein folding and conformational transitions. Physical Chemistry Chemical Physics, 2008, 10, 471-481.	2.8	130
155	Recent advances in implicit solvent-based methods for biomolecular simulations. Current Opinion in Structural Biology, 2008, 18, 140-148.	5.7	294
156	Coevolution of Function and the Folding Landscape: Correlation with Density of Native Contacts. Biophysical Journal, 2008, 95, L57-L59.	0.5	18
157	Subdomain Competition, Cooperativity, and Topological Frustration in the Folding of CheY. Journal of Molecular Biology, 2008, 382, 485-495.	4.2	51
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	De Novo Prediction of the Structures of M. tuberculosis Membrane Proteins. Journal of the American Chemical Society, 2008, 130, 5384-5385.	13.7	10
160	Deprotonation by Dehydration: The Origin of Ammonium Sensing in the AmtB Channel. PLoS Computational Biology, 2007, 3, e22.	3.2	40
161	Chapter 1 Molecular Simulations of pH-Mediated Biological Processes. Annual Reports in Computational Chemistry, 2007, , 3-13.	1.7	7
162	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

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163	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
164	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
165	Membrane Assembly of Simple Helix Homo-Oligomers Studied via Molecular Dynamics Simulations. Biophysical Journal, 2007, 92, 854-863.	0.5	75
166	Can molecular dynamics simulations provide high-resolution refinement of protein structure?. Proteins: Structure, Function and Bioinformatics, 2007, 67, 922-930.	2.6	124
167	Conformational change of the methionine 20 loop ofEscherichia colidihydrofolate reductase modulates pKaof the bound dihydrofolate. Protein Science, 2007, 16, 1087-1100.	7.6	34
168	Fluctuating charge force fields: recent developments and applications from small molecules to macromolecular biological systems. Molecular Simulation, 2006, 32, 231-249.	2.0	116
169	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
170	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
171	Toward the Accurate First-Principles Prediction of Ionization Equilibria in Proteinsâ€. Biochemistry, 2006, 45, 9363-9373.	2.5	170
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