

Robert B Best

List of Publications by Year in descending order

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Version: 2024-02-01

170
papers

20,340
citations

14655

66
h-index

12272

133
g-index

193
all docs

193
docs citations

193
times ranked

16330
citing authors

#	ARTICLE	IF	CITATIONS
1	Optimization of the Additive CHARMM All-Atom Protein Force Field Targeting Improved Sampling of the Backbone ϕ , ψ and Side-Chain χ_1 and χ_2 Dihedral Angles. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3257-3273.	5.3	3,696
2	Optimized Molecular Dynamics Force Fields Applied to the Helix \rightarrow Coil Transition of Polypeptides. <i>Journal of Physical Chemistry B</i> , 2009, 113, 9004-9015.	2.6	767
3	Simultaneous determination of protein structure and dynamics. <i>Nature</i> , 2005, 433, 128-132.	27.8	641
4	Balanced Protein-Water Interactions Improve Properties of Disordered Proteins and Non-Specific Protein Association. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5113-5124.	5.3	564
5	Martini 3: a general purpose force field for coarse-grained molecular dynamics. <i>Nature Methods</i> , 2021, 18, 382-388.	19.0	557
6	Phosphorylation of the α -FUS low-complexity domain disrupts phase separation, aggregation, and toxicity. <i>EMBO Journal</i> , 2017, 36, 2951-2967.	7.8	544
7	Extreme disorder in an ultrahigh-affinity protein complex. <i>Nature</i> , 2018, 555, 61-66.	27.8	538
8	Polarizable Atomic Multipole-Based AMOEBA Force Field for Proteins. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4046-4063.	5.3	524
9	Native contacts determine protein folding mechanisms in atomistic simulations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 17874-17879.	7.1	490
10	Reaction coordinates and rates from transition paths. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 6732-6737.	7.1	483
11	Sequence determinants of protein phase behavior from a coarse-grained model. <i>PLoS Computational Biology</i> , 2018, 14, e1005941.	3.2	427
12	Are Current Molecular Dynamics Force Fields too Helical?. <i>Biophysical Journal</i> , 2008, 95, L07-L09.	0.5	419
13	Biomolecular Phase Separation: From Molecular Driving Forces to Macroscopic Properties. <i>Annual Review of Physical Chemistry</i> , 2020, 71, 53-75.	10.8	368
14	Characterizing the unfolded states of proteins using single-molecule FRET spectroscopy and molecular simulations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 1528-1533.	7.1	327
15	Relation between single-molecule properties and phase behavior of intrinsically disordered proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 9929-9934.	7.1	283
16	Hidden complexity in the mechanical properties of titin. <i>Nature</i> , 2003, 422, 446-449.	27.8	268
17	Coordinate-dependent diffusion in protein folding. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 1088-1093.	7.1	253
18	Can Non-Mechanical Proteins Withstand Force? Stretching Barnase by Atomic Force Microscopy and Molecular Dynamics Simulation. <i>Biophysical Journal</i> , 2001, 81, 2344-2356.	0.5	234

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19	Protein Simulations with an Optimized Water Model: Cooperative Helix Formation and Temperature-Induced Unfolded State Collapse. <i>Journal of Physical Chemistry B</i> , 2010, 114, 14916-14923.	2.6	233
20	Single-molecule spectroscopy of the temperature-induced collapse of unfolded proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 20740-20745.	7.1	211
21	Effect of flexibility and <i>cis</i> residues in single-molecule FRET studies of polyproline. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 18964-18969.	7.1	201
22	Mechanical Unfolding of a Titin Ig Domain: Structure of Unfolding Intermediate Revealed by Combining AFM, Molecular Dynamics Simulations, NMR and Protein Engineering. <i>Journal of Molecular Biology</i> , 2002, 322, 841-849.	4.2	200
23	Binding-Induced Folding of a Natively Unstructured Transcription Factor. <i>PLoS Computational Biology</i> , 2008, 4, e1000060.	3.2	189
24	Computational and theoretical advances in studies of intrinsically disordered proteins. <i>Current Opinion in Structural Biology</i> , 2017, 42, 147-154.	5.7	186
25	Consistent View of Polypeptide Chain Expansion in Chemical Denaturants from Multiple Experimental Methods. <i>Journal of the American Chemical Society</i> , 2016, 138, 11714-11726.	13.7	171
26	Mechanical Unfolding of a Titin Ig Domain: Structure of Transition State Revealed by Combining Atomic Force Microscopy, Protein Engineering and Molecular Dynamics Simulations. <i>Journal of Molecular Biology</i> , 2003, 330, 867-877.	4.2	168
27	Diffusive Model of Protein Folding Dynamics with Kramers Turnover in Rate. <i>Physical Review Letters</i> , 2006, 96, 228104.	7.8	165
28	Temperature-dependent solvation modulates the dimensions of disordered proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 5213-5218.	7.1	161
29	Slow Protein Conformational Dynamics from Multiple Experimental Structures: The Helix/Sheet Transition of Arc Repressor. <i>Structure</i> , 2005, 13, 1755-1763.	3.3	160
30	Single-molecule fluorescence reveals sequence-specific misfolding in multidomain proteins. <i>Nature</i> , 2011, 474, 662-665.	27.8	158
31	Thermodynamics and kinetics of protein folding under confinement. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 20233-20238.	7.1	146
32	Relation between native ensembles and experimental structures of proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 10901-10906.	7.1	136
33	Pulling Direction as a Reaction Coordinate for the Mechanical Unfolding of Single Molecules. <i>Journal of Physical Chemistry B</i> , 2008, 112, 5968-5976.	2.6	135
34	Inclusion of Many-Body Effects in the Additive CHARMM Protein CMAP Potential Results in Enhanced Cooperativity of I [±] -Helix and I ² -Hairpin Formation. <i>Biophysical Journal</i> , 2012, 103, 1045-1051.	0.5	130
35	Atomistic molecular simulations of protein folding. <i>Current Opinion in Structural Biology</i> , 2012, 22, 52-61.	5.7	129
36	Molecular Details of Protein Condensates Probed by Microsecond Long Atomistic Simulations. <i>Journal of Physical Chemistry B</i> , 2020, 124, 11671-11679.	2.6	127

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37	Determination of Protein Structures Consistent with NMR Order Parameters. <i>Journal of the American Chemical Society</i> , 2004, 126, 8090-8091.	13.7	126
38	Computer Folding of RNA Tetraloops: Identification of Key Force Field Deficiencies. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4534-4548.	5.3	125
39	Probing the Action of Chemical Denaturant on an Intrinsically Disordered Protein by Simulation and Experiment. <i>Journal of the American Chemical Society</i> , 2016, 138, 11702-11713.	13.7	121
40	Force mode atomic force microscopy as a tool for protein folding studies. <i>Analytica Chimica Acta</i> , 2003, 479, 87-105.	5.4	120
41	Structural Interpretation of Hydrogen Exchange Protection Factors in Proteins: Characterization of the Native State Fluctuations of Cl2. <i>Structure</i> , 2006, 14, 97-106.	3.3	115
42	Free energy landscape of the GB1 hairpin in all-atom explicit solvent simulations with different force fields: Similarities and differences. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 1318-1328.	2.6	112
43	Tackling Force-Field Bias in Protein Folding Simulations: Folding of Villin HP35 and Pin WW Domains in Explicit Water. <i>Biophysical Journal</i> , 2010, 99, L26-L28.	0.5	105
44	Mechanism of O2 diffusion and reduction in FeFe hydrogenases. <i>Nature Chemistry</i> , 2017, 9, 88-95.	13.6	105
45	A Preformed Binding Interface in the Unbound Ensemble of an Intrinsically Disordered Protein: Evidence from Molecular Simulations. <i>PLoS Computational Biology</i> , 2012, 8, e1002605.	3.2	104
46	Physics-based computational and theoretical approaches to intrinsically disordered proteins. <i>Current Opinion in Structural Biology</i> , 2021, 67, 219-225.	5.7	101
47	Molecular origins of internal friction effects on protein-folding rates. <i>Nature Communications</i> , 2014, 5, 4307.	12.8	98
48	Residue-Specific α -Helix Propensities from Molecular Simulation. <i>Biophysical Journal</i> , 2012, 102, 1462-1467.	0.5	97
49	Transient misfolding dominates multidomain protein folding. <i>Nature Communications</i> , 2015, 6, 8861.	12.8	97
50	Improving the Performance of the Amber RNA Force Field by Tuning the Hydrogen-Bonding Interactions. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3288-3305.	5.3	97
51	Balance between α and β Structures in Ab Initio Protein Folding. <i>Journal of Physical Chemistry B</i> , 2010, 114, 8790-8798.	2.6	96
52	Comparing a simple theoretical model for protein folding with all-atom molecular dynamics simulations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 17880-17885.	7.1	94
53	A simple method for probing the mechanical unfolding pathway of proteins in detail. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002, 99, 12143-12148.	7.1	93
54	Convergence and Sampling in Determining Free Energy Landscapes for Membrane Protein Association. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3364-3375.	2.6	93

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55	What Contributions to Protein Side-chain Dynamics are Probed by NMR Experiments? A Molecular Dynamics Simulation Analysis. <i>Journal of Molecular Biology</i> , 2005, 349, 185-203.	4.2	92
56	Highly Disordered Amyloid- β^2 Monomer Probed by Single-Molecule FRET and MD Simulation. <i>Biophysical Journal</i> , 2018, 114, 870-884.	0.5	88
57	Peptide Chain Dynamics in Light and Heavy Water: Zooming in on Internal Friction. <i>Journal of the American Chemical Society</i> , 2012, 134, 6273-6279.	13.7	86
58	Folding pathway of an Ig domain is conserved on and off the ribosome. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E11284-E11293.	7.1	86
59	Computer Folding of RNA Tetraloops? Are We There Yet?. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2115-2125.	5.3	84
60	Inferring properties of disordered chains from FRET transfer efficiencies. <i>Journal of Chemical Physics</i> , 2018, 148, 123329.	3.0	84
61	Modulation of an IDP binding mechanism and rates by helix propensity and non-native interactions: association of HIF1 β with CBP. <i>Molecular BioSystems</i> , 2012, 8, 256-267.	2.9	83
62	Dependence of Protein Folding Stability and Dynamics on the Density and Composition of Macromolecular Crowders. <i>Biophysical Journal</i> , 2010, 98, 315-320.	0.5	81
63	Diffusion models of protein folding. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 16902.	2.8	76
64	Mechanism of membrane-tethered mitochondrial protein synthesis. <i>Science</i> , 2021, 371, 846-849.	12.6	76
65	Polyelectrolyte interactions enable rapid association and dissociation in high-affinity disordered protein complexes. <i>Nature Communications</i> , 2020, 11, 5736.	12.8	74
66	Using Ligand-Mapping Simulations to Design a Ligand Selectively Targeting a Cryptic Surface Pocket of Polo-Like Kinase 1. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 10078-10081.	13.8	71
67	Force-Field Dependence of Chignolin Folding and Misfolding: Comparison with Experiment and Redesign. <i>Biophysical Journal</i> , 2012, 102, 1897-1906.	0.5	71
68	A Data-Driven Hydrophobicity Scale for Predicting Liquid-Liquid Phase Separation of Proteins. <i>Journal of Physical Chemistry B</i> , 2021, 125, 4046-4056.	2.6	71
69	Sequence- and Temperature-Dependent Properties of Unfolded and Disordered Proteins from Atomistic Simulations. <i>Journal of Physical Chemistry B</i> , 2015, 119, 14622-14630.	2.6	70
70	Locating the Barrier for Folding of Single Molecules under an External Force. <i>Physical Review Letters</i> , 2011, 107, 208301.	7.8	69
71	Macromolecular crowding effects on protein-protein binding affinity and specificity. <i>Journal of Chemical Physics</i> , 2010, 133, 205101.	3.0	68
72	What Is the Time Scale for β -Helix Nucleation?. <i>Journal of the American Chemical Society</i> , 2011, 133, 6809-6816.	13.7	68

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73	Microscopic events in β -hairpin folding from alternative unfolded ensembles. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 11087-11092.	7.1	67
74	Designing an extracellular matrix protein with enhanced mechanical stability. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 9633-9637.	7.1	66
75	Multiscale Simulation Reveals Multiple Pathways for H ₂ and O ₂ Transport in a [NiFe]-Hydrogenase. Journal of the American Chemical Society, 2011, 133, 3548-3556.	13.7	65
76	Evolution of All-Atom Protein Force Fields to Improve Local and Global Properties. Journal of Physical Chemistry Letters, 2019, 10, 2227-2234.	4.6	65
77	The shape of the bacterial ribosome exit tunnel affects cotranslational protein folding. ELife, 2018, 7, .	6.0	65
78	An Extended Guinier Analysis for Intrinsically Disordered Proteins. Journal of Molecular Biology, 2018, 430, 2540-2553.	4.2	64
79	Molecular Dynamics and NMR Study of the β 1-4 and β 1-6 Glycosidic Linkages: Maltose and Isomaltose. Journal of Physical Chemistry B, 2001, 105, 4742-4751.	2.6	61
80	The Origin of Protein Sidechain Order Parameter Distributions. Journal of the American Chemical Society, 2004, 126, 7734-7735.	13.7	59
81	Quantitative Interpretation of FRET Experiments via Molecular Simulation: Force Field and Validation. Biophysical Journal, 2015, 108, 2721-2731.	0.5	59
82	Disordered RNA chaperones can enhance nucleic acid folding via local charge screening. Nature Communications, 2019, 10, 2453.	12.8	59
83	Co-Evolutionary Fitness Landscapes for Sequence Design. Angewandte Chemie - International Edition, 2018, 57, 5674-5678.	13.8	58
84	Insights into the binding of intrinsically disordered proteins from molecular dynamics simulation. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 182-198.	14.6	56
85	Microscopic interpretation of folding Δ -values using the transition path ensemble. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 3263-3268.	7.1	55
86	Treatment of sickle cell disease by increasing oxygen affinity of hemoglobin. Blood, 2021, 138, 1172-1181.	1.4	52
87	A small single-domain protein folds through the same pathway on and off the ribosome. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 12206-12211.	7.1	51
88	What can atomic force microscopy tell us about protein folding?. Chemical Communications, 2002, , 183-192.	4.1	50
89	Force-Induced Change in Protein Unfolding Mechanism: Discrete or Continuous Switch?. Journal of Physical Chemistry B, 2011, 115, 1546-1561.	2.6	50
90	Interpreting Dynamically-Averaged Scalar Couplings in Proteins. Journal of Biomolecular NMR, 2005, 32, 273-280.	2.8	46

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91	Variational Optimization of an All-Atom Implicit Solvent Force Field To Match Explicit Solvent Simulation Data. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5641-5652.	5.3	46
92	Discriminating binding mechanisms of an intrinsically disordered protein via a multi-state coarse-grained model. <i>Journal of Chemical Physics</i> , 2014, 140, 175102.	3.0	46
93	Accurate Transfer Efficiencies, Distance Distributions, and Ensembles of Unfolded and Intrinsically Disordered Proteins From Single-Molecule FRET. <i>Methods in Enzymology</i> , 2018, 611, 287-325.	1.0	46
94	Evidence for a Partially Structured State of the Amylin Monomer. <i>Biophysical Journal</i> , 2009, 97, 2948-2957.	0.5	45
95	Multiple lipid binding sites determine the affinity of PH domains for phosphoinositide-containing membranes. <i>Science Advances</i> , 2020, 6, eaay5736.	10.3	44
96	Dependence of Internal Friction on Folding Mechanism. <i>Journal of the American Chemical Society</i> , 2015, 137, 3283-3290.	13.7	41
97	Protein Folding Kinetics Under Force from Molecular Simulation. <i>Journal of the American Chemical Society</i> , 2008, 130, 3706-3707.	13.7	40
98	Balancing Force Field Protein-Lipid Interactions To Capture Transmembrane Helix-Helix Association. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1706-1715.	5.3	40
99	A mutant chaperonin with rearranged inter-ring electrostatic contacts and temperature-sensitive dissociation. <i>Nature Structural and Molecular Biology</i> , 2004, 11, 1128-1133.	8.2	39
100	Hydrophobic Core Fluidity of Homologous Protein Domains: A Relation of Side-Chain Dynamics to Core Composition and Packing. <i>Biochemistry</i> , 2004, 43, 1145-1155.	2.5	38
101	Characterization of the residual structure in the unfolded state of the $\hat{1}^{131}$ fragment of staphylococcal nuclease. <i>Proteins: Structure, Function and Bioinformatics</i> , 2006, 65, 145-152.	2.6	38
102	How Many Protein Sequences Fold to a Given Structure? A Coevolutionary Analysis. <i>Biophysical Journal</i> , 2017, 113, 1719-1730.	0.5	38
103	Comment on "Force-Clamp Spectroscopy Monitors the Folding Trajectory of a Single Protein". <i>Science</i> , 2005, 308, 498b-498b.	12.6	37
104	Release of linker histone from the nucleosome driven by polyelectrolyte competition with a disordered protein. <i>Nature Chemistry</i> , 2022, 14, 224-231.	13.6	37
105	Comment on "Innovative scattering analysis shows that hydrophobic disordered proteins are expanded in water". <i>Science</i> , 2018, 361, .	12.6	36
106	Atomistic Insights into Rhodopsin Activation from a Dynamic Model. <i>Journal of the American Chemical Society</i> , 2008, 130, 10141-10149.	13.7	35
107	Folding Kinetics and Unfolded State Dynamics of the GB1 Hairpin from Molecular Simulation. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1743-1753.	5.3	35
108	Effects of Interactions with the GroEL Cavity on Protein Folding Rates. <i>Biophysical Journal</i> , 2013, 104, 1098-1106.	0.5	34

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109	Complex Energy Landscape of a Giant Repeat Protein. <i>Structure</i> , 2013, 21, 1954-1965.	3.3	33
110	Reduction of All-Atom Protein Folding Dynamics to One-Dimensional Diffusion. <i>Journal of Physical Chemistry B</i> , 2015, 119, 15247-15255.	2.6	31
111	Structural Determinants of Misfolding in Multidomain Proteins. <i>PLoS Computational Biology</i> , 2016, 12, e1004933.	3.2	30
112	Modest Influence of FRET Chromophores on the Properties of Unfolded Proteins. <i>Biophysical Journal</i> , 2014, 107, 1654-1660.	0.5	29
113	Tandem domain swapping: determinants of multidomain protein misfolding. <i>Current Opinion in Structural Biology</i> , 2019, 58, 97-104.	5.7	28
114	A microscopic model for gas diffusion dynamics in a [NiFe]-hydrogenase. <i>Physical Chemistry Chemical Physics</i> , 2011, 13, 7708.	2.8	27
115	The ribosome modulates folding inside the ribosomal exit tunnel. <i>Communications Biology</i> , 2021, 4, 523.	4.4	27
116	Aerobic Damage to [FeFe]-Hydrogenases: Activation Barriers for the Chemical Attachment of O ₂ . <i>Angewandte Chemie - International Edition</i> , 2014, 53, 4081-4084.	13.8	26
117	Markov state models of protein misfolding. <i>Journal of Chemical Physics</i> , 2016, 144, 075101.	3.0	26
118	Emerging consensus on the collapse of unfolded and intrinsically disordered proteins in water. <i>Current Opinion in Structural Biology</i> , 2020, 60, 27-38.	5.7	26
119	Cutting antiparallel DNA strands in a single active site. <i>Nature Structural and Molecular Biology</i> , 2020, 27, 119-126.	8.2	25
120	Matching of Additive and Polarizable Force Fields for Multiscale Condensed Phase Simulations. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2826-2837.	5.3	24
121	Cotranslational folding cooperativity of contiguous domains of α -spectrin. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 14119-14126.	7.1	24
122	Crosstalk between the Protein Surface and Hydrophobic Core in a Core-swapped Fibronectin Type III Domain. <i>Journal of Molecular Biology</i> , 2008, 375, 560-571.	4.2	23
123	Empirical Optimization of Interactions between Proteins and Chemical Denaturants in Molecular Simulations. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 5543-5553.	5.3	23
124	Structural Comparison of the Two Alternative Transition States for Folding of TI I27. <i>Biophysical Journal</i> , 2006, 91, 263-275.	0.5	21
125	Smoothing of the GB1 Hairpin Folding Landscape by Interfacial Confinement. <i>Biophysical Journal</i> , 2012, 103, 596-600.	0.5	21
126	Pressure-induced structural transition of mature HIV-1 protease from a combined μ -NMR/MD simulation approach. <i>Proteins: Structure, Function and Bioinformatics</i> , 2015, 83, 2117-2123.	2.6	21

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127	Diffusive Dynamics of Contact Formation in Disordered Polypeptides. <i>Physical Review Letters</i> , 2016, 116, 068102.	7.8	21
128	Exploring the sequence fitness landscape of a bridge between protein folds. <i>PLoS Computational Biology</i> , 2020, 16, e1008285.	3.2	20
129	Origin of Internal Friction in Disordered Proteins Depends on Solvent Quality. <i>Journal of Physical Chemistry B</i> , 2018, 122, 11478-11487.	2.6	19
130	Molecular Determinants of Al^{2+} Adsorption to Amyloid Fibril Surfaces. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 6437-6443.	4.6	19
131	Modeling the β Branch Point of Amylopectin in Solution. <i>Journal of Physical Chemistry B</i> , 2002, 106, 5091-5098.	2.6	18
132	Single-molecule Detection of Ultrafast Biomolecular Dynamics with Nanophotonics. <i>Journal of the American Chemical Society</i> , 2022, 144, 52-56.	13.7	18
133	Effect of interactions with the chaperonin cavity on protein folding and misfolding. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 6358-6366.	2.8	17
134	How Well Does a Funneled Energy Landscape Capture the Folding Mechanism of Spectrin Domains?. <i>Journal of Physical Chemistry B</i> , 2013, 117, 13235-13244.	2.6	16
135	Role of solvation in pressure-induced helix stabilization. <i>Journal of Chemical Physics</i> , 2014, 141, 22D522.	3.0	16
136	Reversible two-state folding of the ultrafast protein gpW under mechanical force. <i>Communications Chemistry</i> , 2018, 1, .	4.5	16
137	Atomistic mechanism of transmembrane helix association. <i>PLoS Computational Biology</i> , 2020, 16, e1007919.	3.2	16
138	Modulation of Folding Internal Friction by Local and Global Barrier Heights. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 1028-1034.	4.6	15
139	Instrumental Effects in the Dynamics of an Ultrafast Folding Protein under Mechanical Force. <i>Journal of Physical Chemistry B</i> , 2018, 122, 11147-11154.	2.6	15
140	Atomistic Force Fields for Proteins. <i>Methods in Molecular Biology</i> , 2019, 2022, 3-19.	0.9	14
141	Unfolding the Secrets of Calmodulin. <i>Science</i> , 2009, 323, 593-594.	12.6	13
142	Reconciling Intermediates in Mechanical Unfolding Experiments with Two-State Protein Folding in Bulk. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 3798-3803.	4.6	13
143	Atomic view of cosolute-induced protein denaturation probed by NMR solvent paramagnetic relaxation enhancement. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	7.1	13
144	Mechanism of Hydrogen Sulfide-Dependent Inhibition of FeFe Hydrogenase. <i>ACS Catalysis</i> , 2021, 11, 15162-15176.	11.2	13

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145	Identification of Mutational Hot Spots for Substrate Diffusion: Application to Myoglobin. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1919-1927.	5.3	12
146	Simulation of Coarse-Grained Protein-Protein Interactions with Graphics Processing Units. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3588-3600.	5.3	11
147	Engineering Folding Dynamics from Two-State to Downhill: Application to λ -Repressor. <i>Journal of Physical Chemistry B</i> , 2013, 117, 13435-13443.	2.6	11
148	Tuning Formation of Protein-DNA Coacervates by Sequence and Environment. <i>Journal of Physical Chemistry B</i> , 2022, 126, 2407-2419.	2.6	10
149	Cyclic N-Terminal Loop of Amylin Forms Non Amyloid Fibers. <i>Biophysical Journal</i> , 2013, 105, 1661-1669.	0.5	9
150	TADOSS: computational estimation of tandem domain swap stability. <i>Bioinformatics</i> , 2019, 35, 2507-2508.	4.1	6
151	(Ala) ₄ as a model system for the optimization of the ϕ and ψ amino acid sidechain dihedral empirical force field parameters. <i>Journal of Computational Chemistry</i> , 2013, 34, 593-603.	3.3	5
152	Co-Evolutionary Fitness Landscapes for Sequence Design. <i>Angewandte Chemie</i> , 2018, 130, 5776-5780.	2.0	5
153	Editorial overview: Theory and simulation: Interpreting experimental data at the molecular level. <i>Current Opinion in Structural Biology</i> , 2018, 49, iv-v.	5.7	4
154	Analysis of Molecular Dynamics Simulations of Protein Folding. <i>Methods in Molecular Biology</i> , 2022, 2376, 317-329.	0.9	4
155	AN NMR INVESTIGATION INTO THE DYNAMICS OF PANOSE, AN $\alpha(1\rightarrow4)$ AND $\alpha(1\rightarrow6)$ -LINKED TRISACCHARIDE. <i>Spectroscopy Letters</i> , 2002, 35, 625-632.	1.0	3
156	A β -protein folds quickly in the end. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 5744-5745.	7.1	3
157	Bootstrapping New Protein Folds. <i>Biophysical Journal</i> , 2014, 107, 1040-1041.	0.5	3
158	Estimating transition path times and shapes from single-molecule photon trajectories: A simulation analysis. <i>Journal of Chemical Physics</i> , 2021, 154, 115101.	3.0	3
159	Folding and Binding: When the Force is Against You. <i>Biophysical Journal</i> , 2013, 105, 2611-2612.	0.5	2
160	Protein Folding Landscapes for Alpha- and Beta-Miniproteins Using All-Atom Simulations with an Optimized Force-Field. <i>Biophysical Journal</i> , 2010, 98, 200a.	0.5	1
161	Race to the native state. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 2267-2269.	7.1	1
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