Robert B Best

List of Publications by Year
in descending order

170	20,340	14644 66	12258 133
papers	citations	h-index	g-index

193	193	193	16330
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Optimization of the Additive CHARMM All-Atom Protein Force Field Targeting Improved Sampling of the Backbone Ï•, Ï^ and Side-Chain Ï‡₁ and Ï‡₂ Dihedral Angles. Journal of Chemical Theory and Computation, 2012, 8, 3257-3273.	2.3	3,696
2	Optimized Molecular Dynamics Force Fields Applied to the Helixâ^'Coil Transition of Polypeptides. Journal of Physical Chemistry B, 2009, 113, 9004-9015.	1.2	767
3	Simultaneous determination of protein structure and dynamics. Nature, 2005, 433, 128-132.	13.7	641
4	Balanced Proteinâ€"Water Interactions Improve Properties of Disordered Proteins and Non-Specific Protein Association. Journal of Chemical Theory and Computation, 2014, 10, 5113-5124.	2.3	564
5	Martini 3: a general purpose force field for coarse-grained molecular dynamics. Nature Methods, 2021, 18, 382-388.	9.0	557
6	Phosphorylation of the <scp>FUS</scp> lowâ€complexity domain disrupts phase separation, aggregation, and toxicity. EMBO Journal, 2017, 36, 2951-2967.	3.5	544
7	Extreme disorder in an ultrahigh-affinity protein complex. Nature, 2018, 555, 61-66.	13.7	538
8	Polarizable Atomic Multipole-Based AMOEBA Force Field for Proteins. Journal of Chemical Theory and Computation, 2013, 9, 4046-4063.	2.3	524
9	Native contacts determine protein folding mechanisms in atomistic simulations. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 17874-17879.	3.3	490
10	Reaction coordinates and rates from transition paths. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 6732-6737.	3.3	433
11	Sequence determinants of protein phase behavior from a coarse-grained model. PLoS Computational Biology, 2018, 14, e1005941.	1.5	427
12	Are Current Molecular Dynamics Force Fields too Helical?. Biophysical Journal, 2008, 95, L07-L09.	0.2	419
13	Biomolecular Phase Separation: From Molecular Driving Forces to Macroscopic Properties. Annual Review of Physical Chemistry, 2020, 71, 53-75.	4.8	368
14	Characterizing the unfolded states of proteins using single-molecule FRET spectroscopy and molecular simulations. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 1528-1533.	3.3	327
15	Relation between single-molecule properties and phase behavior of intrinsically disordered proteins. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 9929-9934.	3.3	283
16	Hidden complexity in the mechanical properties of titin. Nature, 2003, 422, 446-449.	13.7	268
17	Coordinate-dependent diffusion in protein folding. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 1088-1093.	3.3	253
18	Can Non-Mechanical Proteins Withstand Force? Stretching Barnase by Atomic Force Microscopy and Molecular Dynamics Simulation. Biophysical Journal, 2001, 81, 2344-2356.	0.2	234

#	Article	IF	Citations
19	Protein Simulations with an Optimized Water Model: Cooperative Helix Formation and Temperature-Induced Unfolded State Collapse. Journal of Physical Chemistry B, 2010, 114, 14916-14923.	1.2	233
20	Single-molecule spectroscopy of the temperature-induced collapse of unfolded proteins. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 20740-20745.	3.3	211
21	Effect of flexibility and cis residues in single-molecule FRET studies of polyproline. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 18964-18969.	3.3	201
22	Mechanical Unfolding of a Titin Ig Domain: Structure of Unfolding Intermediate Revealed by Combining AFM, Molecular Dynamics Simulations, NMR and Protein Engineering. Journal of Molecular Biology, 2002, 322, 841-849.	2.0	200
23	Binding-Induced Folding of a Natively Unstructured Transcription Factor. PLoS Computational Biology, 2008, 4, e1000060.	1.5	189
24	Computational and theoretical advances in studies of intrinsically disordered proteins. Current Opinion in Structural Biology, 2017, 42, 147-154.	2.6	186
25	Consistent View of Polypeptide Chain Expansion in Chemical Denaturants from Multiple Experimental Methods. Journal of the American Chemical Society, 2016, 138, 11714-11726.	6.6	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. Journal of Molecular Biology, 2003, 330, 867-877.	2.0	168
27	Diffusive Model of Protein Folding Dynamics with Kramers Turnover in Rate. Physical Review Letters, 2006, 96, 228104.	2.9	165
28	Temperature-dependent solvation modulates the dimensions of disordered proteins. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 5213-5218.	3.3	161
29	Slow Protein Conformational Dynamics from Multiple Experimental Structures: The Helix/Sheet Transition of Arc Repressor. Structure, 2005, 13, 1755-1763.	1.6	160
30	Single-molecule fluorescence reveals sequence-specific misfolding in multidomain proteins. Nature, 2011, 474, 662-665.	13.7	158
31	Thermodynamics and kinetics of protein folding under confinement. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 20233-20238.	3.3	146
32	Relation between native ensembles and experimental structures of proteins. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 10901-10906.	3.3	136
33	Pulling Direction as a Reaction Coordinate for the Mechanical Unfolding of Single Molecules. Journal of Physical Chemistry B, 2008, 112, 5968-5976.	1.2	135
34	Inclusion of Many-Body Effects in the Additive CHARMM Protein CMAP Potential Results in Enhanced Cooperativity of Î±-Helix and Î²-Hairpin Formation. Biophysical Journal, 2012, 103, 1045-1051.	0.2	130
35	Atomistic molecular simulations of protein folding. Current Opinion in Structural Biology, 2012, 22, 52-61.	2.6	129
36	Molecular Details of Protein Condensates Probed by Microsecond Long Atomistic Simulations. Journal of Physical Chemistry B, 2020, 124, 11671-11679.	1.2	127

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37	Determination of Protein Structures Consistent with NMR Order Parameters. Journal of the American Chemical Society, 2004, 126, 8090-8091.	6.6	126
38	Computer Folding of RNA Tetraloops: Identification of Key Force Field Deficiencies. Journal of Chemical Theory and Computation, 2016, 12, 4534-4548.	2.3	125
39	Probing the Action of Chemical Denaturant on an Intrinsically Disordered Protein by Simulation and Experiment. Journal of the American Chemical Society, 2016, 138, 11702-11713.	6.6	121
40	Force mode atomic force microscopy as a tool for protein folding studies. Analytica Chimica Acta, 2003, 479, 87-105.	2.6	120
41	Structural Interpretation of Hydrogen Exchange Protection Factors in Proteins: Characterization of the Native State Fluctuations of CI2. Structure, 2006, 14, 97-106.	1.6	115
42	Freeâ€energy landscape of the GB1 hairpin in allâ€atom explicit solvent simulations with different force fields: Similarities and differences. Proteins: Structure, Function and Bioinformatics, 2011, 79, 1318-1328.	1.5	112
43	Tackling Force-Field Bias in Protein Folding Simulations: Folding of Villin HP35 and Pin WW Domains in Explicit Water. Biophysical Journal, 2010, 99, L26-L28.	0.2	105
44	Mechanism of O2 diffusion and reduction in FeFe hydrogenases. Nature Chemistry, 2017, 9, 88-95.	6.6	105
45	A Preformed Binding Interface in the Unbound Ensemble of an Intrinsically Disordered Protein: Evidence from Molecular Simulations. PLoS Computational Biology, 2012, 8, e1002605.	1.5	104
46	Physics-based computational and theoretical approaches to intrinsically disordered proteins. Current Opinion in Structural Biology, 2021, 67, 219-225.	2.6	101
47	Molecular origins of internal friction effects on protein-folding rates. Nature Communications, 2014, 5, 4307.	5.8	98
48	Residue-Specific Î±-Helix Propensities from Molecular Simulation. Biophysical Journal, 2012, 102, 1462-1467.	0.2	97
49	Transient misfolding dominates multidomain protein folding. Nature Communications, 2015, 6, 8861.	5.8	97
50	Improving the Performance of the Amber RNA Force Field by Tuning the Hydrogen-Bonding Interactions. Journal of Chemical Theory and Computation, 2019, 15, 3288-3305.	2.3	97
51	Balance between Î± and Î² Structures in Ab Initio Protein Folding. Journal of Physical Chemistry B, 2010, 114, 8790-8798.	1.2	96
52	Comparing a simple theoretical model for protein folding with all-atom molecular dynamics simulations. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 17880-17885.	3.3	94
53	A simple method for probing the mechanical unfolding pathway of proteins in detail. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 12143-12148.	3.3	93
54	Convergence and Sampling in Determining Free Energy Landscapes for Membrane Protein Association. Journal of Physical Chemistry B, 2017, 121, 3364-3375.	1.2	93

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55	What Contributions to Protein Side-chain Dynamics are Probed by NMR Experiments? A Molecular Dynamics Simulation Analysis. Journal of Molecular Biology, 2005, 349, 185-203.	2.0	92
56	Highly Disordered Amyloid-Î² Monomer Probed by Single-Molecule FRET and MD Simulation. Biophysical Journal, 2018, 114, 870-884.	0.2	88
57	Peptide Chain Dynamics in Light and Heavy Water: Zooming in on Internal Friction. Journal of the American Chemical Society, 2012, 134, 6273-6279.	6.6	86
58	Folding pathway of an Ig domain is conserved on and off the ribosome. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E11284-E11293.	3.3	86
59	Computer Folding of RNA Tetraloops? Are We There Yet?. Journal of Chemical Theory and Computation, 2013, 9, 2115-2125.	2.3	84
60	Inferring properties of disordered chains from FRET transfer efficiencies. Journal of Chemical Physics, 2018, 148, 123329.	1.2	84
61	Modulation of an IDP binding mechanism and rates by helix propensity and non-native interactions: association of HIF1Î± with CBP. Molecular BioSystems, 2012, 8, 256-267.	2.9	83
62	Dependence of Protein Folding Stability and Dynamics on the Density and Composition of Macromolecular Crowders. Biophysical Journal, 2010, 98, 315-320.	0.2	81
63	Diffusion models of protein folding. Physical Chemistry Chemical Physics, 2011, 13, 16902.	1.3	76
64	Mechanism of membrane-tethered mitochondrial protein synthesis. Science, 2021, 371, 846-849.	6.0	76
65	Polyelectrolyte interactions enable rapid association and dissociation in high-affinity disordered protein complexes. Nature Communications, 2020, 11, 5736.	5.8	74
66	Using Ligandâ€Mapping Simulations to Design a Ligand Selectively Targeting a Cryptic Surface Pocket of Poloâ€Like Kinase 1. Angewandte Chemie - International Edition, 2012, 51, 10078-10081.	7.2	71
67	Force-Field Dependence of Chignolin Folding and Misfolding: Comparison with Experiment and Redesign. Biophysical Journal, 2012, 102, 1897-1906.	0.2	71
68	A Data-Driven Hydrophobicity Scale for Predicting Liquidâ€“Liquid Phase Separation of Proteins. Journal of Physical Chemistry B, 2021, 125, 4046-4056.	1.2	71
69	Sequence- and Temperature-Dependent Properties of Unfolded and Disordered Proteins from Atomistic Simulations. Journal of Physical Chemistry B, 2015, 119, 14622-14630.	1.2	70
70	Locating the Barrier for Folding of Single Molecules under an External Force. Physical Review Letters, 2011, 107, 208301.	2.9	69
71	Macromolecular crowding effects on proteinâ€“protein binding affinity and specificity. Journal of Chemical Physics, 2010, 133, 205101.	1.2	68
72	What Is the Time Scale for Î±-Helix Nucleation?. Journal of the American Chemical Society, 2011, 133, 6809-6816.	6.6	68

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73	Microscopic events in Î²-hairpin folding from alternative unfolded ensembles. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 11087-11092.	3.3	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.	3.3	66
75	Multiscale Simulation Reveals Multiple Pathways for H2and O2Transport in a [NiFe]-Hydrogenase. Journal of the American Chemical Society, 2011, 133, 3548-3556.	6.6	65
76	Evolution of All-Atom Protein Force Fields to Improve Local and Global Properties. Journal of Physical Chemistry Letters, 2019, 10, 2227-2234.	2.1	65
77	The shape of the bacterial ribosome exit tunnel affects cotranslational protein folding. ELife, 2018, 7, .	2.8	65
78	An Extended Guinier Analysis for Intrinsically Disordered Proteins. Journal of Molecular Biology, 2018, 430, 2540-2553.	2.0	64
79	Molecular Dynamics and NMR Study of the Î±(1â†'4) and Î±(1â†'6) Glycosidic Linkages:Â Maltose and Isomaltose. Journal of Physical Chemistry B, 2001, 105, 4742-4751.	1.2	61
80	The Origin of Protein Sidechain Order Parameter Distributions. Journal of the American Chemical Society, 2004, 126, 7734-7735.	6.6	59
81	Quantitative Interpretation of FRET Experiments via Molecular Simulation: Force Field and Validation. Biophysical Journal, 2015, 108, 2721-2731.	0.2	59
82	Disordered RNA chaperones can enhance nucleic acid folding via local charge screening. Nature Communications, 2019, 10, 2453.	5.8	59
83	Coâ€Evolutionary Fitness Landscapes for Sequence Design. Angewandte Chemie - International Edition, 2018, 57, 5674-5678.	7.2	58
84	Insights into the binding of intrinsically disordered proteins from molecular dynamics simulation. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 182-198.	6.2	56
85	Microscopic interpretation of folding Ï•-values using the transition path ensemble. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 3263-3268.	3.3	55
86	Treatment of sickle cell disease by increasing oxygen affinity of hemoglobin. Blood, 2021, 138, 1172-1181.	0.6	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.	3.3	51
88	What can atomic force microscopy tell us about protein folding?. Chemical Communications, 2002, , 183-192.	2.2	50
89	Force-Induced Change in Protein Unfolding Mechanism: Discrete or Continuous Switch?. Journal of Physical Chemistry B, 2011, 115, 1546-1561.	1.2	50
90	Interpreting Dynamically-Averaged Scalar Couplings in Proteins. Journal of Biomolecular NMR, 2005, 32, 273-280.	1.6	46

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91	Variational Optimization of an All-Atom Implicit Solvent Force Field To Match Explicit Solvent Simulation Data. Journal of Chemical Theory and Computation, 2013, 9, 5641-5652.	2.3	46
92	Discriminating binding mechanisms of an intrinsically disordered protein via a multi-state coarse-grained model. Journal of Chemical Physics, 2014, 140, 175102.	1.2	46
93	Accurate Transfer Efficiencies, Distance Distributions, and Ensembles of Unfolded and Intrinsically Disordered Proteins From Single-Molecule FRET. Methods in Enzymology, 2018, 611, 287-325.	0.4	46
94	Evidence for a Partially Structured State of the Amylin Monomer. Biophysical Journal, 2009, 97, 2948-2957.	0.2	45
95	Multiple lipid binding sites determine the affinity of PH domains for phosphoinositide-containing membranes. Science Advances, 2020, 6, eaay5736.	4.7	44
96	Dependence of Internal Friction on Folding Mechanism. Journal of the American Chemical Society, 2015, 137, 3283-3290.	6.6	41
97	Protein Folding Kinetics Under Force from Molecular Simulation. Journal of the American Chemical Society, 2008, 130, 3706-3707.	6.6	40
98	Balancing Force Field Proteinâ€“Lipid Interactions To Capture Transmembrane Helixâ€“Helix Association. Journal of Chemical Theory and Computation, 2018, 14, 1706-1715.	2.3	40
99	A mutant chaperonin with rearranged inter-ring electrostatic contacts and temperature-sensitive dissociation. Nature Structural and Molecular Biology, 2004, 11, 1128-1133.	3.6	39
100	Hydrophobic Core Fluidity of Homologous Protein Domains:Â Relation of Side-Chain Dynamics to Core Composition and Packingâ€. Biochemistry, 2004, 43, 1145-1155.	1.2	38
101	Characterization of the residual structure in the unfolded state of the Î”131Î” fragment of staphylococcal nuclease. Proteins: Structure, Function and Bioinformatics, 2006, 65, 145-152.	1.5	38
102	How Many Protein Sequences Fold to a Given Structure? A Coevolutionary Analysis. Biophysical Journal, 2017, 113, 1719-1730.	0.2	38
103	Comment on "Force-Clamp Spectroscopy Monitors the Folding Trajectory of a Single Protein". Science, 2005, 308, 498b-498b.	6.0	37
104	Release of linker histone from the nucleosome driven by polyelectrolyte competition with a disordered protein. Nature Chemistry, 2022, 14, 224-231.	6.6	37
105	Comment on â€œInnovative scattering analysis shows that hydrophobic disordered proteins are expanded in waterâ€. Science, 2018, 361, .	6.0	36
106	Atomistic Insights into Rhodopsin Activation from a Dynamic Model. Journal of the American Chemical Society, 2008, 130, 10141-10149.	6.6	35
107	Folding Kinetics and Unfolded State Dynamics of the GB1 Hairpin from Molecular Simulation. Journal of Chemical Theory and Computation, 2013, 9, 1743-1753.	2.3	35
108	Effects of Interactions with the GroEL Cavity on Protein Folding Rates. Biophysical Journal, 2013, 104, 1098-1106.	0.2	34

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109	Complex Energy Landscape of a Giant Repeat Protein. Structure, 2013, 21, 1954-1965.	1.6	33
110	Reduction of All-Atom Protein Folding Dynamics to One-Dimensional Diffusion. Journal of Physical Chemistry B, 2015, 119, 15247-15255.	1.2	31
111	Structural Determinants of Misfolding in Multidomain Proteins. PLoS Computational Biology, 2016, 12, e1004933.	1.5	30
112	Modest Influence of FRET Chromophores on the Properties of Unfolded Proteins. Biophysical Journal, 2014, 107, 1654-1660.	0.2	29
113	Tandem domain swapping: determinants of multidomain protein misfolding. Current Opinion in Structural Biology, 2019, 58, 97-104.	2.6	28
114	A microscopic model for gas diffusion dynamics in a [NiFe]-hydrogenase. Physical Chemistry Chemical Physics, 2011, 13, 7708.	1.3	27
115	The ribosome modulates folding inside the ribosomal exit tunnel. Communications Biology, 2021, 4, 523.	2.0	27
116	Aerobic Damage to [FeFe]â€Hydrogenases: Activation Barriers for the Chemical Attachment of O₂. Angewandte Chemie - International Edition, 2014, 53, 4081-4084.	7.2	26
117	Markov state models of protein misfolding. Journal of Chemical Physics, 2016, 144, 075101.	1.2	26
118	Emerging consensus on the collapse of unfolded and intrinsically disordered proteins in water. Current Opinion in Structural Biology, 2020, 60, 27-38.	2.6	26
119	Cutting antiparallel DNA strands in a single active site. Nature Structural and Molecular Biology, 2020, 27, 119-126.	3.6	25
120	Matching of Additive and Polarizable Force Fields for Multiscale Condensed Phase Simulations. Journal of Chemical Theory and Computation, 2013, 9, 2826-2837.	2.3	24
121	Cotranslational folding cooperativity of contiguous domains of Î±-spectrin. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 14119-14126.	3.3	24
122	Crosstalk between the Protein Surface and Hydrophobic Core in a Core-swapped Fibronectin Type III Domain. Journal of Molecular Biology, 2008, 375, 560-571.	2.0	23
123	Empirical Optimization of Interactions between Proteins and Chemical Denaturants in Molecular Simulations. Journal of Chemical Theory and Computation, 2015, 11, 5543-5553.	2.3	23
124	Structural Comparison of the Two Alternative Transition States for Folding of TI I27. Biophysical Journal, 2006, 91, 263-275.	0.2	21
125	Smoothing of the GB1 Hairpin Folding Landscape by Interfacial Confinement. Biophysical Journal, 2012, 103, 596-600.	0.2	21
126	Pressureâ€induced structural transition of mature <scp>HIV</scp>â€1 protease from a combined <scp>NMR/MD</scp> simulation approach. Proteins: Structure, Function and Bioinformatics, 2015, 83, 2117-2123.	1.5	21

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127	Diffusive Dynamics of Contact Formation in Disordered Polypeptides. Physical Review Letters, 2016, 116, 068102.	2.9	21
128	Exploring the sequence fitness landscape of a bridge between protein folds. PLoS Computational Biology, 2020, 16, e1008285.	1.5	20
129	Origin of Internal Friction in Disordered Proteins Depends on Solvent Quality. Journal of Physical Chemistry B, 2018, 122, 11478-11487.	1.2	19
130	Molecular Determinants of AÎ²₄₂ Adsorption to Amyloid Fibril Surfaces. Journal of Physical Chemistry Letters, 2018, 9, 6437-6443.	2.1	19
131	Modeling the Î±(1â†'6) Branch Point of Amylopectin in Solution. Journal of Physical Chemistry B, 2002, 106, 5091-5098.	1.2	18
132	Single-molecule Detection of Ultrafast Biomolecular Dynamics with Nanophotonics. Journal of the American Chemical Society, 2022, 144, 52-56.	6.6	18
133	Effect of interactions with the chaperonin cavity on protein folding and misfolding. Physical Chemistry Chemical Physics, 2014, 16, 6358-6366.	1.3	17
134	How Well Does a Funneled Energy Landscape Capture the Folding Mechanism of Spectrin Domains?. Journal of Physical Chemistry B, 2013, 117, 13235-13244.	1.2	16
135	Role of solvation in pressure-induced helix stabilization. Journal of Chemical Physics, 2014, 141, 22D522.	1.2	16
136	Reversible two-state folding of the ultrafast protein gpW under mechanical force. Communications Chemistry, 2018, 1, .	2.0	16
137	Atomistic mechanism of transmembrane helix association. PLoS Computational Biology, 2020, 16, e1007919.	1.5	16
138	Modulation of Folding Internal Friction by Local and Global Barrier Heights. Journal of Physical Chemistry Letters, 2016, 7, 1028-1034.	2.1	15
139	Instrumental Effects in the Dynamics of an Ultrafast Folding Protein under Mechanical Force. Journal of Physical Chemistry B, 2018, 122, 11147-11154.	1.2	15
140	Atomistic Force Fields for Proteins. Methods in Molecular Biology, 2019, 2022, 3-19.	0.4	14
141	Unfolding the Secrets of Calmodulin. Science, 2009, 323, 593-594.	6.0	13
142	Reconciling Intermediates in Mechanical Unfolding Experiments with Two-State Protein Folding in Bulk. Journal of Physical Chemistry Letters, 2016, 7, 3798-3803.	2.1	13
143	Atomic view of cosolute-induced protein denaturation probed by NMR solvent paramagnetic relaxation enhancement. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	13
144	Mechanism of Hydrogen Sulfide-Dependent Inhibition of FeFe Hydrogenase. ACS Catalysis, 2021, 11, 15162-15176.	5.5	13

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145	Identification of Mutational Hot Spots for Substrate Diffusion: Application to Myoglobin. Journal of Chemical Theory and Computation, 2015, 11, 1919-1927.	2.3	12
146	Simulation of Coarse-Grained Proteinâ^'Protein Interactions with Graphics Processing Units. Journal of Chemical Theory and Computation, 2010, 6, 3588-3600.	2.3	11
147	Engineering Folding Dynamics from Two-State to Downhill: Application to Î»-Repressor. Journal of Physical Chemistry B, 2013, 117, 13435-13443.	1.2	11
148	Tuning Formation of Proteinâ€"DNA Coacervates by Sequence and Environment. Journal of Physical Chemistry B, 2022, 126, 2407-2419.	1.2	10
149	Cyclic N-Terminal Loop of Amylin Forms Non Amyloid Fibers. Biophysical Journal, 2013, 105, 1661-1669.	0.2	9
150	TADOSS: computational estimation of tandem domain swap stability. Bioinformatics, 2019, 35, 2507-2508.	1.8	6
151	(Ala)₄â€Xâ€(Ala)₄ as a model system for the optimization of the Ï‡₁ and Ï‡₂ amino acid sideâ€chain dihedral empirical force field parameters. Journal of Computational Chemistry, 2013, 34, 593-603.	1.5	5
152	Coâ€Evolutionary Fitness Landscapes for Sequence Design. Angewandte Chemie, 2018, 130, 5776-5780.	1.6	5
153	Editorial overview: Theory and simulation: Interpreting experimental data at the molecular level. Current Opinion in Structural Biology, 2018, 49, iv-v.	2.6	4
154	Analysis of Molecular Dynamics Simulations of Protein Folding. Methods in Molecular Biology, 2022, 2376, 317-329.	0.4	4
155	AN NMR INVESTIGATION INTO THE DYNAMICS OF PANOSE, AN Î±(1â†'4) AND Î±(1â†'6)-LINKED TRISACCHARIDE. Spectroscopy Letters, 2002, 35, 625-632.	0.5	3
156	A â€œslowâ€•protein folds quickly in the end. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 5744-5745.	3.3	3
157	Bootstrapping New Protein Folds. Biophysical Journal, 2014, 107, 1040-1041.	0.2	3
158	Estimating transition path times and shapes from single-molecule photon trajectories: A simulation analysis. Journal of Chemical Physics, 2021, 154, 115101.	1.2	3
159	Folding and Binding: When the Force is Against You. Biophysical Journal, 2013, 105, 2611-2612.	0.2	2
160	Protein Folding Landscapes for Alpha- and Beta-Miniproteins Using All-Atom Simulations with an Optimized Force-Field. Biophysical Journal, 2010, 98, 200a.	0.2	1
161	Race to the native state. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 2267-2269.	3.3	1
162	InnenrÃ¼cktitelbild: Co-Evolutionary Fitness Landscapes for Sequence Design (Angew. Chem. 20/2018). Angewandte Chemie, 2018, 130, 6061-6061.	1.6	1

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163	Computational Protocol for Determining Conformational Ensembles of Intrinsically Disordered Proteins. Methods in Molecular Biology, 2020, 2141, 413-427.	0.4	1
164	Insights from Molecular Simulations into the Temperature-Induced Collapse of Unfolded Proteins. Biophysical Journal, 2010, 98, 634a.	0.2	0
165	Replica Exchange Simulations For Macromolecular Crowding Effects on Multiprotein Binding. Biophysical Journal, 2010, 98, 57a.	0.2	0
166	Cyclic N Terminal Fragment of Amylin Forms Non Amyloid Fibers: Implications for Intra- and Inter-Molecular Interactions in Amylin. Biophysical Journal, 2013, 104, 389a-390a.	0.2	0
167	Surprising Abundance of Misfolding during Refolding of Multidomain Proteins. Biophysical Journal, 2015, 108, 501a.	0.2	0
168	Dependence of Internal Friction on Native Topology. Biophysical Journal, 2015, 108, 518a.	0.2	0
169	Molecular Simulations of Unfolded and Intrinsically Disordered Proteins. Biophysical Journal, 2015, 108, 194a.	0.2	0
170	A Tale of Two Tyrosines. Biophysical Journal, 2020, 119, 1927-1928.	0.2	0