Kresten Lindorff-Larsen

List of Publications by Year
in descending order

161 papers	20,479 citations	41344 49 h-index	12597 132 g-index
234 all docs	234 docs citations	234 times ranked	18743 citing authors

#	Article	IF	Citations
1	Improved sideâ€chain torsion potentials for the Amber ff99SB protein force field. Proteins: Structure, Function and Bioinformatics, 2010, 78, 1950-1958.	2.6	4,694
2	How Fast-Folding Proteins Fold. Science, 2011, 334, 517-520.	12.6	1,609
3	Atomic-Level Characterization of the Structural Dynamics of Proteins. Science, 2010, 330, 341-346.	12.6	1,583
4	How Robust Are Protein Folding Simulations with Respect to Force Field Parameterization?. Biophysical Journal, 2011, 100, L47-L49.	0.5	725
5	Long-timescale molecular dynamics simulations of protein structure and function. Current Opinion in Structural Biology, 2009, 19, 120-127.	5.7	671
6	Mapping Long-Range Interactions in Î±-Synuclein using Spin-Label NMR and Ensemble Molecular Dynamics Simulations. Journal of the American Chemical Society, 2005, 127, 476-477.	13.7	658
7	Promoting transparency and reproducibility in enhanced molecular simulations. Nature Methods, 2019, 16, 670-673.	19.0	655
8	Simultaneous determination of protein structure and dynamics. Nature, 2005, 433, 128-132.	27.8	641
9	Systematic Validation of Protein Force Fields against Experimental Data. PLoS ONE, 2012, 7, e32131.	2.5	570
10	The Role of Protein Loops and Linkers in Conformational Dynamics and Allostery. Chemical Reviews, 2016, 116, 6391-6423.	47.7	302
11	Principles of conduction and hydrophobic gating in K ⁺ channels. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 5833-5838.	7.1	298
12	Cancer Mutations of the Tumor Suppressor SPOP Disrupt the Formation of Active, Phase-Separated Compartments. Molecular Cell, 2018, 72, 19-36.e8.	9.7	286
13	Atomic-level description of ubiquitin folding. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 5915-5920.	7.1	281
14	Protein folding kinetics and thermodynamics from atomistic simulation. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 17845-17850.	7.1	262
15	Millisecond-scale molecular dynamics simulations on Anton. , 2009, , .		238
16	Structure and Dynamics of an Unfolded Protein Examined by Molecular Dynamics Simulation. Journal of the American Chemical Society, 2012, 134, 3787-3791.	13.7	222
17	Biophysical experiments and biomolecular simulations: A perfect match?. Science, 2018, 361, 355-360.	12.6	205
18	Microsecond Molecular Dynamics Simulation Shows Effect of Slow Loop Dynamics on Backbone Amide Order Parameters of Proteinsâ€. Journal of Physical Chemistry B, 2008, 112, 6155-6158.	2.6	188

#	Article	IF	Citations
19	Combining Experiments and Simulations Using the Maximum Entropy Principle. PLoS Computational Biology, 2014, 10, e1003406.	3.2	167
20	Determination of an Ensemble of Structures Representing the Denatured State of the Bovine Acyl-Coenzyme A Binding Protein. Journal of the American Chemical Society, 2004, 126, 3291-3299.	13.7	155
21	Parallel protein-unfolding pathways revealed and mapped. Nature Structural and Molecular Biology, 2003, 10, 658-662.	8.2	153
22	Accurate model of liquidâ€“liquid phase behavior of intrinsically disordered proteins from optimization of single-chain properties. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	151
23	Biophysical and Mechanistic Models for Disease-Causing Protein Variants. Trends in Biochemical Sciences, 2019, 44, 575-588.	7.5	143
24	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.	7.1	136
25	Integrating Molecular Simulation and Experimental Data: A Bayesian/Maximum Entropy Reweighting Approach. Methods in Molecular Biology, 2020, 2112, 219-240.	0.9	129
26	Surprisingly high stability of barley lipid transfer protein, LTP1, towards denaturant, heat and proteases. FEBS Letters, 2001, 488, 145-148.	2.8	126
27	An Efficient Method for Estimating the Hydrodynamic Radius of Disordered Protein Conformations. Biophysical Journal, 2017, 113, 550-557.	0.5	110
28	Computational Design and Experimental Testing of the Fastest-Folding Î²-Sheet Protein. Journal of Molecular Biology, 2011, 405, 43-48.	4.2	106
29	Protein folding and the organization of the protein topology universe. Trends in Biochemical Sciences, 2005, 30, 13-19.	7.5	101
30	Conformational ensembles of RNA oligonucleotides from integrating NMR and molecular simulations. Science Advances, 2018, 4, eaar8521.	10.3	99
31	Structure of a Functional Amyloid Protein Subunit Computed Using Sequence Variation. Journal of the American Chemical Society, 2015, 137, 22-25.	13.7	98
32	Conformational Rigidity and Protein Dynamics at Distinct Timescales Regulate PTP1B Activity and Allostery. Molecular Cell, 2017, 65, 644-658.e5.	9.7	96
33	Picosecond to Millisecond Structural Dynamics in Human Ubiquitin. Journal of Physical Chemistry B, 2016, 120, 8313-8320.	2.6	93
34	Formation of Native and Non-native Interactions in Ensembles of Denatured ACBP Molecules from Paramagnetic Relaxation Enhancement Studies. Journal of Molecular Biology, 2005, 347, 1053-1062.	4.2	90
35	Predicting the impact of Lynch syndrome-causing missense mutations from structural calculations. PLoS Genetics, 2017, 13, e1006739.	3.5	90
36	Transition states for protein folding have native topologies despite high structural variability. Nature Structural and Molecular Biology, 2004, 11, 443-449.	8.2	88

#	Article	IF	Citations
37	Structural Basis of Membrane Protein Chaperoning through the Mitochondrial Intermembrane Space. Cell, 2018, 175, 1365-1379.e25.	28.9	87
38	Evaluating the Effects of Cutoffs and Treatment of Long-range Electrostatics in Protein Folding Simulations. PLoS ONE, 2012, 7, e39918.	2.5	83
39	Interplay of folded domains and the disordered low-complexity domain in mediating hnRNPA1 phase separation. Nucleic Acids Research, 2021, 49, 2931-2945.	14.5	81
40	Comparing Molecular Dynamics Force Fields in the Essential Subspace. PLoS ONE, 2015, 10, e0121114.	2.5	80
41	Side chain to main chain hydrogen bonds stabilize a polyglutamine helix in a transcription factor. Nature Communications, 2019, 10, 2034.	12.8	78
42	Interaction Networks in Protein Folding via Atomic-Resolution Experiments and Long-Time-Scale Molecular Dynamics Simulations. Journal of the American Chemical Society, 2015, 137, 6506-6516.	13.7	76
43	Combining molecular dynamics simulations with small-angle X-ray and neutron scattering data to study multi-domain proteins in solution. PLoS Computational Biology, 2020, 16, e1007870.	3.2	76
44	How to learn from inconsistencies: Integrating molecular simulations with experimental data. Progress in Molecular Biology and Translational Science, 2020, 170, 123-176.	1.7	76
45	Experimental Parameterization of an Energy Function for the Simulation of Unfolded Proteins. Biophysical Journal, 2008, 94, 182-192.	0.5	70
46	Understanding the Origins of Loss of Protein Function by Analyzing the Effects of Thousands of Variants on Activity and Abundance. Molecular Biology and Evolution, 2021, 38, 3235-3246.	8.9	65
47	Similarity Measures for Protein Ensembles. PLoS ONE, 2009, 4, e4203.	2.5	65
48	Transition State Contact Orders Correlate with Protein Folding Rates. Journal of Molecular Biology, 2005, 352, 495-500.	4.2	64
49	Structure of the Regulatory Apparatus of a Calcium-dependent Protein Kinase (CDPK): A Novel Mode of Calmodulin-target Recognition. Journal of Molecular Biology, 2006, 357, 400-410.	4.2	64
50	ENCORE: Software for Quantitative Ensemble Comparison. PLoS Computational Biology, 2015, 11, e1004415.	3.2	64
51	On the Calculation of SAXS Profiles of Folded and Intrinsically Disordered Proteins from Computer Simulations. Journal of Molecular Biology, 2018, 430, 2521-2539.	4.2	64
52	Mapping transiently formed and sparsely populated conformations on a complex energy landscape. ELife, 2016, 5, .	6.0	63
53	Predicting and interpreting large-scale mutagenesis data using analyses of protein stability and conservation. Cell Reports, 2022, 38, 110207.	6.4	62
54	How well do force fields capture the strength of salt bridges in proteins?. PeerJ, 2018, 6, e4967.	2.0	58

#	Article	IF	Citations
55	Toward mechanistic models for genotypeâ€“phenotype correlations in phenylketonuria using protein stability calculations. Human Mutation, 2019, 40, 444-457.	2.5	56
56	BPPred: A Web-based computational tool for predicting biophysical parameters of proteins. Protein Science, 2006, 16, 125-134.	7.6	55
57	Frequency adaptive metadynamics for the calculation of rare-event kinetics. Journal of Chemical Physics, 2018, 149, 072309.	3.0	54
58	Fitting Corrections to an RNA Force Field Using Experimental Data. Journal of Chemical Theory and Computation, 2019, 15, 3425-3431.	5.3	54
59	Improving Martini 3 for Disordered and Multidomain Proteins. Journal of Chemical Theory and Computation, 2022, 18, 2033-2041.	5.3	54
60	A combined computational and structural model of the full-length human prolactin receptor. Nature Communications, 2016, 7, 11578.	12.8	52
61	Dynamic activation and regulation of the mitogen-activated protein kinase p38. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 4655-4660.	7.1	52
62	Biomolecular conformational changes and ligand binding: from kinetics to thermodynamics. Chemical Science, 2017, 8, 6466-6473.	7.4	51
63	Refinement of Î±-Synuclein Ensembles Against SAXS Data: Comparison of Force Fields and Methods. Frontiers in Molecular Biosciences, 2021, 8, 654333.	3.5	51
64	On the Potential of Machine Learning to Examine the Relationship Between Sequence, Structure, Dynamics and Function of Intrinsically Disordered Proteins. Journal of Molecular Biology, 2021, 433, 167196.	4.2	51
65	Barnaba: software for analysis of nucleic acid structures and trajectories. Rna, 2019, 25, 219-231.	3.5	50
66	Understanding singleâ€pass transmembrane receptor signaling from a structural viewpointâ€”what are we missing?. FEBS Journal, 2016, 283, 4424-4451.	4.7	49
67	Computational and cellular studies reveal structural destabilization and degradation of MLH1 variants in Lynch syndrome. ELife, 2019, 8, .	6.0	49
68	Structure and dynamics of a nanodisc by integrating NMR, SAXS and SANS experiments with molecular dynamics simulations. ELife, 2020, 9, .	6.0	49
69	Conformational ensembles of intrinsically disordered proteins and flexible multidomain proteins. Biochemical Society Transactions, 2022, 50, 541-554.	3.4	49
70	Detection of initiation sites in protein folding of the four helix bundle ACBP by chemical shift analysis. FEBS Letters, 2007, 581, 4965-4971.	2.8	47
71	Automated Event Detection and Activity Monitoring in Long Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2009, 5, 2595-2605.	5.3	47
72	Structural Basis for Properdin Oligomerization and Convertase Stimulation in the Human Complement System. Frontiers in Immunology, 2019, 10, 2007.	4.8	47

#	Article	IF	Citations
73	DEER-PREdict: Software for efficient calculation of spin-labeling EPR and NMR data from conformational ensembles. PLoS Computational Biology, 2021, 17, e1008551.	3.2	47
74	Interpreting Dynamically-Averaged Scalar Couplings in Proteins. Journal of Biomolecular NMR, 2005, 32, 273-280.	2.8	46
75	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.	5.3	46
76	Conformational Changes and Free Energies in a Proline Isomerase. Journal of Chemical Theory and Computation, 2014, 10, 4169-4174.	5.3	46
77	Substrate-induced conformational dynamics of the dopamine transporter. Nature Communications, 2019, 10, 2714.	12.8	46
78	Atomistic Description of the Folding of a Dimeric Protein. Journal of Physical Chemistry B, 2013, 117, 12935-12942.	2.6	45
79	Structural heterogeneity and dynamics in protein evolution and design. Current Opinion in Structural Biology, 2018, 48, 157-163.	5.7	42
80	Comparison of the transition state ensembles for folding of Im7 and Im9 determined using all-atom molecular dynamics simulations with Ï• value restraints. Proteins: Structure, Function and Bioinformatics, 2003, 54, 513-525.	2.6	41
81	Communication Routes in ARID Domains between Distal Residues in Helix 5 and the DNA-Binding Loops. PLoS Computational Biology, 2014, 10, e1003744.	3.2	40
82	DNA-binding protects p53 from interactions with cofactors involved in transcription-independent functions. Nucleic Acids Research, 2016, 44, gkw770.	14.5	40
83	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.	2.6	38
84	Probabilistic Determination of Native State Ensembles of Proteins. Journal of Chemical Theory and Computation, 2014, 10, 3484-3491.	5.3	38
85	Mapping the Universe of RNA Tetraloop Folds. Biophysical Journal, 2017, 113, 257-267.	0.5	37
86	Barley Lipid Transfer Protein, LTP1, Contains a New Type of Lipid-like Post-translational Modification*. Journal of Biological Chemistry, 2001, 276, 33547-33553.	3.4	36
87	PHAISTOS: A framework for Markov chain Monte Carlo simulation and inference of protein structure. Journal of Computational Chemistry, 2013, 34, 1697-1705.	3.3	35
88	Bayesian-Maximum-Entropy Reweighting of IDP Ensembles Based on NMR Chemical Shifts. Entropy, 2019, 21, 898.	2.2	35
89	Molecular dynamics-guided discovery of an ago-allosteric modulator for GPR40/FFAR1. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 7123-7128.	7.1	35
90	A Soluble, Folded Protein without Charged Amino Acid Residues. Biochemistry, 2016, 55, 3949-3956.	2.5	34

#	Article	IF	Citations
91	A phosphorylation-motif for tuneable helix stabilisation in intrinsically disordered proteins â€“ Lessons from the sodium proton exchanger 1 (NHE1). Cellular Signalling, 2017, 37, 40-51.	3.6	34
92	Paths of long-range communication in the E2 enzymes of family 3: a molecular dynamics investigation. Physical Chemistry Chemical Physics, 2012, 14, 12515.	2.8	33
93	Equilibrium simulations of proteins using molecular fragment replacement and NMR chemical shifts. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 13852-13857.	7.1	33
94	Calculation of Mutational Free Energy Changes in Transition States for Protein Folding. Biophysical Journal, 2003, 85, 1207-1214.	0.5	31
95	Protein stability and degradation in health and disease. Advances in Protein Chemistry and Structural Biology, 2019, 114, 61-83.	2.3	31
96	Integrating NMR and simulations reveals motions in the UUCG tetraloop. Nucleic Acids Research, 2020, 48, 5839-5848.	14.5	31
97	Cryo-EM reveals the architecture of placental malaria VAR2CSA and provides molecular insight into chondroitin sulfate binding. Nature Communications, 2021, 12, 2956.	12.8	30
98	Thiol Alkylation below Neutral pH. Analytical Biochemistry, 2000, 286, 308-310.	2.4	29
99	Co-Chaperones in Targeting and Delivery of Misfolded Proteins to the 26S Proteasome. Biomolecules, 2020, 10, 1141.	4.0	29
100	Conformational Fluctuations Affect Protein Alignment in Dilute Liquid Crystal Media. Journal of the American Chemical Society, 2006, 128, 4371-4376.	13.7	26
101	Role of protein dynamics in transmembrane receptor signalling. Current Opinion in Structural Biology, 2018, 48, 74-82.	5.7	26
102	Order and disorderâ€”An integrative structure of the full-length human growth hormone receptor. Science Advances, 2021, 7, .	10.3	25
103	Molecular dynamics ensemble refinement of the heterogeneous native state of NCBD using chemical shifts and NOEs. PeerJ, 2018, 6, e5125.	2.0	25
104	Force Field Effects in Simulations of Flexible Peptides with Varying Polyproline II Propensity. Journal of Chemical Theory and Computation, 2021, 17, 6634-6646.	5.3	24
105	Computing, Analyzing, and Comparing the Radius of Gyration and Hydrodynamic Radius in Conformational Ensembles of Intrinsically Disordered Proteins. Methods in Molecular Biology, 2020, 2141, 429-445.	0.9	24
106	Bioinformatics analysis identifies several intrinsically disordered human E3 ubiquitin-protein ligases. PeerJ, 2016, 4, e1725.	2.0	24
107	Refining conformational ensembles of flexible proteins against small-angle x-ray scattering data. Biophysical Journal, 2021, 120, 5124-5135.	0.5	24
108	Blocking protein quality control to counter hereditary cancers. Genes Chromosomes and Cancer, 2017, 56, 823-831.	2.8	23

#	Article	IF	Citations
109	Fitting Side-Chain NMR Relaxation Data Using Molecular Simulations. Journal of Chemical Theory and Computation, 2021, 17, 5262-5275.	5.3	23
110	A Two-step Protein Quality Control Pathway for a Misfolded DJ-1 Variant in Fission Yeast. Journal of Biological Chemistry, 2015, 290, 21141-21153.	3.4	22
111	Protein Structure Validation and Refinement Using Amide Proton Chemical Shifts Derived from Quantum Mechanics. PLoS ONE, 2013, 8, e84123.	2.5	21
112	Computational Redesign of Thioredoxin Is Hypersensitive toward Minor Conformational Changes in the Backbone Template. Journal of Molecular Biology, 2016, 428, 4361-4377.	4.2	21
113	Topological constraints and modular structure in the folding and functional motions of GlpG, an intramembrane protease. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 2098-2103.	7.1	21
114	Diversityâ€Oriented Peptide Stapling: A Third Generation Copperâ€Catalysed Azideâ€“Alkyne Cycloaddition Stapling and Functionalisation Strategy. Chemistry - A European Journal, 2017, 23, 3490-3495.	3.3	21
115	Protein Dynamics Enables Phosphorylation of Buried Residues in Cdk2/Cyclin-A-Bound p27. Biophysical Journal, 2020, 119, 2010-2018.	0.5	21
116	Classifying disease-associated variants using measures of protein activity and stability. , 2020, , 91-107.		21
117	Structural basis of client specificity in mitochondrial membrane-protein chaperones. Science Advances, 2020, 6, .	10.3	21
118	Global analysis of protein stability by temperature and chemical denaturation. Analytical Biochemistry, 2020, 605, 113863.	2.4	20
119	Conformational Ensembles of Noncoding Elements in the SARS-CoV-2 Genome from Molecular Dynamics Simulations. Journal of the American Chemical Society, 2021, 143, 8333-8343.	13.7	17
120	Insight into Calcium-Binding Motifs of Intrinsically Disordered Proteins. Biomolecules, 2021, 11, 1173.	4.0	16
121	Structural and functional variation of chitin-binding domains of a lytic polysaccharide monooxygenase from Cellvibrio japonicus. Journal of Biological Chemistry, 2021, 297, 101084.	3.4	16
122	Folliculin variants linked to Birt-Hogg-DubÃ© syndrome are targeted for proteasomal degradation. PLoS Genetics, 2020, 16, e1009187.	3.5	16
123	Ensuring scientific reproducibility in bio-macromolecular modeling via extensive, automated benchmarks. Nature Communications, 2021, 12, 6947.	12.8	16
124	Structure of the Bacterial Cytoskeleton Protein Bactofilin by NMR Chemical Shifts and Sequence Variation. Biophysical Journal, 2016, 110, 2342-2348.	0.5	15
125	A Robust Proton Flux (pHlux) Assay for Studying the Function and Inhibition of the Influenza A M2 Proton Channel. Biochemistry, 2018, 57, 5949-5956.	2.5	15
126	What Will Computational Modeling Approaches Have to Say in the Era of Atomistic Cryo-EM Data?. Journal of Chemical Information and Modeling, 2020, 60, 2410-2412.	5.4	15

#	Article	IF	Citations
127	Charge Interactions in a Highly Charge-Depleted Protein. Journal of the American Chemical Society, 2021, 143, 2500-2508.	13.7	15
128	Disease-linked mutations cause exposure of a protein quality control degron. Structure, 2022, 30, 1245-1253.e5.	3.3	14
129	Linking thermodynamics and measurements of protein stability. Protein Engineering, Design and Selection, 2021, 34, .	2.1	13
130	Multiplexed assays reveal effects of missense variants in MSH2 and cancer predisposition. PLoS Genetics, 2021, 17, e1009496.	3.5	13
131	Synergistic stabilization of a double mutant in chymotrypsin inhibitor 2 from a library screen in E. coli. Communications Biology, 2021, 4, 980.	4.4	13
132	Robust Estimation of Diffusion-Optimized Ensembles for Enhanced Sampling. Journal of Chemical Theory and Computation, 2014, 10, 543-553.	5.3	12
133	Mapping the degradation pathway of a disease-linked aspartoacylase variant. PLoS Genetics, 2021, 17, e1009539.	3.5	12
134	A dual-reporter system for investigating and optimizing protein translation and folding in E. coli. Nature Communications, 2021, 12, 6093.	12.8	12
135	Exploiting Hydrophobicity for Efficient Production of Transmembrane Helices for Structure Determination by NMR Spectroscopy. Analytical Chemistry, 2015, 87, 9126-9131.	6.5	11
136	Random Mutagenesis Analysis of the Influenza A M2 Proton Channel Reveals Novel Resistance Mutants. Biochemistry, 2018, 57, 5957-5968.	2.5	11
137	Properdin oligomers adopt rigid extended conformations supporting function. ELife, 2021, 10, .	6.0	10
138	Architecture and assembly dynamics of the essential mitochondrial chaperone complex TIM9Â·10Â·12. Structure, 2021, 29, 1065-1073.e4.	3.3	10
139	Mg2+-dependent conformational equilibria in CorA and an integrated view on transport regulation. ELife, 2022, 11, .	6.0	10
140	Gs protein peptidomimetics as allosteric modulators of the Î²2-adrenergic receptor. RSC Advances, 2018, 8, 2219-2228.	3.6	9
141	Novel HARS2 missense variants identified in individuals with sensorineural hearing impairment and Perrault syndrome. European Journal of Medical Genetics, 2020, 63, 103733.	1.3	9
142	A Monte Carlo Study of the Early Steps of Functional Amyloid Formation. PLoS ONE, 2016, 11, e0146096.	2.5	9
143	Transient exposure of a buried phosphorylation site in an autoinhibited protein. Biophysical Journal, 2022, 121, 91-101.	0.5	8
144	Allosteric modulation of the sarcoplasmic reticulum Ca2+ATPase by thapsigarginviadecoupling of functional motions. Physical Chemistry Chemical Physics, 2019, 21, 21991-21995.	2.8	7

#	Article	IF	Citations
145	Ubiquitin Interacting Motifs: Duality Between Structured and Disordered Motifs. Frontiers in Molecular Biosciences, 2021, 8, 676235.	3.5	6
146	Double Mutant of Chymotrypsin Inhibitor 2 Stabilized through Increased Conformational Entropy. Biochemistry, 2022, 61, 160-170.	2.5	6
147	PSX, Proteinâ€“Solvent Exchange: software for calculation of deuterium-exchange effects in small-angle neutron scattering measurements from protein coordinates. Journal of Applied Crystallography, 2019, 52, 1427-1436.	4.5	5
148	Dissecting the statistical properties of the linear extrapolation method of determining protein stability. Protein Engineering, Design and Selection, 2019, 32, 471-479.	2.1	5
149	Protein destabilization and degradation as a mechanism for hereditary disease. , 2020, , 111-125.		5
150	Computational and Experimental Assessment of Backbone Templates for Computational Redesign of the Thioredoxin Fold. Journal of Physical Chemistry B, 2021, 125, 11141-11149.	2.6	5
151	Editorial overview: Theory and simulation: Interpreting experimental data at the molecular level. Current Opinion in Structural Biology, 2018, 49, iv-v.	5.7	4
152	Enhancing coevolution-based contact prediction by imposing structural self-consistency of the contacts. Scientific Reports, 2018, 8, 11112.	3.3	3
153	Monte Carlo Sampling of Protein Folding by Combining an All-Atom Physics-Based Model with a Native State Bias. Journal of Physical Chemistry B, 2018, 122, 11174-11185.	2.6	3
154	The role of water coordination in the pH-dependent gating of hAQP10. Biochimica Et Biophysica Acta - Biomembranes, 2022, 1864, 183809.	2.6	3
155	A Sticky Cage can Slow Down Folding. Biophysical Journal, 2013, 104, 964-965.	0.5	1
156	Co-evolution of drug resistance and broadened substrate recognition in HIV protease variants isolated from an Escherichia coli genetic selection system. Biochemical Journal, 2022, 479, 479-501.	3.7	1
157	Reply to Domene and Furini: Distinguishing knock-on and vacancy diffusion mechanisms. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, .	7.1	0
158	Title is missing!. , 2020, 16, e1007870.		0
159	Title is missing!. , 2020, 16, e1007870.		0
160	Title is missing!. , 2020, 16, e1007870.		0
161	Title is missing!. , 2020, 16, e1007870.		0