Nikolay V Dokholyan

List of Publications by Year
in descending order

335 papers	17,525 citations	12330 69 h-index	22832 112 g-index
447 all docs	447 docs citations	447 times ranked	15684 citing authors

#	Article	IF	Citations
1	Amyloid Oligomers: A Joint Experimental/Computational Perspective on Alzheimerâ€™s Disease, Parkinsonâ€™s Disease, Type II Diabetes, and Amyotrophic Lateral Sclerosis. Chemical Reviews, 2021, 121, 2545-2647.	47.7	406
2	Automated minimization of steric clashes in protein structures. Proteins: Structure, Function and Bioinformatics, 2011, 79, 261-270.	2.6	372
3	Eris: an automated estimator of protein stability. Nature Methods, 2007, 4, 466-467.	19.0	355
4	Phenylalanine-508 mediates a cytoplasmicâ€“membrane domain contact in the CFTR 3D structure crucial to assembly and channel function. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 3256-3261.	7.1	354
5	Small-world view of the amino acids that play a key role in protein folding. Physical Review E, 2002, 65, 061910.	2.1	336
6	Ab Initio Folding of Proteins with All-Atom Discrete Molecular Dynamics. Structure, 2008, 16, 1010-1018.	3.3	287
7	Allostery in Its Many Disguises: From Theory to Applications. Structure, 2019, 27, 566-578.	3.3	285
8	Discrete molecular dynamics studies of the folding of a protein-like model. Folding & Design, 1998, 3, 577-587.	4.5	283
9	Potentiator ivacaftor abrogates pharmacological correction of Î”F508 CFTR in cystic fibrosis. Science Translational Medicine, 2014, 6, 246ra96.	12.4	279
10	Topological determinants of protein folding. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 8637-8641.	7.1	278
11	Community-wide assessment of GPCR structure modelling and ligand docking: GPCR Dock 2008. Nature Reviews Drug Discovery, 2009, 8, 455-463.	46.4	260
12	Ab initio RNA folding by discrete molecular dynamics: From structure prediction to folding mechanisms. Rna, 2008, 14, 1164-1173.	3.5	258
13	Mechanism for the ?-helix to ?-hairpin transition. Proteins: Structure, Function and Bioinformatics, 2003, 53, 220-228.	2.6	252
14	RNA-Puzzles: A CASP-like evaluation of RNA three-dimensional structure prediction. Rna, 2012, 18, 610-625.	3.5	241
15	Controlling Allosteric Networks in Proteins. Chemical Reviews, 2016, 116, 6463-6487.	47.7	207
16	iFoldRNA: three-dimensional RNA structure prediction and folding. Bioinformatics, 2008, 24, 1951-1952.	4.1	200
17	Molecular Dynamics Simulation of Amyloid Î² Dimer Formation. Biophysical Journal, 2004, 87, 2310-2321.	0.5	194
18	The interface of protein structure, protein biophysics, and molecular evolution. Protein Science, 2012, 21, 769-785.	7.6	188

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19	Engineering extrinsic disorder to control protein activity in living cells. Science, 2016, 354, 1441-1444.	12.6	185
20	Discrete Molecular Dynamics: An Efficient And Versatile Simulation Method For Fine Protein Characterization. Journal of Physical Chemistry B, 2012, 116, 8375-8382.	2.6	179
21	Emergence of Protein Fold Families through Rational Design. PLoS Computational Biology, 2006, 2, e85.	3.2	177
22	Engineered allosteric activation of kinases in living cells. Nature Biotechnology, 2010, 28, 743-747.	17.5	177
23	Expanding protein universe and its origin from the biological Big Bang. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 14132-14136.	7.1	174
24	MedusaScore: An Accurate Force Field-Based Scoring Function for Virtual Drug Screening. Journal of Chemical Information and Modeling, 2008, 48, 1656-1662.	5.4	165
25	RNA-Puzzles Round II: assessment of RNA structure prediction programs applied to three large RNA structures. Rna, 2015, 21, 1066-1084.	3.5	161
26	Understanding hierarchical protein evolution from first principles 1 1Edited by J. Thornton. Journal of Molecular Biology, 2001, 312, 289-307.	4.2	158
27	RNA-Puzzles Round III: 3D RNA structure prediction of five riboswitches and one ribozyme. Rna, 2017, 23, 655-672.	3.5	158
28	Molecular Dynamics Simulation of the SH3 Domain Aggregation Suggests a Generic Amyloidogenesis Mechanism. Journal of Molecular Biology, 2002, 324, 851-857.	4.2	157
29	Modeling Backbone Flexibility Improves Protein Stability Estimation. Structure, 2007, 15, 1567-1576.	3.3	147
30	Analysis of DNA sequences using methods of statistical physics. Physica A: Statistical Mechanics and Its Applications, 1998, 249, 430-438.	2.6	140
31	Light Regulation of Protein Dimerization and Kinase Activity in Living Cells Using Photocaged Rapamycin and Engineered FKBP. Journal of the American Chemical Society, 2011, 133, 420-423.	13.7	140
32	Single-molecule correlated chemical probing of RNA. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 13858-13863.	7.1	140
33	Identifying the protein folding nucleus using molecular dynamics 1 1Edited by A. R. Fersht. Journal of Molecular Biology, 2000, 296, 1183-1188.	4.2	137
34	The rate and equilibrium constants for a multistep reaction sequence for the aggregation of superoxide dismutase in amyotrophic lateral sclerosis. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 15094-15099.	7.1	137
35	Correctors of Î”F508 CFTR restore global conformational maturation without thermally stabilizing the mutant protein. FASEB Journal, 2013, 27, 536-545.	0.5	135
36	Direct Molecular Dynamics Observation of Protein Folding Transition State Ensemble. Biophysical Journal, 2002, 83, 3525-3532.	0.5	133

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37	Dynamical roles of metal ions and the disulfide bond in Cu, Zn superoxide dismutase folding and aggregation. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 19696-19701.	7.1	131
38	The Complex Molecular Biology of Amyotrophic Lateral Sclerosis (ALS). Progress in Molecular Biology and Translational Science, 2012, 107, 215-262.	1.7	131
39	Folding Trp-Cage to NMR Resolution Native Structure Using a Coarse-Grained Protein Model. Biophysical Journal, 2005, 88, 147-155.	0.5	130
40	Rational design of a ligand-controlled protein conformational switch. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 6800-6804.	7.1	111
41	Multiple Membrane-Cytoplasmic Domain Contacts in the Cystic Fibrosis Transmembrane Conductance Regulator (CFTR) Mediate Regulation of Channel Gating. Journal of Biological Chemistry, 2008, 283, 26383-26390.	3.4	109
42	Modifications of Superoxide Dismutase (SOD1) in Human Erythrocytes. Journal of Biological Chemistry, 2009, 284, 13940-13947.	3.4	106
43	Regulatory Insertion Removal Restores Maturation, Stability and Function of Î”F508 CFTR. Journal of Molecular Biology, 2010, 401, 194-210.	4.2	105
44	Multiscale Modeling of Nucleosome Dynamics. Biophysical Journal, 2007, 92, 1457-1470.	0.5	104
45	On the significance of an RNA tertiary structure prediction. Rna, 2010, 16, 1340-1349.	3.5	103
46	Physicochemical code for quinary protein interactions in Escherichia coli. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E4556-E4563.	7.1	103
47	Mapping allosteric communications within individual proteins. Nature Communications, 2020, 11, 3862.	12.8	101
48	RNA-Puzzles Round IV: 3D structure predictions of four ribozymes and two aptamers. Rna, 2020, 26, 982-995.	3.5	100
49	Nonnative SOD1 trimer is toxic to motor neurons in a model of amyotrophic lateral sclerosis. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 614-619.	7.1	97
50	iFoldRNA v2: folding RNA with constraints. Bioinformatics, 2015, 31, 2891-2893.	4.1	96
51	Possible Mechanism for Cold Denaturation of Proteins at High Pressure. Physical Review Letters, 2003, 91, 138103.	7.8	95
52	Common dynamical signatures of familial amyotrophic lateral sclerosis-associated structurally diverse Cu, Zn superoxide dismutase mutants. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 3147-3152.	7.1	94
53	Traveling time and traveling length in critical percolation clusters. Physical Review E, 1999, 60, 3425-3428.	2.1	92
54	Molecular Origin of Polyglutamine Aggregation in Neurodegenerative Diseases. PLoS Computational Biology, 2005, 1, e30.	3.2	92

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55	Discrete molecular dynamics. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 80-92.	14.6	91
56	Allosteric Modulation Balances Thermodynamic Stability and Restores Function of Î”F508 CFTR. Journal of Molecular Biology, 2012, 419, 41-60.	4.2	90
57	Protein folding: Then and now. Archives of Biochemistry and Biophysics, 2008, 469, 4-19.	3.0	88
58	Polyglutamine Induced Misfolding of Huntingtin Exon1 is Modulated by the Flanking Sequences. PLoS Computational Biology, 2010, 6, e1000772.	3.2	86
59	Pharmacological Chaperones: Design and Development of New Therapeutic Strategies for the Treatment of Conformational Diseases. ACS Chemical Biology, 2016, 11, 1471-1489.	3.4	85
60	Rapid Flexible Docking Using a Stochastic Rotamer Library of Ligands. Journal of Chemical Information and Modeling, 2010, 50, 1623-1632.	5.4	80
61	Solving protein structures using short-distance cross-linking constraints as a guide for discrete molecular dynamics simulations. Science Advances, 2017, 3, e1700479.	10.3	80
62	Regulation of the epithelial Na+ channel and airway surface liquid volume by serine proteases. Pflugers Archiv European Journal of Physiology, 2010, 460, 1-17.	2.8	79
63	Structural and Dynamic Determinants of Protein-Peptide Recognition. Structure, 2011, 19, 1837-1845.	3.3	79
64	miRNA-711 Binds and Activates TRPA1 Extracellularly to Evoke Acute and Chronic Pruritus. Neuron, 2018, 99, 449-463.e6.	8.1	79
65	Direct Observation of Protein Folding, Aggregation, and a Prion-like Conformational Conversion. Journal of Biological Chemistry, 2005, 280, 40235-40240.	3.4	77
66	Three-dimensional RNA structure refinement by hydroxyl radical probing. Nature Methods, 2012, 9, 603-608.	19.0	77
67	Large SOD1 aggregates, unlike trimeric SOD1, do not impact cell viability in a model of amyotrophic lateral sclerosis. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 4661-4665.	7.1	77
68	Glutathionylation at Cys-111 Induces Dissociation of Wild Type and FALS Mutant SOD1 Dimers. Biochemistry, 2011, 50, 7057-7066.	2.5	75
69	Predicting the functional consequences of non-synonymous single nucleotide polymorphisms in IL8 gene. Scientific Reports, 2017, 7, 6525.	3.3	75
70	Computational design of chemogenetic and optogenetic split proteins. Nature Communications, 2018, 9, 4042.	12.8	75
71	Discrete molecular dynamics simulations of peptide aggregation. Physical Review E, 2004, 69, 041908.	2.1	74
72	Local Unfolding of Cu, Zn Superoxide Dismutase Monomer Determines the Morphology of Fibrillar Aggregates. Journal of Molecular Biology, 2012, 421, 548-560.	4.2	74

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73	Simple but predictive protein models. Trends in Biotechnology, 2005, 23, 450-455.	9.3	73
74	Topological Determinants of Protein Domain Swapping. Structure, 2006, 14, 5-14.	3.3	73
75	Fast complementation of split fluorescent protein triggered by DNA hybridization. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 2052-2056.	7.1	73
76	Reconstruction of the src-SH3 Protein Domain Transition State Ensemble using Multiscale Molecular Dynamics Simulations. Journal of Molecular Biology, 2005, 350, 1035-1050.	4.2	72
77	Deciphering Protein Dynamics from NMR Data Using Explicit Structure Sampling and Selection. Biophysical Journal, 2007, 93, 2300-2306.	0.5	72
78	Can Contact Potentials Reliably Predict Stability of Proteins?. Journal of Molecular Biology, 2004, 336, 1223-1238.	4.2	69
79	Computational Design of a PAK1 Binding Protein. Journal of Molecular Biology, 2010, 400, 257-270.	4.2	69
80	Flow between two sites on a percolation cluster. Physical Review E, 2000, 62, 8270-8281.	2.1	67
81	Studies of folding and misfolding using simplified models. Current Opinion in Structural Biology, 2006, 16, 79-85.	5.7	67
82	Native-like RNA Tertiary Structures Using a Sequence-Encoded Cleavage Agent and Refinement by Discrete Molecular Dynamics. Journal of the American Chemical Society, 2009, 131, 2541-2546.	13.7	65
83	Harnessing a Physiologic Mechanism for siRNA Delivery With Mimetic Lipoprotein Particles. Molecular Therapy, 2012, 20, 1582-1589.	8.2	65
84	RNAâ€“DNA fibers and polygons with controlled immunorecognition activate RNAi, FRET and transcriptional regulation of NF-ÎºB in human cells. Nucleic Acids Research, 2019, 47, 1350-1361.	14.5	64
85	New Insights into FAK Signaling and Localization Based on Detection of a FAT Domain Folding Intermediate. Structure, 2004, 12, 2161-2171.	3.3	62
86	Natural Selection against Protein Aggregation on Self-Interacting and Essential Proteins in Yeast, Fly, and Worm. Molecular Biology and Evolution, 2008, 25, 1530-1533.	8.9	61
87	The coordinated evolution of yeast proteins is constrained by functional modularity. Trends in Genetics, 2006, 22, 416-419.	6.7	60
88	Folding of Cu, Zn Superoxide Dismutase and Familial Amyotrophic Lateral Sclerosis. Journal of Molecular Biology, 2003, 334, 515-525.	4.2	59
89	Applications of Discrete Molecular Dynamics in biology and medicine. Current Opinion in Structural Biology, 2016, 37, 9-13.	5.7	59
90	Scaling Behavior and Structure of Denatured Proteins. Structure, 2005, 13, 1047-1054.	3.3	58

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91	Fast screening of protein surfaces using geometric invariant fingerprints. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 16622-16626.	7.1	58
92	Viral DNA Binding to NLRC3, an Inhibitory Nucleic Acid Sensor, Unleashes STING, a Cyclic Dinucleotide Receptor that Activates Type I Interferon. Immunity, 2019, 50, 591-599.e6.	14.3	58
93	High-speed atomic force microscopy reveals structural dynamics of Î±-synuclein monomers and dimers. Journal of Chemical Physics, 2018, 148, 123322.	3.0	57
94	RNA Fibers as Optimized Nanoscaffolds for siRNA Coordination and Reduced Immunological Recognition. Advanced Functional Materials, 2018, 28, 1805959.	14.9	57
95	Imprint of evolution on protein structures. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 2846-2851.	7.1	55
96	BiPS, a Photocleavable, Isotopically Coded, Fluorescent Cross-linker for Structural Proteomics. Molecular and Cellular Proteomics, 2009, 8, 273-286.	3.8	55
97	Conformational ensemble of native Î±-synuclein in solution as determined by short-distance crosslinking constraint-guided discrete molecular dynamics simulations. PLoS Computational Biology, 2019, 15, e1006859.	3.2	55
98	Thermodynamics and Folding Kinetics Analysis of the SH3 Domain form Discrete Molecular Dynamics. Journal of Molecular Biology, 2002, 318, 863-876.	4.2	54
99	Computational Studies Reveal Phosphorylation-dependent Changes in the Unstructured R Domain of CFTR. Journal of Molecular Biology, 2008, 378, 1052-1063.	4.2	54
100	Identification and Rational Redesign of Peptide Ligands to CRIP1, A Novel Biomarker for Cancers. PLoS Computational Biology, 2008, 4, e1000138.	3.2	53
101	Scaling of the Distribution of Shortest Paths in Percolation. Journal of Statistical Physics, 1998, 93, 603-613.	1.2	52
102	A Single Disulfide Bond Differentiates Aggregation Pathways of ÃŸ2-Microglobulin. Journal of Molecular Biology, 2005, 354, 473-482.	4.2	52
103	FALS mutations in Cu, Zn superoxide dismutase destabilize the dimer and increase dimer dissociation propensity: A large-scale thermodynamic analysis. Amyloid: the International Journal of Experimental and Clinical Investigation: the Official Journal of the International Society of Amyloidosis, 2006, 13, 226-235.	3.0	52
104	Protein Destabilization as a Common Factor in Diverse Inherited Disorders. Journal of Molecular Evolution, 2016, 82, 11-16.	1.8	52
105	Disruptive mRNA folding increases translational efficiency of catechol-O-methyltransferase variant. Nucleic Acids Research, 2011, 39, 6201-6212.	14.5	51
106	Functional Fingerprints of Folds: Evidence for Correlated Structureâ€“Function Evolution. Journal of Molecular Biology, 2003, 326, 1-9.	4.2	50
107	Knowledge-Based Design of a Biosensor to Quantify Localized ERK Activation in Living Cells. Chemistry and Biology, 2013, 20, 847-856.	6.0	49
108	Identification of an Actin Binding Surface on Vinculin that Mediates Mechanical Cell and Focal Adhesion Properties. Structure, 2014, 22, 697-706.	3.3	49

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109	Rational coupled dynamics network manipulation rescues disease-relevant mutant cystic fibrosis transmembrane conductance regulator. Chemical Science, 2015, 6, 1237-1246.	7.4	49
110	Structural Determinants of Skeletal Muscle Ryanodine Receptor Gating*. Journal of Biological Chemistry, 2013, 288, 6154-6165.	3.4	48
111	Cu,Zn-Superoxide Dismutase without Zn Is Folded but Catalytically Inactive. Journal of Molecular Biology, 2014, 426, 4112-4124.	4.2	47
112	Molecular Dynamic Simulations of Cisplatin- and Oxaliplatin-d(GG) Intrastand Cross-links Reveal Differences in their Conformational Dynamics. Journal of Molecular Biology, 2007, 373, 1123-1140.	4.2	46
113	Diminished Self-Chaperoning Activity of the Î”F508 Mutant of CFTR Results in Protein Misfolding. PLoS Computational Biology, 2008, 4, e1000008.	3.2	46
114	Engineering proteins for allosteric control by light or ligands. Nature Protocols, 2019, 14, 1863-1883.	12.0	46
115	MedusaDock 2.0: Efficient and Accurate Proteinâ€“Ligand Docking With Constraints. Journal of Chemical Information and Modeling, 2019, 59, 2509-2515.	5.4	46
116	AlphaFold illuminates half of the dark human proteins. Current Opinion in Structural Biology, 2022, 74, 102372.	5.7	45
117	Distribution of Base Pair Repeats in Coding and Noncoding DNA Sequences. Physical Review Letters, 1997, 79, 5182-5185.	7.8	44
118	Gaia: automated quality assessment of protein structure models. Bioinformatics, 2011, 27, 2209-2215.	4.1	44
119	Structural and Thermodynamic Effects of Post-translational Modifications in Mutant and Wild Type Cu, Zn Superoxide Dismutase. Journal of Molecular Biology, 2011, 408, 555-567.	4.2	43
120	Computational approaches to understanding protein aggregation in neurodegeneration. Journal of Molecular Cell Biology, 2014, 6, 104-115.	3.3	43
121	Restoration of R117H CFTR folding and function in human airway cells through combination treatment with VX-809 and VX-770. American Journal of Physiology - Lung Cellular and Molecular Physiology, 2016, 311, L550-L559.	2.9	42
122	Active Nuclear Receptors Exhibit Highly Correlated AF-2 Domain Motions. PLoS Computational Biology, 2008, 4, e1000111.	3.2	42
123	Principles for Understanding the Accuracy of SHAPE-Directed RNA Structure Modeling. Biochemistry, 2013, 52, 588-595.	2.5	41
124	Non-native Soluble Oligomers of Cu/Zn Superoxide Dismutase (SOD1) Contain a Conformational Epitope Linked to Cytotoxicity in Amyotrophic Lateral Sclerosis (ALS). Biochemistry, 2014, 53, 2423-2432.	2.5	41
125	Light-cleavable rapamycin dimer as an optical trigger for protein dimerization. Chemical Communications, 2015, 51, 5702-5705.	4.1	41
126	A Phosphomimetic Mutation Stabilizes SOD1 and Rescues Cell Viability in the Context of an ALS-Associated Mutation. Structure, 2016, 24, 1898-1906.	3.3	41

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127	Predicting oil recovery using percolation. Physica A: Statistical Mechanics and Its Applications, 1999, 266, 107-114.	2.6	40
128	The Length Dependence of the PolyQ-mediated Protein Aggregation. Journal of Biological Chemistry, 2007, 282, 25487-25492.	3.4	40
129	Reversible and Tunable Photoswitching of Protein Function through Genetic Encoding of Azobenzene Amino Acids in Mammalian Cells. ChemBioChem, 2018, 19, 2178-2185.	2.6	40
130	Dynamic Docking of Conformationally Constrained Macrocycles: Methods and Applications. ACS Chemical Biology, 2016, 11, 10-24.	3.4	39
131	Insight into the Structure of the â€œUnstructuredâ€•Tau Protein. Structure, 2019, 27, 1710-1715.e4.	3.3	39
132	Distributions of Dimeric Tandem Repeats in Non-coding and Coding DNA Sequences. Journal of Theoretical Biology, 2000, 202, 273-282.	1.7	38
133	Hierarchy in social organization. Physica A: Statistical Mechanics and Its Applications, 2003, 330, 653-659.	2.6	38
134	Multiple Folding Pathways of the SH3 Domain. Biophysical Journal, 2004, 87, 521-533.	0.5	38
135	ATP hydrolysis at one of the two sites in ABC transporters initiates transport related conformational transitions. Biochimica Et Biophysica Acta - Biomembranes, 2011, 1808, 2954-2964.	2.6	38
136	Predicting oil recovery using percolation theory. Petroleum Geoscience, 2001, 7, .	1.5	37
137	Protein Evolution within a Structural Space. Biophysical Journal, 2003, 85, 2962-2972.	0.5	37
138	Interaction with the 5D3 Monoclonal Antibody Is Regulated by Intramolecular Rearrangements but Not by Covalent Dimer Formation of the Human ABCG2 Multidrug Transporter. Journal of Biological Chemistry, 2008, 283, 26059-26070.	3.4	37
139	Identification of a consensus motif in substrates bound by a Type I Hsp40. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 11073-11078.	7.1	37
140	Cheminformatics Meets Molecular Mechanics: A Combined Application of Knowledge-Based Pose Scoring and Physical Force Field-Based Hit Scoring Functions Improves the Accuracy of Structure-Based Virtual Screening. Journal of Chemical Information and Modeling, 2012, 52, 16-28.	5.4	37
141	Incorporating Backbone Flexibility in MedusaDock Improves Ligand-Binding Pose Prediction in the CSAR2011 Docking Benchmark. Journal of Chemical Information and Modeling, 2013, 53, 1871-1879.	5.4	37
142	Applications of statistical physics to the oil industry: predicting oil recovery using percolation theory. Physica A: Statistical Mechanics and Its Applications, 1999, 274, 60-66.	2.6	35
143	Sequence and structural determinants of Cu, Zn superoxide dismutase aggregation. Proteins: Structure, Function and Bioinformatics, 2005, 61, 617-632.	2.6	35
144	The path of DNA in the kinetochore. Current Biology, 2006, 16, R276-R278.	3.9	35

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145	Submillisecond Elastic Recoil Reveals Molecular Origins of Fibrin Fiber Mechanics. Biophysical Journal, 2013, 104, 2671-2680.	0.5	35
146	Comparative Visualization of the RNA Suboptimal Conformational Ensemble InÂVivo. Biophysical Journal, 2017, 113, 290-301.	0.5	35
147	A structural model reveals energy transduction in dynein. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 18540-18545.	7.1	34
148	Structural and functional interactions between six-transmembrane Î¼-opioid receptors and Î²2-adrenoreceptors modulate opioid signaling. Scientific Reports, 2016, 5, 18198.	3.3	34
149	Macromolecular crowding induces polypeptide compaction and decreases folding cooperativity. Physical Chemistry Chemical Physics, 2010, 12, 3491.	2.8	33
150	The structural heterogeneity of Î±-synuclein is governed by several distinct subpopulations with interconversion times slower than milliseconds. Structure, 2021, 29, 1048-1064.e6.	3.3	32
151	Robust and Generic RNA Modeling Using Inferred Constraints: A Structure for the Hepatitis C Virus IRES Pseudoknot Domain. Biochemistry, 2010, 49, 4931-4933.	2.5	31
152	Discrete Molecular Dynamics Distinguishes Nativelike Binding Poses from Decoys in Difficult Targets. Biophysical Journal, 2012, 102, 144-151.	0.5	31
153	Direct identification of base-paired RNA nucleotides by correlated chemical probing. Rna, 2017, 23, 6-13.	3.5	31
154	Structural complexity and functional diversity of plant NADPH oxidases. Amino Acids, 2018, 50, 79-94.	2.7	31
155	Structural Mechanism of S-Adenosyl Methionine Binding to Catechol O-Methyltransferase. PLoS ONE, 2011, 6, e24287.	2.5	31
156	Insights into Allosteric Control of Vinculin Function from Its Large Scale Conformational Dynamics. Journal of Biological Chemistry, 2006, 281, 29148-29154.	3.4	30
157	Structural Basis for Î¼-Opioid Receptor Binding and Activation. Structure, 2011, 19, 1683-1690.	3.3	30
158	Rational design and implementation of a chemically inducible heterotrimerization system. Nature Methods, 2020, 17, 928-936.	19.0	30
159	Combining Fluorescence Detection and Mass Spectrometric Analysis for Comprehensive and Quantitative Analysis of Redox-Sensitive Cysteines in Native Membrane Proteins. Analytical Chemistry, 2006, 78, 7959-7966.	6.5	29
160	Parallel Folding Pathways in the SH3 Domain Protein. Journal of Molecular Biology, 2007, 373, 1348-1360.	4.2	29
161	Nâ€terminal strands of filamin Ig domains act as a conformational switch under biological forces. Proteins: Structure, Function and Bioinformatics, 2010, 78, 12-24.	2.6	29
162	Rigid substructure search. Bioinformatics, 2011, 27, 1327-1329.	4.1	28

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163	COMT gene locus. Pain, 2015, 156, 2072-2083.	4.2	28
164	iFold: a platform for interactive folding simulations of proteins. Bioinformatics, 2006, 22, 2693-2694.	4.1	27
165	A cost effectiveness analysis of omitting radiography in diagnosis of acute bronchiolitis. Pediatric Pulmonology, 2009, 44, 122-127.	2.0	27
166	Structural basis for the sequence-dependent effects of platinumâ€“DNA adducts. Nucleic Acids Research, 2009, 37, 2434-2448.	14.5	27
167	Differences in the Antinociceptive Effects and Binding Properties of Propranolol and Bupranolol Enantiomers. Journal of Pain, 2015, 16, 1321-1333.	1.4	27
168	Ca2+-mediated activation of the skeletal-muscle ryanodine receptor ion channel. Journal of Biological Chemistry, 2018, 293, 19501-19509.	3.4	27
169	Î²-Methylamino-L-alanine substitution of serine in SOD1 suggests a direct role in ALS etiology. PLoS Computational Biology, 2019, 15, e1007225.	3.2	27
170	Hybrid Dynamics Simulation Engine for Metalloproteins. Biophysical Journal, 2012, 103, 767-776.	0.5	26
171	Î¼-Opioid receptor 6-transmembrane isoform: A potential therapeutic target for new effective opioids. Progress in Neuro-Psychopharmacology and Biological Psychiatry, 2015, 62, 61-67.	4.8	26
172	A modified PATH algorithm rapidly generates transition states comparable to those found by other well established algorithms. Structural Dynamics, 2016, 3, 012101.	2.3	26
173	Engineering Pak1 Allosteric Switches. ACS Synthetic Biology, 2017, 6, 1257-1262.	3.8	26
174	Distribution of shortest paths in percolation. Physica A: Statistical Mechanics and Its Applications, 1999, 266, 55-61.	2.6	25
175	G Protein Mono-ubiquitination by the Rsp5 Ubiquitin Ligase. Journal of Biological Chemistry, 2009, 284, 8940-8950.	3.4	25
176	A Structural Model of the Pore-Forming Region of the Skeletal Muscle Ryanodine Receptor (RyR1). PLoS Computational Biology, 2009, 5, e1000367.	3.2	25
177	MERTK mediated novel site Akt phosphorylation alleviates SAV1 suppression. Nature Communications, 2019, 10, 1515.	12.8	25
178	Modifications to the Framework Regions Eliminate Chimeric Antigen Receptor Tonic Signaling. Cancer Immunology Research, 2021, 9, 441-453.	3.4	25
179	Using protein design for homology detection and active site searches. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 11361-11366.	7.1	24
180	Energetic and Structural Basis for Activation of the Epithelial Sodium Channel by Matriptase. Biochemistry, 2012, 51, 3460-3469.	2.5	24

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181	Dynamics Intrinsic to Cystic Fibrosis Transmembrane Conductance Regulator Function and Stability. Cold Spring Harbor Perspectives in Medicine, 2013, 3, a009522-a009522.	6.2	24
182	Intrinsic Disorder Mediates Cooperative Signal Transduction in STIM1. Journal of Molecular Biology, 2014, 426, 2082-2097.	4.2	24
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