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	Mapping coâ€regulatory interactions among ligandâ€binding sites in ryanodine receptor 1. Proteins: Structure, Function and Bioinformatics, 2022, 90, 385-394.	2.6	2
2	Yuel: Improving the Generalizability of Structure-Free Compoundâ€“Protein Interaction Prediction. Journal of Chemical Information and Modeling, 2022, 62, 463-471.	5.4	17
3	Toward rational vaccine engineering. Advanced Drug Delivery Reviews, 2022, 183, 114142.	13.7	10
4	Anhydrous Nucleic Acid Nanoparticles for Storage and Handling at Broad Range of Temperatures. Small, 2022, 18, e2104814.	10.0	13
5	NeuralDock: Rapid and Conformation-Agnostic Docking of Small Molecules. Frontiers in Molecular Biosciences, 2022, 9, 867241.	3.5	3
6	Design and engineering of allosteric communications in proteins. Current Opinion in Structural Biology, 2022, 73, 102334.	5.7	19
7	Identification of a Vitamin-D Receptor Antagonist, MeTC7, which Inhibits the Growth of Xenograft and Transgenic Tumors In Vivo. Journal of Medicinal Chemistry, 2022, 65, 6039-6055.	6.4	3
8	AlphaFold illuminates half of the dark human proteins. Current Opinion in Structural Biology, 2022, 74, 102372.	5.7	45
9	Multifunctions of Î±â€Synuclein Explained by Its Dynamic Heterogeneous Conformations with a Hierarchy of Transition Times. FASEB Journal, 2022, 36, .	0.5	0
10	Toxic SOD1 trimers are off-pathway in the formation of amyloid-like fibrils in ALS. Biophysical Journal, 2022, 121, 2084-2095.	0.5	7
11	Evaluation of pH change effects on the HSA folding and its drug binding characteristics, a computational biology investigation. Proteins: Structure, Function and Bioinformatics, 2022, 90, 1908-1925.	2.6	3
12	Predicting Proteinâ€“Ligand Docking Structure with Graph Neural Network. Journal of Chemical Information and Modeling, 2022, 62, 2923-2932.	5.4	23
13	Monosialotetrahexosylganglioside Promotes Early AÎ²42 Oligomer Formation and Maintenance. ACS Chemical Neuroscience, 2022, 13, 1979-1991.	3.5	6
14	Locking and Unlocking Thrombin Function Using Immunoquiescent Nucleic Acid Nanoparticles with Regulated Retention In Vivo. Nano Letters, 2022, 22, 5961-5972.	9.1	9
15	Alternative Splicing of Opioid Receptor Genes Shows a Conserved Pattern for 6TM Receptor Variants. Cellular and Molecular Neurobiology, 2021, 41, 1039-1055.	3.3	5
16	Prefusion spike protein stabilization through computational mutagenesis. Proteins: Structure, Function and Bioinformatics, 2021, 89, 399-408.	2.6	5
17	GPU-Accelerated Flexible Molecular Docking. Journal of Physical Chemistry B, 2021, 125, 1049-1060.	2.6	14
18	SOD1 oligomers in amyotrophic lateral sclerosis. Current Opinion in Structural Biology, 2021, 66, 225-230.	5.7	17

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19	Modifications to the Framework Regions Eliminate Chimeric Antigen Receptor Tonic Signaling. Cancer Immunology Research, 2021, 9, 441-453.	3.4	25
20	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
21	Engineering an Allosteric Control of Protein Function. Journal of Physical Chemistry B, 2021, 125, 1806-1814.	2.6	18
22	Nanoscale programming of cellular and physiological phenotypes: inorganic meets organic programming. Npj Systems Biology and Applications, 2021, 7, 15.	3.0	9
23	Identification and characterization of novel candidate compounds targeting 6â€•and 7â€transmembrane Î¼â€opioid receptor isoforms. British Journal of Pharmacology, 2021, 178, 2709-2726.	5.4	4
24	Activating Sphingosine-1-phospahte signaling in endothelial cells increases myosin light chain phosphorylation to decrease endothelial permeability thereby inhibiting cancer metastasis. Cancer Letters, 2021, 506, 107-119.	7.2	4
25	Direct Mapping of Higher-Order RNA Interactions by SHAPE-JuMP. Biochemistry, 2021, 60, 1971-1982.	2.5	24
26	Titr-DMDâ€”A Rapid, Coarse-Grained Quasi-All-Atom Constant pH Molecular Dynamics Framework. Journal of Chemical Theory and Computation, 2021, 17, 4538-4549.	5.3	6
27	Structure of prion Î²â€oligomers as determined by shortâ€distance crosslinking constraintâ€guided discrete molecular dynamics simulations. Proteomics, 2021, 21, e2000298.	2.2	10
28	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
29	Searching for methyllysine-binding aromatic cages. Biochemical Journal, 2021, 478, 3613-3619.	3.7	3
30	Mechanical Counterbalance of Kinesin and Dynein Motors in a Microtubular Network Regulates Cell Mechanics, 3D Architecture, and Mechanosensing. ACS Nano, 2021, 15, 17528-17548.	14.6	9
31	Invited: Drug Discovery Approaches using Quantum Machine Learning. , 2021, , .		12
32	IL-1 Via IRAK1/4 Sustains Acute Myeloid Leukemia Stem Cells Following Treatment and Relapse. Blood, 2021, 138, 1175-1175.	1.4	1
33	Two-input protein logic gate for computation in living cells. Nature Communications, 2021, 12, 6615.	12.8	20
34	Development of a Novel Multi-Isoform ALDH Inhibitor Effective as an Antimelanoma Agent. Molecular Cancer Therapeutics, 2020, 19, 447-459.	4.1	15
35	Ligand-induced disorder-to-order transitions characterized by structural proteomics and molecular dynamics simulations. Journal of Proteomics, 2020, 211, 103544.	2.4	10
36	Guiding Conventional Proteinâ€“Ligand Docking Software with Convolutional Neural Networks. Journal of Chemical Information and Modeling, 2020, 60, 4594-4602.	5.4	15

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37	Molecular Design for Research and Therapeutics. Biophysical Journal, 2020, 118, 42a.	0.5	0
38	Mapping allosteric communications within individual proteins. Nature Communications, 2020, 11, 3862.	12.8	101
39	Rational design and implementation of a chemically inducible heterotrimerization system. Nature Methods, 2020, 17, 928-936.	19.0	30
40	ASR490, a Small Molecule, Overrides Aberrant Expression ofNotch1in Colorectal Cancer. Molecular Cancer Therapeutics, 2020, 19, 2422-2431.	4.1	4
41	RNA-Puzzles Round IV: 3D structure predictions of four ribozymes and two aptamers. Rna, 2020, 26, 982-995.	3.5	100
42	Various miRNAs compensate the role of miR-122 on HCV replication. PLoS Pathogens, 2020, 16, e1008308.	4.7	14
43	Single-channel properties of skeletal muscle ryanodine receptor pore Î”4923FF4924 in two brothers with a lethal form of fetal akinesia. Cell Calcium, 2020, 87, 102182.	2.4	6
44	Experimentally-driven protein structure modeling. Journal of Proteomics, 2020, 220, 103777.	2.4	21
45	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
46	Inter-Active Site Communication Mediated by the Dimer Interface Î²-Sheet in the Half-the-Sites Enzyme, Thymidylate Synthase. Biochemistry, 2019, 58, 3302-3313.	2.5	9
47	Insight into the Structure of the â€œUnstructuredâ€•Tau Protein. Structure, 2019, 27, 1710-1715.e4.	3.3	39
48	Computationally Guided Design of Single-Chain Variable Fragment Improves Specificity of Chimeric Antigen Receptors. Molecular Therapy - Oncolytics, 2019, 15, 30-37.	4.4	20
49	Distinct Binding Modes of Vinculin Isoforms Underlie Their Functional Differences. Structure, 2019, 27, 1527-1536.e3.	3.3	4
50	A central core disease mutation in the Ca²⁺-binding site of skeletal muscle ryanodine receptor impairs single-channel regulation. American Journal of Physiology - Cell Physiology, 2019, 317, C358-C365.	4.6	22
51	Stabilization of Î¼â€opioid receptor facilitates its cellular translocation and signaling. Proteins: Structure, Function and Bioinformatics, 2019, 87, 878-884.	2.6	6
52	Limits in accuracy and a strategy of RNA structure prediction using experimental information. Nucleic Acids Research, 2019, 47, 5563-5572.	14.5	10
53	Engineering proteins for allosteric control by light or ligands. Nature Protocols, 2019, 14, 1863-1883.	12.0	46
54	Molecular mechanisms of heterogeneous oligomerization of huntingtin proteins. Scientific Reports, 2019, 9, 7615.	3.3	21

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55	Mutation Analysis of the Calcium Binding Site of Skeletal Muscle Ryanodine Receptor Calcium Release Channel. Biophysical Journal, 2019, 116, 520a-521a.	0.5	0
56	Uncovered Dynamic Coupling Resolves the Ambiguous Mechanism of Phenylalanine Hydroxylase Oxygen Binding. Journal of Physical Chemistry B, 2019, 123, 4534-4539.	2.6	7
57	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
58	Cardiomyopathy Mutations in Metavinculin Disrupt Regulation of Vinculin-Induced F-Actin Assemblies. Journal of Molecular Biology, 2019, 431, 1604-1618.	4.2	11
59	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
60	MedusaDock 2.0: Efficient and Accurate Proteinâ€“Ligand Docking With Constraints. Journal of Chemical Information and Modeling, 2019, 59, 2509-2515.	5.4	46
61	MERTK mediated novel site Akt phosphorylation alleviates SAV1 suppression. Nature Communications, 2019, 10, 1515.	12.8	25
62	Allostery in Its Many Disguises: From Theory to Applications. Structure, 2019, 27, 566-578.	3.3	285
63	Rationally designed carbohydrate-occluded epitopes elicit HIV-1 Env-specific antibodies. Nature Communications, 2019, 10, 948.	12.8	19
64	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
65	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
66	Mapping allosteric linkage to channel gating by extracellular domains in the human epithelial sodium channel. Journal of Biological Chemistry, 2018, 293, 3675-3684.	3.4	0
67	High-speed atomic force microscopy reveals structural dynamics of Î±-synuclein monomers and dimers. Journal of Chemical Physics, 2018, 148, 123322.	3.0	57
68	Tyrosine phosphorylation switching of a G protein. Journal of Biological Chemistry, 2018, 293, 4752-4766.	3.4	23
69	G4941K substitution in the pore-lining S6 helix of the skeletal muscle ryanodine receptor increases RyR1 sensitivity to cytosolic and luminal Ca2+. Journal of Biological Chemistry, 2018, 293, 2015-2028.	3.4	10
70	Structural complexity and functional diversity of plant NADPH oxidases. Amino Acids, 2018, 50, 79-94.	2.7	31
71	Ca2+-mediated activation of the skeletal-muscle ryanodine receptor ion channel. Journal of Biological Chemistry, 2018, 293, 19501-19509.	3.4	27
72	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

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73	Computational design of chemogenetic and optogenetic split proteins. Nature Communications, 2018, 9, 4042.	12.8	75
74	RNA Fibers as Optimized Nanoscaffolds for siRNA Coordination and Reduced Immunological Recognition. Advanced Functional Materials, 2018, 28, 1805959.	14.9	57
75	miRNA-711 Binds and Activates TRPA1 Extracellularly to Evoke Acute and Chronic Pruritus. Neuron, 2018, 99, 449-463.e6.	8.1	79
76	Vinculin and its Fundamental Role in Actin Bundling Formation. Biophysical Journal, 2018, 114, 27a.	0.5	1
77	Ligand binding to a remote site thermodynamically corrects the F508del mutation in the human cystic fibrosis transmembrane conductance regulator. Journal of Biological Chemistry, 2018, 293, 17685-17704.	3.4	9
78	Elicitation of HIVâ€specific Antibodies Targeting The Carbohydrateâ€Occluded Neutralization Epitopes Through Rational Protein Design. FASEB Journal, 2018, 32, 798.14.	0.5	1
79	A Structural Model for Vinculin Insertion into PIP2-Containing Membranes and the Effect of Insertion on Vinculin Activation and Localization. Structure, 2017, 25, 264-275.	3.3	23
80	RNA-Puzzles Round III: 3D RNA structure prediction of five riboswitches and one ribozyme. Rna, 2017, 23, 655-672.	3.5	158
81	Comparative Visualization of the RNA Suboptimal Conformational Ensemble InÂVivo. Biophysical Journal, 2017, 113, 290-301.	0.5	35
82	Protein folding: Over half a century lasting quest. Physics of Life Reviews, 2017, 21, 72-74.	2.8	2
83	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
84	Ion-pulling simulations provide insights into the mechanisms of channel opening of the skeletal muscle ryanodine receptor. Journal of Biological Chemistry, 2017, 292, 12947-12958.	3.4	11
85	Engineering Pak1 Allosteric Switches. ACS Synthetic Biology, 2017, 6, 1257-1262.	3.8	26
86	Computational Protein Design Through Grafting and Stabilization. Methods in Molecular Biology, 2017, 1529, 227-241.	0.9	6
87	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
88	Molecular Mechanisms of the R61T Mutation in Apolipoprotein E4: A Dynamic Rescue. Biophysical Journal, 2017, 113, 2192-2198.	0.5	2
89	Redundant Functions for Nap1 and Chz1 in H2A.Z Deposition. Scientific Reports, 2017, 7, 10791.	3.3	13
90	Predicting the functional consequences of non-synonymous single nucleotide polymorphisms in IL8 gene. Scientific Reports, 2017, 7, 6525.	3.3	75

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91	Direct identification of base-paired RNA nucleotides by correlated chemical probing. Rna, 2017, 23, 6-13.	3.5	31
92	Transmembrane helical interactions in the CFTR channel pore. PLoS Computational Biology, 2017, 13, e1005594.	3.2	9
93	Structure modeling of RNA using sparse NMR constraints. Nucleic Acids Research, 2017, 45, 12638-12647.	14.5	15
94	Structural and functional interactions between six-transmembrane Î¼-opioid receptors and Î²2-adrenoreceptors modulate opioid signaling. Scientific Reports, 2016, 5, 18198.	3.3	34
95	Engineering extrinsic disorder to control protein activity in living cells. Science, 2016, 354, 1441-1444.	12.6	185
96	Role of PIP2-Dependent Membrane Interactions in Vinculin Activation, Motility and Force Transmission. Biophysical Journal, 2016, 110, 575a.	0.5	0
97	Docking and Scoring with Target-Specific Pose Classifier Succeeds in Native-Like Pose Identification But Not Binding Affinity Prediction in the CSAR 2014 Benchmark Exercise. Journal of Chemical Information and Modeling, 2016, 56, 1032-1041.	5.4	15
98	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
99	Computational Modeling of Small Molecule Ligand Binding Interactions and Affinities. Methods in Molecular Biology, 2016, 1414, 23-32.	0.9	4
100	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
101	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
102	Harnessing Natureâ€™s Diversity: Discovering organophosphate bioscavenger characteristics among low molecular weight proteins. Scientific Reports, 2016, 6, 37175.	3.3	10
103	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
104	A hidden aggregationâ€prone structure in the heart of hypoxia inducible factor prolyl hydroxylase. Proteins: Structure, Function and Bioinformatics, 2016, 84, 611-623.	2.6	2
105	Controlling Allosteric Networks in Proteins. Chemical Reviews, 2016, 116, 6463-6487.	47.7	207
106	Gain-of-Function Mutation W493R in the Epithelial Sodium Channel Allosterically Reconfigures Intersubunit Coupling. Journal of Biological Chemistry, 2016, 291, 3682-3692.	3.4	6
107	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
108	Protein Destabilization as a Common Factor in Diverse Inherited Disorders. Journal of Molecular Evolution, 2016, 82, 11-16.	1.8	52

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109	Applications of Discrete Molecular Dynamics in biology and medicine. Current Opinion in Structural Biology, 2016, 37, 9-13.	5.7	59
110	Dynamic Docking of Conformationally Constrained Macrocycles: Methods and Applications. ACS Chemical Biology, 2016, 11, 10-24.	3.4	39
111	W493R Gain of Function Mutation in Atypical Cystic Fibrosis Rewires the Epithelial Sodium Channel Dynamics. Biophysical Journal, 2015, 108, 583a-584a.	0.5	0
112	New Models for Regulation of Vinculin by Actin and Phospholipids. Biophysical Journal, 2015, 108, 508a-509a.	0.5	0
113	COMT gene locus. Pain, 2015, 156, 2072-2083.	4.2	28
114	ApoE4-specific Misfolded Intermediate Identified by Molecular Dynamics Simulations. PLoS Computational Biology, 2015, 11, e1004359.	3.2	21
115	Differential Regulation of 6- and 7-Transmembrane Helix Variants of Î¼-Opioid Receptor in Response to Morphine Stimulation. PLoS ONE, 2015, 10, e0142826.	2.5	14
116	Differences in the Antinociceptive Effects and Binding Properties of Propranolol and Bupranolol Enantiomers. Journal of Pain, 2015, 16, 1321-1333.	1.4	27
117	Computational Methods Toward Accurate RNA Structure Prediction Using Coarse-Grained and All-Atom Models. Methods in Enzymology, 2015, 553, 65-89.	1.0	13
118	Light-cleavable rapamycin dimer as an optical trigger for protein dimerization. Chemical Communications, 2015, 51, 5702-5705.	4.1	41
119	Channel Gating Dependence on Pore Lining Helix Glycine Residues in Skeletal Muscle Ryanodine Receptor. Journal of Biological Chemistry, 2015, 290, 17535-17545.	3.4	17
120	Non-canonical Bromodomain within DNA-PKcs Promotes DNA Damage Response and Radioresistance through Recognizing an IR-Induced Acetyl-Lysine on H2AX. Chemistry and Biology, 2015, 22, 849-861.	6.0	15
121	iFoldRNA v2: folding RNA with constraints. Bioinformatics, 2015, 31, 2891-2893.	4.1	96
122	Modeling the Calcium and Integrin Binding Protein 2. Biophysical Journal, 2015, 108, 213a.	0.5	0
123	RNA-Puzzles Round II: assessment of RNA structure prediction programs applied to three large RNA structures. Rna, 2015, 21, 1066-1084.	3.5	161
124	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
125	Rational coupled dynamics network manipulation rescues disease-relevant mutant cystic fibrosis transmembrane conductance regulator. Chemical Science, 2015, 6, 1237-1246.	7.4	49
126	PostÂtranslational Modifications Promote Formation of SOD1 Oligomers With Potential Toxicity in ALS. FASEB Journal, 2015, 29, 564.1.	0.5	0

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127	Cu,Zn-Superoxide Dismutase without Zn Is Folded but Catalytically Inactive. Journal of Molecular Biology, 2014, 426, 4112-4124.	4.2	47
128	The N-terminal Domain Allosterically Regulates Cleavage and Activation of the Epithelial Sodium Channel. Journal of Biological Chemistry, 2014, 289, 23029-23042.	3.4	12
129	Identification of an Actin Binding Surface on Vinculin that Mediates Mechanical Cell and Focal Adhesion Properties. Structure, 2014, 22, 697-706.	3.3	49
130	The maturation of HIVâ€1 protease precursor studied by discrete molecular dynamics. Proteins: Structure, Function and Bioinformatics, 2014, 82, 633-639.	2.6	10
131	Computational approaches to understanding protein aggregation in neurodegeneration. Journal of Molecular Cell Biology, 2014, 6, 104-115.	3.3	43
132	Intrinsic Disorder Mediates Cooperative Signal Transduction in STIM1. Journal of Molecular Biology, 2014, 426, 2082-2097.	4.2	24
133	Post-Translational Modifications Promote Formation of SOD1 Oligomers with Potential Toxicity in ALS. Biophysical Journal, 2014, 106, 33a-34a.	0.5	1
134	RNA Tertiary Structure Analysis by 2â€²-Hydroxyl Molecular Interference. Biochemistry, 2014, 53, 6825-6833.	2.5	17
135	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
136	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
137	Potentiator ivacaftor abrogates pharmacological correction of Î”F508 CFTR in cystic fibrosis. Science Translational Medicine, 2014, 6, 246ra96.	12.4	279
138	Traffic within the Cytochrome b6f Lipoprotein Complex: Gating of the Quinone Portal. Biophysical Journal, 2014, 107, 1620-1628.	0.5	20
139	A Robust High-Throughput Assay for Thermodynamic Correctors of the Predominant Molecular Defect Causing Cystic Fibrosis. Biophysical Journal, 2014, 106, 432a.	0.5	0
140	Pore Dynamics and Conductance of RyR1 Transmembrane Domain. Biophysical Journal, 2014, 106, 2375-2384.	0.5	20
141	Discrete Molecular Dynamics Can Predict Helical Prestructured Motifs in Disordered Proteins. PLoS ONE, 2014, 9, e95795.	2.5	19
142	Predicting Binding Affinity of CSAR Ligands Using Both Structure-Based and Ligand-Based Approaches. Journal of Chemical Information and Modeling, 2013, 53, 1915-1922.	5.4	20
143	Identification of Novel Integrin Binding Partners for Calcium and Integrin Binding Protein 1 (CIB1): Structural and Thermodynamic Basis of CIB1 Promiscuity. Biochemistry, 2013, 52, 7082-7090.	2.5	21
144	Is Protein Destabilization a Widespread Factor in Genetic Disease?. Biophysical Journal, 2013, 104, 565a.	0.5	0

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145	Rational Design of a Ligand-Controlled Protein Conformational Switch. Biophysical Journal, 2013, 104, 18a-19a.	0.5	0
146	Generation of a Light Inhibited Src Kinase through Insertion of LOV into the Catalytic Domain. Biophysical Journal, 2013, 104, 679a.	0.5	0
147	Knowledge-Based Design of a Biosensor to Quantify Localized ERK Activation in Living Cells. Chemistry and Biology, 2013, 20, 847-856.	6.0	49
148	Principles for Understanding the Accuracy of SHAPE-Directed RNA Structure Modeling. Biochemistry, 2013, 52, 588-595.	2.5	41
149	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
150	Statistical Analysis of SHAPE-Directed RNA Secondary Structure Modeling. Biochemistry, 2013, 52, 596-599.	2.5	14
151	Structural Determinants of Skeletal Muscle Ryanodine Receptor Gating*. Journal of Biological Chemistry, 2013, 288, 6154-6165.	3.4	48
152	Metric to Distinguish Closely Related Domain Families Using Sequence Information. Journal of Molecular Biology, 2013, 425, 475-478.	4.2	0
153	Correctors of Î”F508 CFTR restore global conformational maturation without thermally stabilizing the mutant protein. FASEB Journal, 2013, 27, 536-545.	0.5	135
154	Highly covarying residues have a functional role in antibody constant domains. Proteins: Structure, Function and Bioinformatics, 2013, 81, 884-895.	2.6	5
155	Submillisecond Elastic Recoil Reveals Molecular Origins of Fibrin Fiber Mechanics. Biophysical Journal, 2013, 104, 2671-2680.	0.5	35
156	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
157	Protein HP1028 from the human pathogenHelicobacter pyloribelongs to the lipocalin family. Acta Crystallographica Section D: Biological Crystallography, 2013, 69, 1387-1394.	2.5	3
158	Dynamics Intrinsic to Cystic Fibrosis Transmembrane Conductance Regulator Function and Stability. Cold Spring Harbor Perspectives in Medicine, 2013, 3, a009522-a009522.	6.2	24
159	RNA-Puzzles: A CASP-like evaluation of RNA three-dimensional structure prediction. Rna, 2012, 18, 610-625.	3.5	241
160	Harnessing a Physiologic Mechanism for siRNA Delivery With Mimetic Lipoprotein Particles. Molecular Therapy, 2012, 20, 1582-1589.	8.2	65
161	Energetic and Structural Basis for Activation of the Epithelial Sodium Channel by Matriptase. Biochemistry, 2012, 51, 3460-3469.	2.5	24
162	New Models of Tetrahymena Telomerase RNA from Experimentally Derived Constraints and Modeling. Journal of the American Chemical Society, 2012, 134, 20070-20080.	13.7	19

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163	Discrete Molecular Dynamics Simulation of Biomolecules. Biological and Medical Physics Series, 2012, , 55-73.	0.4	13
164	Homology Modeling: Generating Structural Models to Understand Protein Function and Mechanism. Biological and Medical Physics Series, 2012, , 97-116.	0.4	9
165	Computational Modeling of Telomerase in Action. Biophysical Journal, 2012, 102, 732a.	0.5	0
166	Recognition of Platinumâ€“DNA Adducts by HMGB1a. Biochemistry, 2012, 51, 7608-7617.	2.5	14
167	Physical Microscopic Model of Proteins Under Force. Journal of Physical Chemistry B, 2012, 116, 6806-6809.	2.6	0
168	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
169	Allosteric Modulation Balances Thermodynamic Stability and Restores Function of Î”F508 CFTR. Journal of Molecular Biology, 2012, 419, 41-60.	4.2	90
170	The Complex Molecular Biology of Amyotrophic Lateral Sclerosis (ALS). Progress in Molecular Biology and Translational Science, 2012, 107, 215-262.	1.7	131
171	Discrete Molecular Dynamics Distinguishes Nativelike Binding Poses from Decoys in Difficult Targets. Biophysical Journal, 2012, 102, 144-151.	0.5	31
172	Hybrid Dynamics Simulation Engine for Metalloproteins. Biophysical Journal, 2012, 103, 767-776.	0.5	26
173	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
174	Serotonin-Induced Hypersensitivity via Inhibition of Catechol O-Methyltransferase Activity. Molecular Pain, 2012, 8, 1744-8069-8-25.	2.1	16
175	Thermal Unfolding Pathway of PHD2 Catalytic Domain in Three Different PHD2 Species: Computational Approaches. PLoS ONE, 2012, 7, e47061.	2.5	4
176	The interface of protein structure, protein biophysics, and molecular evolution. Protein Science, 2012, 21, 769-785.	7.6	188
177	Multiscale Modeling of RNA Structure and Dynamics. Nucleic Acids and Molecular Biology, 2012, , 167-184.	0.2	3
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