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List of Publications by Year
in descending order

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177 papers	14,942 citations	23567 58 h-index	20961 115 g-index
178 all docs	178 docs citations	178 times ranked	14027 citing authors

#	Article	IF	Citations
1	Principles of docking: An overview of search algorithms and a guide to scoring functions. Proteins: Structure, Function and Bioinformatics, 2002, 47, 409-443.	2.6	1,130
2	Is allostery an intrinsic property of all dynamic proteins?. Proteins: Structure, Function and Bioinformatics, 2004, 57, 433-443.	2.6	779
3	AÎ²(1â€“42) fibril structure illuminates self-recognition and replication of amyloid in Alzheimer's disease. Nature Structural and Molecular Biology, 2015, 22, 499-505.	8.2	701
4	Principles of Proteinâ^'Protein Interactions: What are the Preferred Ways For Proteins To Interact?. Chemical Reviews, 2008, 108, 1225-1244.	47.7	568
5	Protein-protein interactions: Structurally conserved residues distinguish between binding sites and exposed protein surfaces. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 5772-5777.	7.1	553
6	Hot Regions in Proteinâ€“Protein Interactions: The Organization and Contribution of Structurally Conserved Hot Spot Residues. Journal of Molecular Biology, 2005, 345, 1281-1294.	4.2	465
7	Stabilities and conformations of Alzheimer's Â-amyloid peptide oligomers (AÂ16-22, AÂ16-35, and AÂ10-35): Sequence effects. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 14126-14131.	7.1	414
8	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
9	Multiple diverse ligands binding at a single protein site: A matter of pre-existing populations. Protein Science, 2009, 11, 184-197.	7.6	364
10	The Origin of Allosteric Functional Modulation: Multiple Pre-existing Pathways. Structure, 2009, 17, 1042-1050.	3.3	347
11	Folding and binding cascades: Shifts in energy landscapes. Proceedings of the National Academy of Sciences of the United States of America, 1999, 96, 9970-9972.	7.1	337
12	Protein Ensembles: How Does Nature Harness Thermodynamic Fluctuations for Life? The Diverse Functional Roles of Conformational Ensembles in the Cell. Chemical Reviews, 2016, 116, 6516-6551.	47.7	302
13	Zinc ions promote Alzheimer AÎ² aggregation via population shift of polymorphic states. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 9490-9495.	7.1	283
14	Polymorphism in Alzheimer AÎ² Amyloid Organization Reflects Conformational Selection in a Rugged Energy Landscape. Chemical Reviews, 2010, 110, 4820-4838.	47.7	265
15	Conservation of polar residues as hot spots at protein interfaces. Proteins: Structure, Function and Bioinformatics, 2000, 39, 331-342.	2.6	253
16	Simulations as analytical tools to understand protein aggregation and predict amyloid conformation. Current Opinion in Chemical Biology, 2006, 10, 445-452.	6.1	214
17	Allosteric Effects of the Oncogenic RasQ61L Mutant on Raf-RBD. Structure, 2015, 23, 505-516.	3.3	201
18	Proteinâ€“Protein Interactions: Hot Spots and Structurally Conserved Residues often Locate in Complemented Pockets that Pre-organized in the Unbound States: Implications for Docking. Journal of Molecular Biology, 2004, 344, 781-795.	4.2	197

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19	Dynamic Allostery: Linkers Are Not Merely Flexible. Structure, 2011, 19, 907-917.	3.3	196
20	Enzyme dynamics point to stepwise conformational selection in catalysis. Current Opinion in Chemical Biology, 2010, 14, 652-659.	6.1	195
21	Principles and Overview of Sampling Methods for Modeling Macromolecular Structure and Dynamics. PLoS Computational Biology, 2016, 12, e1004619.	3.2	188
22	Structured disorder and conformational selection. Proteins: Structure, Function and Bioinformatics, 2001, 44, 418-427.	2.6	184
23	Molecular-Level Examination of Cu²⁺ Binding Structure for Amyloid Fibrils of 40-Residue Alzheimerâ€™s Î² by Solid-State NMR Spectroscopy. Journal of the American Chemical Society, 2011, 133, 3390-3400.	13.7	182
24	Modeling the Alzheimer AÎ²17-42 Fibril Architecture: Tight Intermolecular Sheet-Sheet Association and Intramolecular Hydrated Cavities. Biophysical Journal, 2007, 93, 3046-3057.	0.5	167
25	Molecular dynamics simulations of alanine rich Î²-sheet oligomers: Insight into amyloid formation. Protein Science, 2009, 11, 2335-2350.	7.6	156
26	The Underappreciated Role of Allostery in the Cellular Network. Annual Review of Biophysics, 2013, 42, 169-189.	10.0	152
27	Electrostatic strengths of salt bridges in thermophilic and mesophilic glutamate dehydrogenase monomers. Proteins: Structure, Function and Bioinformatics, 2000, 38, 368-383.	2.6	140
28	Mechanisms of transcription factor selectivity. Trends in Genetics, 2010, 26, 75-83.	6.7	133
29	Structural Stability and Dynamics of an Amyloid-Forming Peptide GNNQQNY from the Yeast Prion Sup-35. Biophysical Journal, 2006, 91, 824-833.	0.5	131
30	Proteinâ€“protein interaction networks: how can a hub protein bind so many different partners?. Trends in Biochemical Sciences, 2009, 34, 594-600.	7.5	125
31	Molecular dynamics simulations of a Î²-hairpin fragment of protein G: balance between side-chain and backbone forces 1 1Edited by F. E. Cohen. Journal of Molecular Biology, 2000, 296, 1091-1104.	4.2	115
32	Protein functional epitopes: hot spots, dynamics and combinatorial libraries. Current Opinion in Structural Biology, 2001, 11, 364-369.	5.7	114
33	Release of Cytochrome C from Bax Pores at the Mitochondrial Membrane. Scientific Reports, 2017, 7, 2635.	3.3	107
34	Multiple conformational selection and induced fit events take place in allosteric propagation. Biophysical Chemistry, 2014, 186, 22-30.	2.8	105
35	Theoretical Studies of the Potential Energy Surfaces and Compositions of thed-Aldo-andd-Ketohexoses. Journal of the American Chemical Society, 1998, 120, 3411-3422.	13.7	101
36	Synergistic Interactions between Repeats in Tau Protein and AÎ² Amyloids May Be Responsible for Accelerated Aggregation via Polymorphic States. Biochemistry, 2011, 50, 5172-5181.	2.5	95

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37	Metal binding sites in amyloid oligomers: Complexes and mechanisms. Coordination Chemistry Reviews, 2012, 256, 2245-2252.	18.8	95
38	Trp/Met/Phe Hot Spots in Protein-Protein Interactions: Potential Targets in Drug Design. Current Topics in Medicinal Chemistry, 2007, 7, 999-1005.	2.1	94
39	Proteinâ€“protein interactions: organization, cooperativity and mapping in a bottom-up Systems Biology approach. Physical Biology, 2005, 2, S24-S35.	1.8	93
40	Models of Toxic Î²-Sheet Channels of Protegrin-1 Suggest a Common Subunit Organization Motif Shared with Toxic Alzheimer Î²-Amyloid Ion Channels. Biophysical Journal, 2008, 95, 4631-4642.	0.5	91
41	Polymorphism of Alzheimer's AÎ²17-42 (p3) Oligomers: The Importance of the Turn Location and Its Conformation. Biophysical Journal, 2009, 97, 1168-1177.	0.5	91
42	Hollow core of Alzheimerâ€™s A Î² ₄₂ amyloid observed by cryoEM is relevant at physiological pH. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 14128-14133.	7.1	81
43	Structural Insight into Tau Proteinâ€™s Paradox of Intrinsically Disordered Behavior, Self-Acetylation Activity, and Aggregation. Journal of Physical Chemistry Letters, 2014, 5, 3026-3031.	4.6	81
44	Selective Molecular Recognition in Amyloid Growth and Transmission and Cross-Species Barriers. Journal of Molecular Biology, 2012, 421, 172-184.	4.2	76
45	How Similar Are Protein Folding and Protein Binding Nuclei? Examination of Vibrational Motions of Energy Hot Spots and Conserved Residues. Biophysical Journal, 2005, 88, 1552-1559.	0.5	75
46	Amylinâ€“AÎ² oligomers at atomic resolution using molecular dynamics simulations: a link between Type 2 diabetes and Alzheimer's disease. Physical Chemistry Chemical Physics, 2016, 18, 2330-2338.	2.8	74
47	Transition-state Ensemble in Enzyme Catalysis: Possibility, Reality, or Necessity?. Journal of Theoretical Biology, 2000, 203, 383-397.	1.7	73
48	A Comparative Study of Amyloid Fibril Formation by Residues 15â€“19 of the Human Calcitonin Hormone: A Single Î²-Sheet Model with a Small Hydrophobic Core. Journal of Molecular Biology, 2005, 345, 1213-1227.	4.2	71
49	Contribution of Salt Bridges Toward Protein Thermostability. Journal of Biomolecular Structure and Dynamics, 2000, 17, 79-85.	3.5	70
50	Annular Structures as Intermediates in Fibril Formation of Alzheimer AÎ²_{17â^'42}. Journal of Physical Chemistry B, 2008, 112, 6856-6865.	2.6	70
51	Replica Exchange Molecular Dynamics: A Practical Application Protocol with Solutions to Common Problems and a Peptide Aggregation and Self-Assembly Example. Methods in Molecular Biology, 2018, 1777, 101-119.	0.9	70
52	Protein dynamics and conformational selection in bidirectional signal transduction. BMC Biology, 2012, 10, 2.	3.8	69
53	Conformational Distribution and Î±-Helix to Î²-Sheet Transition of Human Amylin Fragment Dimer. Biomacromolecules, 2014, 15, 122-131.	5.4	69
54	Interaction of Protegrin-1 with Lipid Bilayers: Membrane Thinning Effect. Biophysical Journal, 2006, 91, 2848-2859.	0.5	65

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55	Conformational Basis for Asymmetric Seeding Barrier in Filaments of Three- and Four-Repeat Tau. Journal of the American Chemical Society, 2012, 134, 10271-10278.	13.7	63
56	Cross-seeding and Conformational Selection between Three- and Four-repeat Human Tau Proteins. Journal of Biological Chemistry, 2012, 287, 14950-14959.	3.4	63
57	The Unique Alzheimerâ€™s Î²-Amyloid Triangular Fibril Has a Cavity along the Fibril Axis under Physiological Conditions. Journal of the American Chemical Society, 2011, 133, 2742-2748.	13.7	62
58	The Stability of Monomeric Intermediates Controls Amyloid Formation: AÎ²25â€“35 and its N27Q Mutant. Biophysical Journal, 2006, 90, 3365-3374.	0.5	59
59	Spectroscopic constants and potential energy surfaces for the possible interstellar molecules A1NC and A1CN. Molecular Physics, 1995, 86, 1331-1337.	1.7	56
60	Mechanisms of recognition of amyloid-Î² (AÎ²) monomer, oligomer, and fibril by homologous antibodies. Journal of Biological Chemistry, 2017, 292, 18325-18343.	3.4	53
61	Towards Drugs Targeting Multiple Proteins in a Systems Biology Approach. Current Topics in Medicinal Chemistry, 2007, 7, 943-951.	2.1	51
62	Local and global anatomy of antibodyâ€protein antigen recognition. Journal of Molecular Recognition, 2018, 31, e2693.	2.1	49
63	In silico protein design by combinatorial assembly of protein building blocks. Protein Science, 2009, 13, 2753-2765.	7.6	48
64	Antigen binding allosterically promotes Fc receptor recognition. MAbs, 2019, 11, 58-74.	5.2	48
65	Sequence analysis of p53 response-elements suggests multiple binding modes of the p53 tetramer to DNA targets. Nucleic Acids Research, 2007, 35, 2986-3001.	14.5	47
66	Allosteric Conformational Barcodes Direct Signaling in the Cell. Structure, 2013, 21, 1509-1521.	3.3	47
67	Mapping the Conformation Space of Wildtype and Mutant H-Ras with a Memetic, Cellular, and Multiscale Evolutionary Algorithm. PLoS Computational Biology, 2015, 11, e1004470.	3.2	47
68	The Stability and Dynamics of the Human Calcitonin Amyloid Peptide DFNKF. Biophysical Journal, 2004, 87, 146-158.	0.5	46
69	Consensus features in amyloid fibrils: sheetâ€“sheet recognition via a (polar or nonpolar) zipper structure. Physical Biology, 2006, 3, P1-P4.	1.8	46
70	A broad view of scaffolding suggests that scaffolding proteins can actively control regulation and signaling of multienzyme complexes through allostery. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2013, 1834, 820-829.	2.3	45
71	Peptideâ€“MHC (pMHC) binding to a human antiviral T cell receptor induces long-range allosteric communication between pMHC- and CD3-binding sites. Journal of Biological Chemistry, 2018, 293, 15991-16005.	3.4	45
72	IKKÎ± inactivation promotes Kras-initiated lung adenocarcinoma development through disrupting major redox regulatory pathways. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E812-E821.	7.1	44

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73	Ligand Binding and Circular Permutation Modify Residue Interaction Network in DHFR. PLoS Computational Biology, 2007, 3, e117.	3.2	42
74	How do transcription factors select specific binding sites in the genome?. Nature Structural and Molecular Biology, 2009, 16, 1118-1120.	8.2	42
75	AÎ² â€œStretching-and-Packingâ€•Cross-Seeding Mechanism Can Trigger Tau Protein Aggregation. Journal of Physical Chemistry Letters, 2015, 6, 3276-3282.	4.6	42
76	Triggering Loops and Enzyme Function: Identification of Loops that Trigger and Modulate Movements. Journal of Molecular Biology, 2003, 332, 143-159.	4.2	41
77	Druggable Orthosteric and Allosteric Hot Spots to Target Protein-protein Interactions. Current Pharmaceutical Design, 2014, 20, 1293-1301.	1.9	41
78	Periodic Trends for Transition Metal Dihydrides MH2, Dihydride Dihydrogen Complexes MH2Â·H2, and Tetrahydrides MH4 (M = Ti, V, and Cr). Journal of the American Chemical Society, 1996, 118, 870-879.	13.7	40
79	Structure, Strain Energy, and Magnetic Susceptibility of [4]Paracyclophane and the Activation Energy for Its Interconversion with 1,4-Tetramethylene Dewar Benzene. Journal of the American Chemical Society, 1995, 117, 8392-8400.	13.7	39
80	Thermal unfolding molecular dynamics simulation ofEscherichia coli dihydrofolate reductase: Thermal stability of protein domains and unfolding pathway. Proteins: Structure, Function and Bioinformatics, 2002, 46, 308-320.	2.6	39
81	Conformational study of the protegrin-1 (PG-1) dimer interaction with lipid bilayers and its effect. BMC Structural Biology, 2007, 7, 21.	2.3	39
82	Polymorphic Triple Î²-Sheet Structures Contribute to Amide Hydrogen/Deuterium (H/D) Exchange Protection in the Alzheimer Amyloid Î²42 Peptide. Journal of Biological Chemistry, 2011, 286, 34244-34253.	3.4	38
83	Single Mutations in Tau Modulate the Populations of Fibril Conformers through Seed Selection. Angewandte Chemie - International Edition, 2014, 53, 1590-1593.	13.8	38
84	Polymorphism in Self-Assembly of Peptide-Based Î²-Hairpin Contributes to Network Morphology and Hydrogel Mechanical Rigidity. Journal of Physical Chemistry B, 2015, 119, 482-490.	2.6	37
85	Amplification of signaling via cellular allosteric relay and protein disorder: Fig. 1.. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 6887-6888.	7.1	36
86	Conformational footprints. Nature Chemical Biology, 2016, 12, 890-891.	8.0	36
87	Singlet Methylcarbene: Equilibrium Geometry or Transition State?. Journal of the American Chemical Society, 1994, 116, 3539-3542.	13.7	35
88	Polymorphic C-terminal Î²-Sheet Interactions Determine the Formation of Fibril or Amyloid Î²-derived Diffusible Ligand-like Globulomer for the Alzheimer AÎ²42 Dodecamer. Journal of Biological Chemistry, 2010, 285, 37102-37110.	3.4	35
89	Promiscuous and specific recognition among ephrins and Eph receptors. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2014, 1844, 1729-1740.	2.3	35
90	Structural disorder in four-repeat Tau fibrils reveals a new mechanism for barriers to cross-seeding of Tau isoforms. Journal of Biological Chemistry, 2018, 293, 17336-17348.	3.4	35

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91	The distinct structural preferences of tau protein repeat domains. Chemical Communications, 2018, 54, 5700-5703.	4.1	35
92	Molecular insights into the reversible formation of tau protein fibrils. Chemical Communications, 2013, 49, 3582.	4.1	34
93	Dimerization of the SP1 Region of HIV-1 Gag Induces a Helical Conformation and Association into Helical Bundles: Implications for Particle Assembly. Journal of Virology, 2016, 90, 1773-1787.	3.4	34
94	A Molecular Mechanics Study of the Cholesteryl Acetate Crystal:â€‰ Evaluation of Interconversion among rg, rz, and rÎ± Bond Lengths. Journal of the American Chemical Society, 1997, 119, 2570-2573.	13.7	33
95	Atomistic-level study of the interactions between hIAPP protofibrils and membranes: Influence of pH and lipid composition. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 1818-1825.	2.6	33
96	From Structure to Function: Methods and Applications. Current Protein and Peptide Science, 2005, 6, 171-183.	1.4	32
97	Critical Nucleus Structure and Aggregation Mechanism of the C-terminal Fragment of Copperâ€“Zinc Superoxide Dismutase Protein. ACS Chemical Neuroscience, 2016, 7, 286-296.	3.5	32
98	Binding of protofibrillar AÎ² trimers to lipid bilayer surface enhances AÎ² structural stability and causes membrane thinning. Physical Chemistry Chemical Physics, 2017, 19, 27556-27569.	2.8	32
99	Release Factors eRF1 and RF2. Journal of Biological Chemistry, 2004, 279, 53875-53885.	3.4	31
100	Toward the observation of silanone (H2SiO) and hydroxysilylene (HSiOH) via microwave spectroscopy. Journal of Chemical Physics, 1994, 101, 2734-2739.	3.0	30
101	Probing potential binding modes of the p53 tetramer to DNA based on the symmetries encoded in p53 response elements. Nucleic Acids Research, 2007, 35, 7733-7747.	14.5	30
102	Characterization of the Conformational State and Flexibility of HIV-1 Glycoprotein gp120 Core Domain. Journal of Biological Chemistry, 2004, 279, 30523-30530.	3.4	29
103	Comparison of the protein-protein interfaces in the p53-DNA crystal structures: Towards elucidation of the biological interface. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 3988-3993.	7.1	29
104	Structured Crowding and Its Effects on Enzyme Catalysis. Topics in Current Chemistry, 2013, 337, 123-137.	4.0	29
105	Disruption of the Rbm38-eIF4E Complex with a Synthetic Peptide Pep8 Increases p53 Expression. Cancer Research, 2019, 79, 807-818.	0.9	29
106	Aquated metaphosphate (PO3-.cntdot.(H2O)n) clusters. Molecular anion structures, energetics, and vibrational frequencies. Journal of the American Chemical Society, 1993, 115, 1943-1951.	13.7	28
107	.pi. Electron Delocalization and Compression in Acyclic Acetylenic Precursors to Multidimensional Carbon Networks: Comparison with Experiment for the Recently Synthesized Tris(trimethylsilyl)-Substituted Tetraethynylmethane. Structures, Thermochemistry, Infrared Spectra, Polarizabilities, and Hyperpolarizabilities. Journal of the American Chemical Society, 1994, 116, 3529-3538.	13.7	28
108	Energy landscape and dynamics of the Î²-hairpin G peptide and its isomers: Topology and sequences. Protein Science, 2003, 12, 1882-1893.	7.6	28

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109	Binding interactions between the core central domain of 16S rRNA and the ribosomal protein S15 determined by molecular dynamics simulations. Nucleic Acids Research, 2003, 31, 629-638.	14.5	28
110	Coupling of the non-amyloid-component (NAC) domain and the KTK(E/Q)GV repeats stabilize the Î±-synuclein fibrils. European Journal of Medicinal Chemistry, 2016, 121, 841-850.	5.5	28
111	Prediction of Hostâ€“Pathogen Interactions for Helicobacter pylori by Interface Mimicry and Implications to Gastric Cancer. Journal of Molecular Biology, 2017, 429, 3925-3941.	4.2	28
112	Isomerization of PO3-.(H2O)n clusters to H2PO4-.(H2O)n-1: transition states and barrier heights. Journal of the American Chemical Society, 1993, 115, 11169-11179.	13.7	27
113	Interdependence of Backbone Flexibility, Residue Conservation, and Enzyme Function:â€‰ A Case Study on Î²1,4-Galactosyltransferase-I. Biochemistry, 2003, 42, 3674-3687.	2.5	27
114	Why Does Binding of Proteins to DNA or Proteins to Proteins Not Necessarily Spell Function?. ACS Chemical Biology, 2010, 5, 265-272.	3.4	27
115	How Does Hyperphopsphorylation Promote Tau Aggregation and Modulate Filament Structure and Stability?. ACS Chemical Neuroscience, 2016, 7, 565-575.	3.5	27
116	Familial Mutations May Switch Conformational Preferences in Î±-Synuclein Fibrils. ACS Chemical Neuroscience, 2017, 8, 837-849.	3.5	27
117	Spectroscopic constants and potential energy surfaces for silanone (H2SiO), hydroxysilylene (HSiOH), the hydroxysilylene dimer, and the disilynyl radical (Si2H). Journal of Chemical Physics, 1996, 105, 5731-5736.	3.0	26
118	Theoretical investigation of the Ca+â€“N2 and Ca2+â€“N2 complexes. Chemical Physics Letters, 1998, 295, 204-210.	2.6	26
119	Structural and Functional Consequences of Phosphateâ€“Arsenate Substitutions in Selected Nucleotides: DNA, RNA, and ATP. Journal of Physical Chemistry B, 2012, 116, 4801-4811.	2.6	25
120	Allosteric stabilization of the amyloid-Î² peptide hairpin by the fluctuating N-terminal. Chemical Communications, 2016, 52, 1733-1736.	4.1	25
121	CD4 Binding Partially Locks the Bridging Sheet in gp120 but Leaves the Î²2/3 Strands Flexible. Journal of Molecular Biology, 2005, 350, 514-527.	4.2	24
122	In the Quest for Stable Rescuing Mutants of p53:â€‰ Computational Mutagenesis of Flexible Loop L1. Biochemistry, 2005, 44, 1423-1432.	2.5	23
123	Conformational selection in amyloid-based immunotherapy: Survey of crystal structures of antibody-amyloid complexes. Biochimica Et Biophysica Acta - General Subjects, 2016, 1860, 2672-2681.	2.4	23
124	Self-aggregation and coaggregation of the p53 core fragment with its aggregation gatekeeper variant. Physical Chemistry Chemical Physics, 2016, 18, 8098-8107.	2.8	23
125	Singlet-triplet energy separation and barrier for ring closure for trimethylenemethane and its complexes. Chemical Physics, 1996, 207, 31-41.	1.9	22
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127	Carbon monoxide in controlling the surface formation of Group VIII metal nanoparticles. Chemical Communications, 2014, 50, 14013-14016.	4.1	22
128	Conformational stability and dynamics of the cancerâ€associated isoform Î”133p53Î² are modulated by p53 peptides and p53â€specific DNA. FASEB Journal, 2019, 33, 4225-4235.	0.5	22
129	Comparison of the Human and Worm p53 Structures Suggests a Way for Enhancing Stabilityâ€. Biochemistry, 2006, 45, 3925-3933.	2.5	21
130	Explicit and implicit water simulations of a ?-hairpin peptide. , 1999, 37, 73-87.		20
131	Protein charge and mass contribute to the spatioâ€temporal dynamics of proteinâ€“protein interactions in a minimal proteome. Proteomics, 2013, 13, 1339-1351.	2.2	20
132	Insights Into the Allosteric Inhibition of the SUMO E2 Enzyme Ubc9. Angewandte Chemie - International Edition, 2016, 55, 5703-5707.	13.8	20
133	Molecular Dynamics Simulations of the Denaturation and Refolding of an RNA Tetraloop. Journal of Biomolecular Structure and Dynamics, 2001, 19, 381-396.	3.5	19
134	Molecular dynamics simulation of Escherichia coli dihydrofolate reductase and its protein fragments: Relative stabilities in experiment and simulations. Protein Science, 2001, 10, 135-148.	7.6	19
135	Insights into amyloid structural formation and assembly through computational approaches. Amyloid: the International Journal of Experimental and Clinical Investigation: the Official Journal of the International Society of Amyloidosis, 2004, 11, 143-161.	3.0	19
136	Side chain interactions determine the amyloid organization: a single layer Â-sheet molecular structure of the calcitonin peptide segment 15â€“19. Physical Biology, 2004, 1, 89-99.	1.8	19
137	Conformational dynamics of cancer-associated MyD88-TIR domain mutant L252P (L265P) allosterically tilts the landscape toward homo-dimerization. Protein Engineering, Design and Selection, 2016, 29, 347-354.	2.1	18
138	Molecular dynamics simulations of Alzheimer Abeta40 elongation and lateral association. Frontiers in Bioscience - Landmark, 2008, Volume, 3919.	3.0	17
139	The growth mechanism of single-walled carbon nanotubes with a controlled diameter. Physica E: Low-Dimensional Systems and Nanostructures, 2012, 44, 2032-2040.	2.7	17
140	Defining the Domain Arrangement of the Mammalian Target of Rapamycin Complex Component Rictor Protein. Journal of Computational Biology, 2015, 22, 876-886.	1.6	17
141	Calculation of rz structures from rs structures. Journal of Molecular Structure, 1997, 413-414, 395-404.	3.6	16
142	The contribution of the Trp/Met/Phe residues to physical interactions of p53 with cellular proteins. Physical Biology, 2005, 2, S56-S66.	1.8	16
143	â€œSimilarity Trapâ€•in Protein-Protein Interactions Could Be Carcinogenic: Simulations of p53 Core Domain Complexed with 53BP1 and BRCA1 BRCT Domains. Structure, 2006, 14, 1811-1821.	3.3	16
144	Coupling of Zinc-Binding and Secondary Structure in Nonfibrillar AÎ²40 Peptide Oligomerization. Journal of Chemical Information and Modeling, 2015, 55, 1218-1230.	5.4	16

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145	Observed and calculated Raman spectra of the Ga2H6 and Ga2D6 molecules. The Journal of Physical Chemistry, 1994, 98, 12824-12827.	2.9	15
146	Multipleâ€Targeting and Conformational Selection in the Estrogen Receptor: Computation and Experiment. Chemical Biology and Drug Design, 2011, 78, 137-149.	3.2	13
147	R102Q Mutation Shifts the Salt-Bridge Network and Reduces the Structural Flexibility of Human Neuronal Calcium Sensor-1 Protein. Journal of Physical Chemistry B, 2014, 118, 13112-13122.	2.6	12
148	Computational Investigation of Gantenerumab and Crenezumab Recognition of AÎ² Fibrils in Alzheimerâ€™s Disease Brain Tissue. ACS Chemical Neuroscience, 2020, 11, 3233-3244.	3.5	12
149	Peptideâ€“MHC Binding Reveals Conserved Allosteric Sites in MHC Class I- and Class II-Restricted T Cell Receptors (TCRs). Journal of Molecular Biology, 2020, 432, 166697.	4.2	12
150	Dynamics differentiate between active and inactive inteins. European Journal of Medicinal Chemistry, 2015, 91, 51-62.	5.5	11
151	Oncogenic Mutations Differentially Affect Bax Monomer, Dimer, and Oligomeric Pore Formation in the Membrane. Scientific Reports, 2016, 6, 33340.	3.3	11
152	Cooperativity among Short Amyloid Stretches in Long Amyloidogenic Sequences. PLoS ONE, 2012, 7, e39369.	2.5	10
153	Investigation of the interactions between the EphB2 receptor and SNEW peptide variants. Growth Factors, 2014, 32, 236-246.	1.7	10
154	Dipeptide analysis of p53 mutations and evolution of p53 family proteins. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2014, 1844, 198-206.	2.3	10
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159	Crystal structure of a plectonemic RNA supercoil. Nature Communications, 2012, 3, 901.	12.8	7
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