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List of Publications by Year in descending order

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177 papers	14,942 citations	28736 57 h-index	24511 114 g-index
178 all docs	178 docs citations	178 times ranked	15951 citing authors

#	Article	IF	Citations
1	IKKÎ±-deficient lung adenocarcinomas generate an immunosuppressive microenvironment by overproducing Treg-inducing cytokines. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	3.3	7
2	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.	23.0	406
3	Trastuzumab Blocks the Receiver Function of HER2 Leading to the Population Shifts of HER2-Containing Homodimers and Heterodimers. Antibodies, 2021, 10, 7.	1.2	10
4	Conformational Ensemble of TteAdoCbl Riboswitch Provides Stable Structural Elements for Conformation Selection and Population Shift in Cobalamin Recognition. Journal of Physical Chemistry B, 2021, 125, 2589-2596.	1.2	6
5	BioChem: A New International and Interdisciplinary Journal. Biochem, 2021, 1, 49-50.	0.5	0
6	Computational Investigation of Gantenerumab and Crenezumab Recognition of AÎ² Fibrils in Alzheimerâ€™s Disease Brain Tissue. ACS Chemical Neuroscience, 2020, 11, 3233-3244.	1.7	12
7	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.	2.0	12
8	Molecular dynamics based improvement of the solubilizing self-cleavable tag Zbasic-Î”I-CM application in the preparation of recombinant proteins in Escherichia coli. Biochemical and Biophysical Research Communications, 2019, 513, 412-418.	1.0	0
9	Antigen binding allosterically promotes Fc receptor recognition. MAbs, 2019, 11, 58-74.	2.6	48
10	Disruption of the Rbm38-eIF4E Complex with a Synthetic Peptide Pep8 Increases p53 Expression. Cancer Research, 2019, 79, 807-818.	0.4	29
11	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.	0.2	22
12	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.	1.4	33
13	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.	3.3	44
14	Local and global anatomy of antibodyâ€protein antigen recognition. Journal of Molecular Recognition, 2018, 31, e2693.	1.1	49
15	Structure and energetic basis of overrepresented Î» light chain in systemic light chain amyloidosis patients. Biochimica Et Biophysica Acta - Molecular Basis of Disease, 2018, 1864, 2294-2303.	1.8	6
16	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.	1.6	35
17	Intermolecular disulfide bonds between unpaired cysteines retard the C-terminal trans-cleavage of Npu DnaE. Enzyme and Microbial Technology, 2018, 118, 6-12.	1.6	8
18	The distinct structural preferences of tau protein repeat domains. Chemical Communications, 2018, 54, 5700-5703.	2.2	35

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19	Experimental and Computational Protocols for Studies of Cross-Seeding Amyloid Assemblies. Methods in Molecular Biology, 2018, 1777, 429-447.	0.4	8
20	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.	0.4	70
21	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.	1.6	45
22	Familial Mutations May Switch Conformational Preferences in Î±-Synuclein Fibrils. ACS Chemical Neuroscience, 2017, 8, 837-849.	1.7	27
23	Probing Oligomerized Conformations of Defensin in the Membrane. Methods in Molecular Biology, 2017, 1529, 353-362.	0.4	4
24	Human Neuronal Calcium Sensor-1 Protein Avoids Histidine Residues To Decrease pH Sensitivity. Journal of Physical Chemistry B, 2017, 121, 508-517.	1.2	2
25	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.	1.3	32
26	Mechanisms of recognition of amyloid-Î² (AÎ²) monomer, oligomer, and fibril by homologous antibodies. Journal of Biological Chemistry, 2017, 292, 18325-18343.	1.6	53
27	Release of Cytochrome C from Bax Pores at the Mitochondrial Membrane. Scientific Reports, 2017, 7, 2635.	1.6	107
28	Prediction of Hostâ€“Pathogen Interactions for Helicobacter pylori by Interface Mimicry and Implications to Gastric Cancer. Journal of Molecular Biology, 2017, 429, 3925-3941.	2.0	28
29	Compilation and Analysis of Enzymes, Engineered Antibodies, and Nanoparticles Designed to Interfere with Amyloidâ€Î² Aggregation. Israel Journal of Chemistry, 2017, 57, 622-633.	1.0	2
30	Insights Into the Allosteric Inhibition of the SUMO E2 Enzyme Ubc9. Angewandte Chemie, 2016, 128, 5797-5801.	1.6	1
31	How Does Hyperphopsphorylation Promote Tau Aggregation and Modulate Filament Structure and Stability?. ACS Chemical Neuroscience, 2016, 7, 565-575.	1.7	27
32	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.	1.0	18
33	Oncogenic Mutations Differentially Affect Bax Monomer, Dimer, and Oligomeric Pore Formation in the Membrane. Scientific Reports, 2016, 6, 33340.	1.6	11
34	Conformational footprints. Nature Chemical Biology, 2016, 12, 890-891.	3.9	36
35	Insights Into the Allosteric Inhibition of the SUMO E2 Enzyme Ubc9. Angewandte Chemie - International Edition, 2016, 55, 5703-5707.	7.2	20
36	Conformational selection in amyloid-based immunotherapy: Survey of crystal structures of antibody-amyloid complexes. Biochimica Et Biophysica Acta - General Subjects, 2016, 1860, 2672-2681.	1.1	23

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37	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.	23.0	302
38	Allosteric stabilization of the amyloid-Î² peptide hairpin by the fluctuating N-terminal. Chemical Communications, 2016, 52, 1733-1736.	2.2	25
39	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.	1.5	34
40	Temperature-Dependent Conformational Properties of Human Neuronal Calcium Sensor-1 Protein Revealed by All-Atom Simulations. Journal of Physical Chemistry B, 2016, 120, 3551-3559.	1.2	4
41	Self-aggregation and coaggregation of the p53 core fragment with its aggregation gatekeeper variant. Physical Chemistry Chemical Physics, 2016, 18, 8098-8107.	1.3	23
42	Critical Nucleus Structure and Aggregation Mechanism of the C-terminal Fragment of Copperâ€“Zinc Superoxide Dismutase Protein. ACS Chemical Neuroscience, 2016, 7, 286-296.	1.7	32
43	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.	2.6	28
44	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.	1.3	74
45	Principles and Overview of Sampling Methods for Modeling Macromolecular Structure and Dynamics. PLoS Computational Biology, 2016, 12, e1004619.	1.5	188
46	Mapping the Conformation Space of Wildtype and Mutant H-Ras with a Memetic, Cellular, and Multiscale Evolutionary Algorithm. PLoS Computational Biology, 2015, 11, e1004470.	1.5	47
47	Coupling of Zinc-Binding and Secondary Structure in Nonfibrillar AÎ²40 Peptide Oligomerization. Journal of Chemical Information and Modeling, 2015, 55, 1218-1230.	2.5	16
48	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.	1.2	37
49	AÎ² â€œStretching-and-Packingâ€•Cross-Seeding Mechanism Can Trigger Tau Protein Aggregation. Journal of Physical Chemistry Letters, 2015, 6, 3276-3282.	2.1	42
50	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.	3.6	701
51	Allosteric Effects of the Oncogenic RasQ61L Mutant on Raf-RBD. Structure, 2015, 23, 505-516.	1.6	201
52	Defining the Domain Arrangement of the Mammalian Target of Rapamycin Complex Component Rictor Protein. Journal of Computational Biology, 2015, 22, 876-886.	0.8	17
53	Effects of the C-Terminal Tail on the Conformational Dynamics of Human Neuronal Calcium Sensor-1 Protein. Journal of Physical Chemistry B, 2015, 119, 14236-14244.	1.2	5
54	Dynamics differentiate between active and inactive inteins. European Journal of Medicinal Chemistry, 2015, 91, 51-62.	2.6	11

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55	Investigation of the interactions between the EphB2 receptor and SNEW peptide variants. Growth Factors, 2014, 32, 236-246.	0.5	10
56	Bioinformatics Study of Cancer-Related Mutations within p53 Phosphorylation Site Motifs. International Journal of Molecular Sciences, 2014, 15, 13275-13298.	1.8	5
57	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.	1.2	12
58	Multiple conformational selection and induced fit events take place in allosteric propagation. Biophysical Chemistry, 2014, 186, 22-30.	1.5	105
59	Conformational Distribution and Î±-Helix to Î²-Sheet Transition of Human Amylin Fragment Dimer. Biomacromolecules, 2014, 15, 122-131.	2.6	69
60	Carbon monoxide in controlling the surface formation of Group VIII metal nanoparticles. Chemical Communications, 2014, 50, 14013-14016.	2.2	22
61	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.	2.1	81
62	Promiscuous and specific recognition among ephrins and Eph receptors. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2014, 1844, 1729-1740.	1.1	35
63	Dipeptide analysis of p53 mutations and evolution of p53 family proteins. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2014, 1844, 198-206.	1.1	10
64	Single Mutations in Tau Modulate the Populations of Fibril Conformers through Seed Selection. Angewandte Chemie - International Edition, 2014, 53, 1590-1593.	7.2	38
65	Network Effect of Wt-mutant p53 Interactions and Implications on p53 Gene Therapy. Current Pharmaceutical Design, 2014, 20, 1259-1267.	0.9	4
66	Druggable Orthosteric and Allosteric Hot Spots to Target Protein-protein Interactions. Current Pharmaceutical Design, 2014, 20, 1293-1301.	0.9	41
67	Editorial (Thematic Issue: Protein-protein interaction: from interface to interaction network). Current Pharmaceutical Design, 2014, 20, 1171-1172.	0.9	1
68	Structured Crowding and Its Effects on Enzyme Catalysis. Topics in Current Chemistry, 2013, 337, 123-137.	4.0	29
69	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.	1.1	45
70	Allosteric Conformational Barcodes Direct Signaling in the Cell. Structure, 2013, 21, 1509-1521.	1.6	47
71	Protein charge and mass contribute to the spatioâ€temporal dynamics of proteinâ€“protein interactions in a minimal proteome. Proteomics, 2013, 13, 1339-1351.	1.3	20
72	Molecular insights into the reversible formation of tau protein fibrils. Chemical Communications, 2013, 49, 3582.	2.2	34

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73	The Underappreciated Role of Allostery in the Cellular Network. Annual Review of Biophysics, 2013, 42, 169-189.	4.5	152
74	Conformational Basis for Asymmetric Seeding Barrier in Filaments of Three- and Four-Repeat Tau. Journal of the American Chemical Society, 2012, 134, 10271-10278.	6.6	63
75	The growth mechanism of single-walled carbon nanotubes with a controlled diameter. Physica E: Low-Dimensional Systems and Nanostructures, 2012, 44, 2032-2040.	1.3	17
76	Selective Molecular Recognition in Amyloid Growth and Transmission and Cross-Species Barriers. Journal of Molecular Biology, 2012, 421, 172-184.	2.0	76
77	Metal binding sites in amyloid oligomers: Complexes and mechanisms. Coordination Chemistry Reviews, 2012, 256, 2245-2252.	9.5	95
78	Crystal structure of a plectonemic RNA supercoil. Nature Communications, 2012, 3, 901.	5.8	7
79	Structural and Functional Consequences of Phosphateâ€“Arsenate Substitutions in Selected Nucleotides: DNA, RNA, and ATP. Journal of Physical Chemistry B, 2012, 116, 4801-4811.	1.2	25
80	Cooperativity among Short Amyloid Stretches in Long Amyloidogenic Sequences. PLoS ONE, 2012, 7, e39369.	1.1	10
81	Protein dynamics and conformational selection in bidirectional signal transduction. BMC Biology, 2012, 10, 2.	1.7	69
82	Cross-seeding and Conformational Selection between Three- and Four-repeat Human Tau Proteins. Journal of Biological Chemistry, 2012, 287, 14950-14959.	1.6	63
83	Synergistic Interactions between Repeats in Tau Protein and Aî² Amyloids May Be Responsible for Accelerated Aggregation via Polymorphic States. Biochemistry, 2011, 50, 5172-5181.	1.2	95
84	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.	6.6	62
85	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.	6.6	182
86	Multipleâ€Targeting and Conformational Selection in the Estrogen Receptor: Computation and Experiment. Chemical Biology and Drug Design, 2011, 78, 137-149.	1.5	13
87	Dynamic Allostery: Linkers Are Not Merely Flexible. Structure, 2011, 19, 907-917.	1.6	196
88	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.	1.6	38
89	Mechanisms of transcription factor selectivity. Trends in Genetics, 2010, 26, 75-83.	2.9	133
90	Enzyme dynamics point to stepwise conformational selection in catalysis. Current Opinion in Chemical Biology, 2010, 14, 652-659.	2.8	195

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91	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.	1.6	35
92	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.	3.3	81
93	Polymophism of A-Beta1-42 Peptide Oligomer - Membrane Interactions. Biophysical Journal, 2010, 98, 650a.	0.2	0
94	Polymorphism in Alzheimer AÎ² Amyloid Organization Reflects Conformational Selection in a Rugged Energy Landscape. Chemical Reviews, 2010, 110, 4820-4838.	23.0	265
95	Why Does Binding of Proteins to DNA or Proteins to Proteins Not Necessarily Spell Function?. ACS Chemical Biology, 2010, 5, 265-272.	1.6	27
96	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.	3.3	283
97	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.	3.3	36
98	The Origin of Allosteric Functional Modulation: Multiple Pre-existing Pathways. Structure, 2009, 17, 1042-1050.	1.6	347
99	Proteinâ€“protein interaction networks: how can a hub protein bind so many different partners?. Trends in Biochemical Sciences, 2009, 34, 594-600.	3.7	125
100	How do transcription factors select specific binding sites in the genome?. Nature Structural and Molecular Biology, 2009, 16, 1118-1120.	3.6	42
101	Multiple diverse ligands binding at a single protein site: A matter of pre-existing populations. Protein Science, 2009, 11, 184-197.	3.1	364
102	Molecular dynamics simulations of alanine rich Î²-sheet oligomers: Insight into amyloid formation. Protein Science, 2009, 11, 2335-2350.	3.1	156
103	Polymorphism of Alzheimer's AÎ²17-42 (p3) Oligomers: The Importance of the Turn Location and Its Conformation. Biophysical Journal, 2009, 97, 1168-1177.	0.2	91
104	In silico protein design by combinatorial assembly of protein building blocks. Protein Science, 2009, 13, 2753-2765.	3.1	48
105	Intra-molecular chaperone: the role of the N-terminal in conformational selection and kinetic control. Physical Biology, 2009, 6, 013001.	0.8	9
106	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.	0.2	91
107	Annular Structures as Intermediates in Fibril Formation of Alzheimer AÎ²_{17â^'42}. Journal of Physical Chemistry B, 2008, 112, 6856-6865.	1.2	70
108	Principles of Proteinâ^'Protein Interactions: What are the Preferred Ways For Proteins To Interact?. Chemical Reviews, 2008, 108, 1225-1244.	23.0	568

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109	Molecular dynamics simulations of Alzheimer Abeta40 elongation and lateral association. Frontiers in Bioscience - Landmark, 2008, Volume, 3919.	3.0	17
110	Trp/Met/Phe Hot Spots in Protein-Protein Interactions: Potential Targets in Drug Design. Current Topics in Medicinal Chemistry, 2007, 7, 999-1005.	1.0	94
111	Ligand Binding and Circular Permutation Modify Residue Interaction Network in DHFR. PLoS Computational Biology, 2007, 3, e117.	1.5	42
112	Towards Drugs Targeting Multiple Proteins in a Systems Biology Approach. Current Topics in Medicinal Chemistry, 2007, 7, 943-951.	1.0	51
113	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.	6.5	30
114	Sequence analysis of p53 response-elements suggests multiple binding modes of the p53 tetramer to DNA targets. Nucleic Acids Research, 2007, 35, 2986-3001.	6.5	47
115	Modeling the Alzheimer AÎ²17-42 Fibril Architecture: Tight Intermolecular Sheet-Sheet Association and Intramolecular Hydrated Cavities. Biophysical Journal, 2007, 93, 3046-3057.	0.2	167
116	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
117	Consensus features in amyloid fibrils: sheetâ€“sheet recognition via a (polar or nonpolar) zipper structure. Physical Biology, 2006, 3, P1-P4.	0.8	46
118	The Stability of Monomeric Intermediates Controls Amyloid Formation: AÎ²25â€“35 and its N27Q Mutant. Biophysical Journal, 2006, 90, 3365-3374.	0.2	59
119	Structural Stability and Dynamics of an Amyloid-Forming Peptide GNNQQNY from the Yeast Prion Sup-35. Biophysical Journal, 2006, 91, 824-833.	0.2	131
120	Interaction of Protegrin-1 with Lipid Bilayers: Membrane Thinning Effect. Biophysical Journal, 2006, 91, 2848-2859.	0.2	65
121	Comparison of the Human and Worm p53 Structures Suggests a Way for Enhancing Stabilityâ€. Biochemistry, 2006, 45, 3925-3933.	1.2	21
122	Simulations as analytical tools to understand protein aggregation and predict amyloid conformation. Current Opinion in Chemical Biology, 2006, 10, 445-452.	2.8	214
123	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.	1.6	16
124	From Structure to Function: Methods and Applications. Current Protein and Peptide Science, 2005, 6, 171-183.	0.7	32
125	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.	3.3	29
126	Proteinâ€“protein interactions: organization, cooperativity and mapping in a bottom-up Systems Biology approach. Physical Biology, 2005, 2, S24-S35.	0.8	93

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127	The contribution of the Trp/Met/Phe residues to physical interactions of p53 with cellular proteins. Physical Biology, 2005, 2, S56-S66.	0.8	16
128	In the Quest for Stable Rescuing Mutants of p53:â€‰ Computational Mutagenesis of Flexible Loop L1. Biochemistry, 2005, 44, 1423-1432.	1.2	23
129	Hot Regions in Proteinâ€“Protein Interactions: The Organization and Contribution of Structurally Conserved Hot Spot Residues. Journal of Molecular Biology, 2005, 345, 1281-1294.	2.0	465
130	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.	2.0	71
131	CD4 Binding Partially Locks the Bridging Sheet in gp120 but Leaves the Î²2/3 Strands Flexible. Journal of Molecular Biology, 2005, 350, 514-527.	2.0	24
132	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.	0.2	75
133	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.	1.4	19
134	From computational quantum chemistry to computational biology: experiments and computations are (full) partners. Physical Biology, 2004, 1, P23-P26.	0.8	4
135	Characterization of the Conformational State and Flexibility of HIV-1 Glycoprotein gp120 Core Domain. Journal of Biological Chemistry, 2004, 279, 30523-30530.	1.6	29
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.	0.8	19
137	Release Factors eRF1 and RF2. Journal of Biological Chemistry, 2004, 279, 53875-53885.	1.6	31
138	Is allostery an intrinsic property of all dynamic proteins?. Proteins: Structure, Function and Bioinformatics, 2004, 57, 433-443.	1.5	779
139	The Stability and Dynamics of the Human Calcitonin Amyloid Peptide DFNKF. Biophysical Journal, 2004, 87, 146-158.	0.2	46
140	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.	2.0	197
141	Interdependence of Backbone Flexibility, Residue Conservation, and Enzyme Function:â€‰ A Case Study on Î²1,4-Galactosyltransferase-I. Biochemistry, 2003, 42, 3674-3687.	1.2	27
142	Energy landscape and dynamics of the Î²-hairpin G peptide and its isomers: Topology and sequences. Protein Science, 2003, 12, 1882-1893.	3.1	28
143	Triggering Loops and Enzyme Function: Identification of Loops that Trigger and Modulate Movements. Journal of Molecular Biology, 2003, 332, 143-159.	2.0	41
144	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.	3.3	553

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145	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.	6.5	28
146	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.	3.3	414
147	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.	1.5	39
148	Principles of docking: An overview of search algorithms and a guide to scoring functions. Proteins: Structure, Function and Bioinformatics, 2002, 47, 409-443.	1.5	1,130
149	Molecular Dynamics Simulations of the Denaturation and Refolding of an RNA Tetraloop. Journal of Biomolecular Structure and Dynamics, 2001, 19, 381-396.	2.0	19
150	Structured disorder and conformational selection. Proteins: Structure, Function and Bioinformatics, 2001, 44, 418-427.	1.5	184
151	Molecular dynamics simulation of Escherichia coli dihydrofolate reductase and its protein fragments: Relative stabilities in experiment and simulations. Protein Science, 2001, 10, 135-148.	3.1	19
152	Protein functional epitopes: hot spots, dynamics and combinatorial libraries. Current Opinion in Structural Biology, 2001, 11, 364-369.	2.6	114
153	Conservation of polar residues as hot spots at protein interfaces. , 2000, 39, 331-342.		253
154	Transition-state Ensemble in Enzyme Catalysis: Possibility, Reality, or Necessity?. Journal of Theoretical Biology, 2000, 203, 383-397.	0.8	73
155	Homology modeling and molecular dynamics simulations of lymphotactin. Protein Science, 2000, 9, 2192-2199.	3.1	2
156	Electrostatic strengths of salt bridges in thermophilic and mesophilic glutamate dehydrogenase monomers. Proteins: Structure, Function and Bioinformatics, 2000, 38, 368-383.	1.5	140
157	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.	2.0	115
158	Contribution of Salt Bridges Toward Protein Thermostability. Journal of Biomolecular Structure and Dynamics, 2000, 17, 79-85.	2.0	70
159	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.	3.3	337
160	Explicit and implicit water simulations of a ?-hairpin peptide. , 1999, 37, 73-87.		20
161	Theoretical investigation of the Ca+â€“N2 and Ca2+â€“N2 complexes. Chemical Physics Letters, 1998, 295, 204-210.	1.2	26
162	Fragmentation surface of triplet ketene. Faraday Discussions, 1998, 110, 23-50.	1.6	22

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163	Theoretical Studies of the Potential Energy Surfaces and Compositions of thed-Aldo-andd-Ketohexoses. Journal of the American Chemical Society, 1998, 120, 3411-3422.	6.6	101
164	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.	6.6	33
165	Calculation of rz structures from rs structures. Journal of Molecular Structure, 1997, 413-414, 395-404.	1.8	16
166	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.	6.6	40
167	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.	1.2	26
168	Singlet-triplet energy separation and barrier for ring closure for trimethylenemethane and its complexes. Chemical Physics, 1996, 207, 31-41.	0.9	22
169	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.	6.6	39
170	Spectroscopic constants and potential energy surfaces for the possible interstellar molecules A1NC and A1CN. Molecular Physics, 1995, 86, 1331-1337.	0.8	56
171	Observed and calculated Raman spectra of the Ga2H6 and Ga2D6 molecules. The Journal of Physical Chemistry, 1994, 98, 12824-12827.	2.9	15
172	Toward the observation of silanone (H2SiO) and hydroxysilylene (HSiOH) via microwave spectroscopy. Journal of Chemical Physics, 1994, 101, 2734-2739.	1.2	30
173	Singlet Methylcarbene: Equilibrium Geometry or Transition State?. Journal of the American Chemical Society, 1994, 116, 3539-3542.	6.6	35
174	.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.	6.6	28
175	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.	6.6	27
176	Aquated metaphosphate (PO3-.cntdot.(H2O)n) clusters. Molecular anion structures, energetics, and vibrational frequencies. Journal of the American Chemical Society, 1993, 115, 1943-1951.	6.6	28
177	Computational Approaches and Tools for Establishing Structural Models for Short Amyloid-forming Peptides. , 0, , 301-315.		1