

Andrzej Kolinski

List of Publications by Year in descending order

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213
papers

11,589
citations

31949

53
h-index

37183

96
g-index

223
all docs

223
docs citations

223
times ranked

7316
citing authors

#	ARTICLE	IF	CITATIONS
1	AAindex: amino acid index database, progress report 2008. <i>Nucleic Acids Research</i> , 2007, 36, D202-D205.	6.5	871
2	Coarse-Grained Protein Models and Their Applications. <i>Chemical Reviews</i> , 2016, 116, 7898-7936.	23.0	721
3	Topology fingerprint approach to the inverse protein folding problem. <i>Journal of Molecular Biology</i> , 1992, 227, 227-238.	2.0	341
4	CABS-dock web server for the flexible docking of peptides to proteins without prior knowledge of the binding site. <i>Nucleic Acids Research</i> , 2015, 43, W419-W424.	6.5	331
5	Protein modeling and structure prediction with a reduced representation.. <i>Acta Biochimica Polonica</i> , 2019, 51, 349-371.	0.3	284
6	Monte carlo simulations of protein folding. I. Lattice model and interaction scheme. <i>Proteins: Structure, Function and Bioinformatics</i> , 1994, 18, 338-352.	1.5	282
7	MONSSTER: a method for folding globular proteins with a small number of distance restraints. <i>Journal of Molecular Biology</i> , 1997, 265, 217-241.	2.0	257
8	CABS-flex 2.0: a web server for fast simulations of flexibility of protein structures. <i>Nucleic Acids Research</i> , 2018, 46, W338-W343.	6.5	249
9	TOUCHSTONE II: A New Approach to Ab Initio Protein Structure Prediction. <i>Biophysical Journal</i> , 2003, 85, 1145-1164.	0.2	243
10	Structural genomics and its importance for gene function analysis. <i>Nature Biotechnology</i> , 2000, 18, 283-287.	9.4	212
11	Protein-peptide docking: opportunities and challenges. <i>Drug Discovery Today</i> , 2018, 23, 1530-1537.	3.2	212
12	A general method for the prediction of the three dimensional structure and folding pathway of globular proteins: Application to designed helical proteins. <i>Journal of Chemical Physics</i> , 1993, 98, 7420-7433.	1.2	192
13	Derivation and testing of pair potentials for protein folding. When is the quasichemical approximation correct?. <i>Protein Science</i> , 1997, 6, 676-688.	3.1	182
14	Reduced models of proteins and their applications. <i>Polymer</i> , 2004, 45, 511-524.	1.8	176
15	Dynamic Monte Carlo simulations of a new lattice model of globular protein folding, structure and dynamics. <i>Journal of Molecular Biology</i> , 1991, 221, 499-531.	2.0	160
16	Monte carlo simulations of protein folding. II. Application to protein A, ROP, and crambin. <i>Proteins: Structure, Function and Bioinformatics</i> , 1994, 18, 353-366.	1.5	148
17	Are proteins ideal mixtures of amino acids? Analysis of energy parameter sets. <i>Protein Science</i> , 1995, 4, 2107-2117.	3.1	146
18	Assessing energy functions for flexible docking. <i>Journal of Computational Chemistry</i> , 1998, 19, 1612-1622.	1.5	144

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19	Modeling of protein-peptide interactions using the CABS-dock web server for binding site search and flexible docking. <i>Methods</i> , 2016, 93, 72-83.	1.9	137
20	CABS-flex: server for fast simulation of protein structure fluctuations. <i>Nucleic Acids Research</i> , 2013, 41, W427-W431.	6.5	132
21	Ab initio folding of proteins using restraints derived from evolutionary information. <i>Proteins: Structure, Function and Bioinformatics</i> , 1999, 37, 177-185.	1.5	119
22	Discretized model of proteins. I. Monte Carlo study of cooperativity in homopolypeptides. <i>Journal of Chemical Physics</i> , 1992, 97, 9412-9426.	1.2	118
23	Prediction of the Folding Pathways and Structure of the GCN4 Leucine Zipper. <i>Journal of Molecular Biology</i> , 1994, 237, 361-367.	2.0	107
24	Does reptation describe the dynamics of entangled, finite length polymer systems? A model simulation. <i>Journal of Chemical Physics</i> , 1987, 86, 1567-1585.	1.2	105
25	Derivation of protein-specific pair potentials based on weak sequence fragment similarity. , 2000, 38, 3-16.		104
26	Backbone building from quadrilaterals: A fast and accurate algorithm for protein backbone reconstruction from alpha carbon coordinates. <i>Journal of Computational Chemistry</i> , 2007, 28, 1593-1597.	1.5	102
27	Assembly of protein structure from sparse experimental data: An efficient Monte Carlo model. <i>Proteins: Structure, Function and Bioinformatics</i> , 1998, 32, 475-494.	1.5	101
28	Generalized protein structure prediction based on combination of fold-recognition with de novo folding and evaluation of models. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005, 61, 84-90.	1.5	99
29	On the origin of the cooperativity of protein folding: Implications from model simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 1996, 26, 271-287.	1.5	98
30	Folding Pathway of the B1 Domain of Protein G Explored by Multiscale Modeling. <i>Biophysical Journal</i> , 2008, 94, 726-736.	0.2	96
31	Fold assembly of small proteins using Monte Carlo simulations driven by restraints derived from multiple sequence alignments. <i>Journal of Molecular Biology</i> , 1998, 277, 419-448.	2.0	92
32	Lattice representations of globular proteins: How good are they?. <i>Journal of Computational Chemistry</i> , 1993, 14, 1194-1202.	1.5	89
33	Dynamics and Thermodynamics of \hat{I}^2 -Hairpin Assembly: Insights from Various Simulation Techniques. <i>Biophysical Journal</i> , 1999, 77, 2942-2952.	0.2	89
34	The collapse transition of semiflexible polymers. A Monte Carlo simulation of a model system. <i>Journal of Chemical Physics</i> , 1986, 85, 3585-3597.	1.2	88
35	Characterization of protein-folding pathways by reduced-space modeling. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 12330-12335.	3.3	87
36	CABS-fold: server for the de novo and consensus-based prediction of protein structure. <i>Nucleic Acids Research</i> , 2013, 41, W406-W411.	6.5	86

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37	Accurate reconstruction of all-atom protein representations from side-chain-based low-resolution models. <i>Proteins: Structure, Function and Bioinformatics</i> , 2000, 41, 86-97.	1.5	85
38	Consistent View of Protein Fluctuations from All-Atom Molecular Dynamics and Coarse-Grained Dynamics with Knowledge-Based Force-Field. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 119-125.	2.3	85
39	De novo and inverse folding predictions of protein structure and dynamics. <i>Journal of Computer-Aided Molecular Design</i> , 1993, 7, 397-438.	1.3	84
40	Protein fragment reconstruction using various modeling techniques. <i>Journal of Computer-Aided Molecular Design</i> , 2003, 17, 725-738.	1.3	81
41	Dynamic Monte Carlo simulations of globular protein folding/unfolding pathways. <i>Journal of Molecular Biology</i> , 1990, 212, 787-817.	2.0	80
42	A method for predicting protein structure from sequence. <i>Current Biology</i> , 1993, 3, 414-423.	1.8	80
43	CABS-flex standalone: a simulation environment for fast modeling of protein flexibility. <i>Bioinformatics</i> , 2019, 35, 694-695.	1.8	79
44	CABS-flex predictions of protein flexibility compared with NMR ensembles. <i>Bioinformatics</i> , 2014, 30, 2150-2154.	1.8	75
45	Monte Carlo studies on the long time dynamic properties of dense cubic lattice multichain systems. I. The homopolymeric melt. <i>Journal of Chemical Physics</i> , 1987, 86, 7164-7173.	1.2	73
46	TOUCHSTONE: A unified approach to protein structure prediction. <i>Proteins: Structure, Function and Bioinformatics</i> , 2003, 53, 469-479.	1.5	72
47	2-Ethyl and 2-Ethylidene Analogues of 1 \pm ,25-Dihydroxy-19-norvitamin D ₃ : \hat{A} Synthesis, Conformational Analysis, Biological Activities, and Docking to the Modeled rVDR Ligand Binding Domain. <i>Journal of Medicinal Chemistry</i> , 2002, 45, 3366-3380.	2.9	70
48	Comparison of three Monte Carlo conformational search strategies for a proteinlike homopolymer model: Folding thermodynamics and identification of low-energy structures. <i>Journal of Chemical Physics</i> , 2000, 113, 5065.	1.2	66
49	Ab initio protein structure prediction via a combination of threading, lattice folding, clustering, and structure refinement. <i>Proteins: Structure, Function and Bioinformatics</i> , 2001, 45, 149-156.	1.5	66
50	Inferring ideal amino acid interaction forms from statistical protein contact potentials. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005, 59, 49-57.	1.5	66
51	DNA Vaccine Expressing the Mimotope of GD2 Ganglioside Induces Protective GD2 Cross-reactive Antibody Responses. <i>Cancer Research</i> , 2005, 65, 3410-3418.	0.4	64
52	On the short time dynamics of dense polymeric systems and the origin of the glass transition: A model system. <i>Journal of Chemical Physics</i> , 1986, 84, 1922-1931.	1.2	63
53	Regularities in interaction patterns of globular proteins. <i>Protein Engineering, Design and Selection</i> , 1993, 6, 801-810.	1.0	63
54	Dynamics of Dense Polymer Systems: Computer Simulations and Analytic Theories. <i>Advances in Chemical Physics</i> , 2007, , 223-278.	0.3	63

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55	Modeling of Protein Structural Flexibility and Large-Scale Dynamics: Coarse-Grained Simulations and Elastic Network Models. <i>International Journal of Molecular Sciences</i> , 2018, 19, 3496.	1.8	60
56	Static and dynamic properties of a new lattice model of polypeptide chains. <i>Journal of Chemical Physics</i> , 1991, 94, 3978-3985.	1.2	57
57	CABS-dock standalone: a toolbox for flexible protein-peptide docking. <i>Bioinformatics</i> , 2019, 35, 4170-4172.	1.8	55
58	A method for the improvement of threading-based protein models. <i>Proteins: Structure, Function and Bioinformatics</i> , 1999, 37, 592-610.	1.5	53
59	Does a backwardly read protein sequence have a unique native state?. <i>Protein Engineering, Design and Selection</i> , 1996, 9, 5-14.	1.0	51
60	A Minimal Physically Realistic Protein-Like Lattice Model: Designing an Energy Landscape that Ensures All-Or-None Folding to a Unique Native State. <i>Biophysical Journal</i> , 2003, 84, 1518-1526.	0.2	51
61	Theoretical model of prion propagation: A misfolded protein induces misfolding. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2005, 102, 7835-7840.	3.3	51
62	Flexible docking of peptides to proteins using CABS-dock. <i>Protein Science</i> , 2020, 29, 211-222.	3.1	48
63	Monte carlo studies on equilibrium globular protein folding. I. Homopolymeric lattice models of β -barrel proteins. <i>Biopolymers</i> , 1987, 26, 937-962.	1.2	47
64	Human telomerase model shows the role of the TEN domain in advancing the double helix for the next polymerization step. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 9443-9448.	3.3	47
65	Monte Carlo studies on the long time dynamic properties of dense cubic lattice multichain systems. II. Probe polymer in a matrix of different degrees of polymerization. <i>Journal of Chemical Physics</i> , 1987, 86, 7174-7180.	1.2	45
66	Phenomenological theory of the dynamics of polymer melts. I. Analytic treatment of self-diffusion. <i>Journal of Chemical Physics</i> , 1988, 88, 1407-1417.	1.2	45
67	Prediction of Quaternary Structure of Coiled Coils. Application to Mutants of the GCN4 Leucine Zipper. <i>Journal of Molecular Biology</i> , 1995, 251, 448-467.	2.0	45
68	Monte Carlo studies of the thermodynamics and kinetics of reduced protein models: Application to small helical, β^2 , and β/β^2 proteins. <i>Journal of Chemical Physics</i> , 1998, 108, 2608-2617.	1.2	45
69	Towards the high-resolution protein structure prediction. Fast refinement of reduced models with all-atom force field. <i>BMC Structural Biology</i> , 2007, 7, 43.	2.3	45
70	Distance matrix-based approach to protein structure prediction. <i>Journal of Structural and Functional Genomics</i> , 2009, 10, 67-81.	1.2	45
71	Modeling of Disordered Protein Structures Using Monte Carlo Simulations and Knowledge-Based Statistical Force Fields. <i>International Journal of Molecular Sciences</i> , 2019, 20, 606.	1.8	45
72	BioShell—a package of tools for structural biology computations. <i>Bioinformatics</i> , 2006, 22, 621-622.	1.8	44

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73	Protein-peptide molecular docking with large-scale conformational changes: the p53-MDM2 interaction. <i>Scientific Reports</i> , 2016, 6, 37532.	1.6	44
74	Computational reconstruction of atomistic protein structures from coarse-grained models. <i>Computational and Structural Biotechnology Journal</i> , 2020, 18, 162-176.	1.9	43
75	Ab initio protein structure prediction on a genomic scale: Application to the <i>Mycoplasma genitalium</i> genome. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002, 99, 5993-5998.	3.3	41
76	Mechanism of Folding and Binding of an Intrinsically Disordered Protein As Revealed by ab Initio Simulations. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2224-2231.	2.3	41
77	Simulation of Chaperonin Effect on Protein Folding: A Shift from Nucleation to Condensation to Framework Mechanism. <i>Journal of the American Chemical Society</i> , 2011, 133, 10283-10289.	6.6	40
78	Monte Carlo dynamics of a dense system of chain molecules constrained to lie near an interface. A simplified membrane model. <i>Journal of Chemical Physics</i> , 1990, 93, 4440-4446.	1.2	39
79	A reduced model of short range interactions in polypeptide chains. <i>Journal of Chemical Physics</i> , 1995, 103, 4312-4323.	1.2	39
80	An Efficient Monte Carlo Model of Protein Chains. Modeling the Short-Range Correlations between Side Group Centers of Mass. <i>Journal of Physical Chemistry B</i> , 1998, 102, 4628-4637.	1.2	38
81	TOUCHSTONEX: Protein structure prediction with sparse NMR data. <i>Proteins: Structure, Function and Bioinformatics</i> , 2003, 53, 290-306.	1.5	38
82	Utility library for structural bioinformatics. <i>Bioinformatics</i> , 2008, 24, 584-585.	1.8	38
83	Multibody coarse-grained potentials for native structure recognition and quality assessment of protein models. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011, 79, 1923-1929.	1.5	38
84	Folding simulations and computer redesign of protein A three-helix bundle motifs. <i>Proteins: Structure, Function and Bioinformatics</i> , 1996, 25, 286-299.	1.5	38
85	Monte carlo studies on equilibrium globular protein folding. II. β -barrel globular protein models. <i>Biopolymers</i> , 1989, 28, 1059-1095.	1.2	36
86	Effect of double bonds on the dynamics of hydrocarbon chains. <i>Journal of Chemical Physics</i> , 1992, 97, 1240-1249.	1.2	36
87	Combining MONSSTER and LES/PME to Predict Protein Structure from Amino Acid Sequence: Application to the Small Protein CMTI-1. <i>Journal of the American Chemical Society</i> , 2000, 122, 8392-8402.	6.6	36
88	Monte Carlo study of local orientational order in a semiflexible polymer melt model. <i>Macromolecules</i> , 1986, 19, 2550-2560.	2.2	35
89	Algorithm for rapid reconstruction of protein backbone from alpha carbon coordinates. <i>Journal of Computational Chemistry</i> , 1997, 18, 80-85.	1.5	35
90	Modeling of loops in proteins: a multi-method approach. <i>BMC Structural Biology</i> , 2010, 10, 5.	2.3	35

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91	Protein-peptide docking using CABS-dock and contact information. <i>Briefings in Bioinformatics</i> , 2019, 20, 2299-2305.	3.2	35
92	Computer design of idealized motifs. <i>Journal of Chemical Physics</i> , 1995, 103, 10286-10297.	1.2	33
93	Highly Flexible Protein-Peptide Docking Using CABS-Dock. <i>Methods in Molecular Biology</i> , 2017, 1561, 69-94.	0.4	33
94	The GOR Method of Protein Secondary Structure Prediction and Its Application as a Protein Aggregation Prediction Tool. <i>Methods in Molecular Biology</i> , 2017, 1484, 7-24.	0.4	33
95	Type II restriction endonuclease R.Eco29kl is a member of the GIY-YIG nuclease superfamily. <i>BMC Structural Biology</i> , 2007, 7, 48.	2.3	32
96	Optimization of protein models. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2012, 2, 479-493.	6.2	32
97	ClusCo: clustering and comparison of protein models. <i>BMC Bioinformatics</i> , 2013, 14, 62.	1.2	32
98	Ab initio folding of proteins using restraints derived from evolutionary information. <i>Proteins: Structure, Function and Bioinformatics</i> , 1999, 37, 177-185.	1.5	32
99	De Novo Simulations of the Folding Thermodynamics of the GCN4 Leucine Zipper. <i>Biophysical Journal</i> , 1999, 77, 54-69.	0.2	31
100	From Coarse-Grained to Atomic-Level Characterization of Protein Dynamics: Transition State for the Folding of B Domain of Protein A. <i>Journal of Physical Chemistry B</i> , 2012, 116, 7026-7032.	1.2	31
101	Correlation between knowledge-based and detailed atomic potentials: Application to the unfolding of the GCN4 leucine zipper. <i>Proteins: Structure, Function and Bioinformatics</i> , 1999, 35, 447-452.	1.5	30
102	HCPM-program for hierarchical clustering of protein models. <i>Bioinformatics</i> , 2005, 21, 3179-3180.	1.8	30
103	Monte Carlo study of star-branched polymers on the tetrahedral lattice. I. Conformation of the macromolecule. <i>Journal of Polymer Science: Polymer Chemistry Edition</i> , 1982, 20, 3147-3154.	0.8	29
104	A new combination of replica exchange Monte Carlo and histogram analysis for protein folding and thermodynamics. <i>Journal of Chemical Physics</i> , 2001, 115, 1569-1574.	1.2	29
105	Protein secondary structure prediction using a small training set (compact model) combined with a Complex-valued neural network approach. <i>BMC Bioinformatics</i> , 2016, 17, 362.	1.2	29
106	A method for the prediction of surface turns and transglobular connections in small proteins. , 1997, 27, 290-308.		28
107	Monte Carlo studies of the long-time dynamics of dense polymer systems. The failure of the reptation model. <i>Accounts of Chemical Research</i> , 1987, 20, 350-356.	7.6	26
108	Efficient scheme for optimization of parallel tempering Monte Carlo method. <i>Journal of Physics Condensed Matter</i> , 2007, 19, 036225.	0.7	25

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109	Protein structure prediction: Combining de novo modeling with sparse experimental data. <i>Journal of Computational Chemistry</i> , 2007, 28, 1668-1676.	1.5	25
110	Denatured proteins and early folding intermediates simulated in a reduced conformational space.. <i>Acta Biochimica Polonica</i> , 2019, 53, 131-143.	0.3	25
111	Order-disorder transitions in tetrahedral lattice polymer systems. <i>Macromolecules</i> , 1986, 19, 2560-2567.	2.2	24
112	Computer Simulations of De Novo Designed Helical Proteins. <i>Biophysical Journal</i> , 1998, 75, 92-105.	0.2	24
113	A lattice dynamics study of a Langmuir monolayer of monounsaturated fatty acids. <i>Journal of Chemical Physics</i> , 1993, 98, 7581-7587.	1.2	23
114	Collapse transitions in protein-like lattice polymers: The effect of sequence patterns. <i>Biopolymers</i> , 1997, 42, 537-548.	1.2	23
115	5-HT ₂ receptor affinity, docking studies and pharmacological evaluation of a series of 1,3-disubstituted thiourea derivatives. <i>European Journal of Medicinal Chemistry</i> , 2016, 116, 173-186.	2.6	23
116	Method for Predicting the State of Association of Discretized Protein Models. Application to Leucine Zippers. <i>Biochemistry</i> , 1996, 35, 955-967.	1.2	22
117	Combining Coarse-Grained Protein Models with Replica-Exchange All-Atom Molecular Dynamics. <i>International Journal of Molecular Sciences</i> , 2013, 14, 9893-9905.	1.8	22
118	Dynamics of star branched polymers in a matrix of linear chains – a Monte Carlo study. <i>Macromolecular Theory and Simulations</i> , 1994, 3, 715-729.	0.6	21
119	A simple lattice model that exhibits a protein-like cooperative all-or-none folding transition. <i>Biopolymers</i> , 2003, 69, 399-405.	1.2	21
120	Exploring protein energy landscapes with hierarchical clustering. <i>International Journal of Quantum Chemistry</i> , 2005, 105, 826-830.	1.0	21
121	Steps towards flexible docking: Modeling of three-dimensional structures of the nuclear receptors bound with peptide ligands mimicking co-activators'™ sequences. <i>Journal of Steroid Biochemistry and Molecular Biology</i> , 2007, 103, 357-360.	1.2	21
122	Kinetics and mechanical stability of the fibril state control fibril formation time of polypeptide chains: A computational study. <i>Journal of Chemical Physics</i> , 2018, 148, 215106.	1.2	21
123	Model of three-dimensional structure of vitamin D receptor and its binding mechanism with 1 α ,25-dihydroxyvitamin D ₃ . <i>Proteins: Structure, Function and Bioinformatics</i> , 2001, 44, 188-199.	1.5	20
124	Coarse-Grained Modeling of Mucus Barrier Properties. <i>Biophysical Journal</i> , 2012, 102, 195-200.	0.2	20
125	Structural features that predict real-time value fluctuations of globular proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2012, 80, 1425-1435.	1.5	20
126	Role of Resultant Dipole Moment in Mechanical Dissociation of Biological Complexes. <i>Molecules</i> , 2018, 23, 1995.	1.7	20

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127	Dynamic Monte Carlo study of the conformational properties of long flexible polymers. <i>Macromolecules</i> , 1987, 20, 438-440.	2.2	19
128	Neural network system for the evaluation of side-chain packing in protein structures. <i>Protein Engineering, Design and Selection</i> , 1995, 8, 225-236.	1.0	19
129	Reduced Protein Models and their Application to the Protein Folding Problem. <i>Journal of Biomolecular Structure and Dynamics</i> , 1998, 16, 381-396.	2.0	19
130	Hierarchical modeling of protein interactions. <i>Journal of Molecular Modeling</i> , 2007, 13, 691-698.	0.8	19
131	Preformed template fluctuations promote fibril formation: Insights from lattice and all-atom models. <i>Journal of Chemical Physics</i> , 2015, 142, 145104.	1.2	18
132	SURPASS Low-Resolution Coarse-Grained Protein Modeling. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5766-5779.	2.3	18
133	Determinants of secondary structure of polypeptide chains: Interplay between short range and burial interactions. <i>Journal of Chemical Physics</i> , 1997, 107, 953-964.	1.2	17
134	Tertiary structure prediction of the KIX domain of CBP using Monte Carlo simulations driven by restraints derived from multiple sequence alignments. , 1998, 30, 287-294.		17
135	Elastic network normal modes provide a basis for protein structure refinement. <i>Journal of Chemical Physics</i> , 2012, 136, 195101.	1.2	17
136	BioShell-Threading: versatile Monte Carlo package for protein 3D threading. <i>BMC Bioinformatics</i> , 2014, 15, 22.	1.2	17
137	Coarse-Grained Simulations of Membrane Insertion and Folding of Small Helical Proteins Using the CABS Model. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 2207-2215.	2.5	17
138	Modeling EphB4-EphrinB2 protein-protein interaction using flexible docking of a short linear motif. <i>BioMedical Engineering OnLine</i> , 2017, 16, 71.	1.3	17
139	Folding simulations and computer redesign of protein A three-helix bundle motifs. <i>Proteins: Structure, Function and Bioinformatics</i> , 1996, 25, 286-299.	1.5	16
140	Protein Folding: Flexible Lattice Models. <i>Progress of Theoretical Physics Supplement</i> , 2000, 138, 292-300.	0.2	16
141	Three-dimensional modeling of the I-TevI homing endonuclease catalytic domain, a GIY-YIG superfamily member, using NMR restraints and Monte Carlo dynamics. <i>Protein Engineering, Design and Selection</i> , 2001, 14, 717-721.	1.0	16
142	Use of residual dipolar couplings as restraints in ab initio protein structure prediction. <i>Biopolymers</i> , 2003, 70, 548-562.	1.2	16
143	Comparative modeling without implicit sequence alignments. <i>Bioinformatics</i> , 2007, 23, 2522-2527.	1.8	16
144	Monte carlo study of star-branched polymers on the tetrahedral lattice. II. Statistical thermodynamics of single macromolecules. <i>Journal of Polymer Science: Polymer Chemistry Edition</i> , 1984, 22, 97-106.	0.8	15

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145	Contact prediction in protein modeling: Scoring, folding and refinement of coarse-grained models. BMC Structural Biology, 2008, 8, 36.	2.3	15
146	Protocols for Fast Simulations of Protein Structure Flexibility Using CABS-Flex and SURPASS. Methods in Molecular Biology, 2020, 2165, 337-353.	0.4	15
147	Monte carlo calculations of the α -point of star-branched macromolecules on tetrahedral lattice. Journal of Polymer Science, Polymer Letters Edition, 1982, 20, 177-180.	0.4	14
148	CABS-NMR De novo tool for rapid global fold determination from chemical shifts, residual dipolar couplings and sparse methyl-methyl NOEs. Journal of Computational Chemistry, 2011, 32, 536-544.	1.5	14
149	Helix-coil and beta sheet-coil transitions in a simplified, yet realistic protein model. Macromolecular Theory and Simulations, 2000, 9, 523-533.	0.6	13
150	Unfolding of Globular Proteins: Monte Carlo Dynamics of a Realistic Reduced Model. Biophysical Journal, 2003, 85, 3271-3278.	0.2	13
151	Coarse-Grained Monte Carlo Simulations of Mucus: Structure, Dynamics, and Thermodynamics. Biophysical Journal, 2010, 99, 3507-3516.	0.2	13
152	A structure-based model fails to probe the mechanical unfolding pathways of the titin I27 domain. Journal of Chemical Physics, 2013, 139, 065103.	1.2	13
153	Protocols for Efficient Simulations of Long-Time Protein Dynamics Using Coarse-Grained CABS Model. Methods in Molecular Biology, 2014, 1137, 235-250.	0.4	13
154	A simple technique to estimate partition functions and equilibrium constants from Monte Carlo simulations. Journal of Chemical Physics, 1995, 102, 6189-6193.	1.2	12
155	Numerical Study of the Entropy Loss of Dimerization and the Folding Thermodynamics of the GCN4 Leucine Zipper. Biophysical Journal, 2002, 83, 2801-2811.	0.2	12
156	A minimal proteinlike lattice model: An alpha-helix motif. Journal of Chemical Physics, 2005, 122, 214915.	1.2	12
157	Analysis and optimization of interactions between peptides mimicking the GD2 ganglioside and the monoclonal antibody 14G2a. International Journal of Molecular Medicine, 2011, 28, 47-57.	1.8	12
158	Ideal amino acid exchange forms for approximating substitution matrices. Proteins: Structure, Function and Bioinformatics, 2007, 69, 379-393.	1.5	11
159	Predicting the Complex Structure and Functional Motions of the Outer Membrane Transporter and Signal Transducer FecA. Biophysical Journal, 2008, 94, 2482-2491.	0.2	11
160	Multiscale Approach to Protein Folding Dynamics. , 2011, , 281-293.		11
161	Coarse-Grained Modeling of Peptide Docking Associated with Large Conformation Transitions of the Binding Protein: Troponin I Fragment-Troponin C System. Molecules, 2015, 20, 10763-10780.	1.7	11
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