

Andrzej Kolinski

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211
papers

9,489
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90
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223
ext. papers

10,521
ext. citations

5.2
avg. IF

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L-index

#	Paper	IF	Citations
211	AAindex: amino acid index database, progress report 2008. <i>Nucleic Acids Research</i> , 2008 , 36, D202-5	20.1	623
210	Coarse-Grained Protein Models and Their Applications. <i>Chemical Reviews</i> , 2016 , 116, 7898-936	68.1	489
209	Topology fingerprint approach to the inverse protein folding problem. <i>Journal of Molecular Biology</i> , 1992 , 227, 227-38	6.5	317
208	Monte Carlo simulations of protein folding. I. Lattice model and interaction scheme. <i>Proteins: Structure, Function and Bioinformatics</i> , 1994 , 18, 338-52	4.2	257
207	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, W419-24	20.1	237
206	MONSSTER: a method for folding globular proteins with a small number of distance restraints. <i>Journal of Molecular Biology</i> , 1997 , 265, 217-41	6.5	234
205	TOUCHSTONE II: a new approach to ab initio protein structure prediction. <i>Biophysical Journal</i> , 2003 , 85, 1145-64	2.9	223
204	Protein modeling and structure prediction with a reduced representation.. <i>Acta Biochimica Polonica</i> , 2019 , 51, 349-371	2	221
203	Structural genomics and its importance for gene function analysis. <i>Nature Biotechnology</i> , 2000 , 18, 283-744.5	177	
202	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	2.9	177
201	Derivation and testing of pair potentials for protein folding. When is the quasichemical approximation correct?. <i>Protein Science</i> , 1997 , 6, 676-88	6.3	159
200	Reduced models of proteins and their applications. <i>Polymer</i> , 2004 , 45, 511-524	3.9	159
199	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	6.5	155
198	Assessing energy functions for flexible docking. <i>Journal of Computational Chemistry</i> , 1998 , 19, 1612-1623.5	132	
197	Are proteins ideal mixtures of amino acids? Analysis of energy parameter sets. <i>Protein Science</i> , 1995 , 4, 2107-17	6.3	131
196	Monte Carlo simulations of protein folding. II. Application to protein A, ROP, and crambin. <i>Proteins: Structure, Function and Bioinformatics</i> , 1994 , 18, 353-66	4.2	126
195	Protein-peptide docking: opportunities and challenges. <i>Drug Discovery Today</i> , 2018 , 23, 1530-1537	8.8	118

194	CABS-flex 2.0: a web server for fast simulations of flexibility of protein structures. <i>Nucleic Acids Research</i> , 2018 , 46, W338-W343	20.1	118
193	Discretized model of proteins. I. Monte Carlo study of cooperativity in homopolypeptides. <i>Journal of Chemical Physics</i> , 1992 , 97, 9412-9426	3.9	105
192	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	4.6	104
191	Prediction of the folding pathways and structure of the GCN4 leucine zipper. <i>Journal of Molecular Biology</i> , 1994 , 237, 361-7	6.5	101
190	CABS-flex: Server for fast simulation of protein structure fluctuations. <i>Nucleic Acids Research</i> , 2013 , 41, W427-31	20.1	98
189	Does reptation describe the dynamics of entangled, finite length polymer systems? A model simulation. <i>Journal of Chemical Physics</i> , 1987 , 86, 1567-1585	3.9	94
188	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 Suppl 7, 84-90	4.2	92
187	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	3.5	90
186	Assembly of protein structure from sparse experimental data: An efficient Monte Carlo model. <i>Proteins: Structure, Function and Bioinformatics</i> , 1998 , 32, 475-494	4.2	89
185	Ab initio folding of proteins using restraints derived from evolutionary information. <i>Proteins: Structure, Function and Bioinformatics</i> , 1999 , 37, 177-185	4.2	89
184	On the origin of the cooperativity of protein folding: implications from model simulations. <i>Proteins: Structure, Function and Bioinformatics</i> , 1996 , 26, 271-87	4.2	89
183	Folding pathway of the b1 domain of protein G explored by multiscale modeling. <i>Biophysical Journal</i> , 2008 , 94, 726-36	2.9	85
182	Derivation of protein-specific pair potentials based on weak sequence fragment similarity 2000 , 38, 3-16		84
181	Dynamics and thermodynamics of beta-hairpin assembly: insights from various simulation techniques. <i>Biophysical Journal</i> , 1999 , 77, 2942-52	2.9	82
180	The collapse transition of semiflexible polymers. A Monte Carlo simulation of a model system. <i>Journal of Chemical Physics</i> , 1986 , 85, 3585-3597	3.9	82
179	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	4.2	80
178	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, 419-48	6.5	79
177	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, 12330-5	11.5	78

176	Lattice representations of globular proteins: How good are they?. <i>Journal of Computational Chemistry</i> , 1993 , 14, 1194-1202	3.5	77
175	CABS-fold: Server for the de novo and consensus-based prediction of protein structure. <i>Nucleic Acids Research</i> , 2013 , 41, W406-11	20.1	75
174	A method for predicting protein structure from sequence. <i>Current Biology</i> , 1993 , 3, 414-23	6.3	73
173	Dynamic Monte Carlo simulations of globular protein folding/unfolding pathways. I. Six-member, Greek key beta-barrel proteins. <i>Journal of Molecular Biology</i> , 1990 , 212, 787-817	6.5	73
172	Protein fragment reconstruction using various modeling techniques. <i>Journal of Computer-Aided Molecular Design</i> , 2003 , 17, 725-38	4.2	72
171	TOUCHSTONE: a unified approach to protein structure prediction. <i>Proteins: Structure, Function and Bioinformatics</i> , 2003 , 53 Suppl 6, 469-79	4.2	69
170	De novo and inverse folding predictions of protein structure and dynamics. <i>Journal of Computer-Aided Molecular Design</i> , 1993 , 7, 397-438	4.2	69
169	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	3.9	64
168	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, 119-254	6.4	63
167	2-Ethyl and 2-ethylidene analogues of 1alpha,25-dihydroxy-19-norvitamin D(3): synthesis, conformational analysis, biological activities, and docking to the modeled rVDR ligand binding domain. <i>Journal of Medicinal Chemistry</i> , 2002 , 45, 3366-80	8.3	62
166	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	3.9	62
165	Ab initio protein structure prediction via a combination of threading, lattice folding, clustering, and structure refinement. <i>Proteins: Structure, Function and Bioinformatics</i> , 2001 , Suppl 5, 149-56	4.2	58
164	Inferring ideal amino acid interaction forms from statistical protein contact potentials. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005 , 59, 49-57	4.2	55
163	Regularities in interaction patterns of globular proteins. <i>Protein Engineering, Design and Selection</i> , 1993 , 6, 801-10	1.9	54
162	Static and dynamic properties of a new lattice model of polypeptide chains. <i>Journal of Chemical Physics</i> , 1991 , 94, 3978-3985	3.9	54
161	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	3.9	54
160	DNA vaccine expressing the mimotope of GD2 ganglioside induces protective GD2 cross-reactive antibody responses. <i>Cancer Research</i> , 2005 , 65, 3410-8	10.1	53
159	Does a backwardly read protein sequence have a unique native state?. <i>Protein Engineering, Design and Selection</i> , 1996 , 9, 5-14	1.9	50

158	CABS-flex predictions of protein flexibility compared with NMR ensembles. <i>Bioinformatics</i> , 2014 , 30, 2150-4	7.2	48
157	Dynamics of Dense Polymer Systems: Computer Simulations and Analytic Theories. <i>Advances in Chemical Physics</i> , 2007 , 223-278		48
156	A method for the improvement of threading-based protein models. <i>Proteins: Structure, Function and Bioinformatics</i> , 1999 , 37, 592-610	4.2	48
155	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, 7835-40	11.5	47
154	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, 1518-26	2.9	46
153	CABS-flex standalone: a simulation environment for fast modeling of protein flexibility. <i>Bioinformatics</i> , 2019 , 35, 694-695	7.2	45
152	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	2.7	44
151	Monte Carlo studies of the thermodynamics and kinetics of reduced protein models: Application to small helical, β and $\beta\alpha$ proteins. <i>Journal of Chemical Physics</i> , 1998 , 108, 2608-2617	3.9	44
150	Prediction of quaternary structure of coiled coils. Application to mutants of the GCN4 leucine zipper. <i>Journal of Molecular Biology</i> , 1995 , 251, 448-67	6.5	44
149	BioShell--a package of tools for structural biology computations. <i>Bioinformatics</i> , 2006 , 22, 621-2	7.2	42
148	Monte Carlo studies on equilibrium globular protein folding. I. Homopolymeric lattice models of beta-barrel proteins. <i>Biopolymers</i> , 1987 , 26, 937-62	2.2	42
147	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, 9443-8	11.5	41
146	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, 5993-8	11.5	39
145	Simulation of chaperonin effect on protein folding: a shift from nucleation-condensation to framework mechanism. <i>Journal of the American Chemical Society</i> , 2011 , 133, 10283-9	16.4	38
144	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	3.9	38
143	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,	6.3	37
142	Multibody coarse-grained potentials for native structure recognition and quality assessment of protein models. <i>Proteins: Structure, Function and Bioinformatics</i> , 2011 , 79, 1923-9	4.2	36
141	Distance matrix-based approach to protein structure prediction. <i>Journal of Structural and Functional Genomics</i> , 2009 , 10, 67-81		36

140	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	3.9	36
139	Phenomenological theory of the dynamics of polymer melts. I. Analytic treatment of self-diffusion. <i>Journal of Chemical Physics</i> , 1988 , 88, 1407-1417	3.9	36
138	Utility library for structural bioinformatics. <i>Bioinformatics</i> , 2008 , 24, 584-5	7.2	35
137	TOUCHSTONEX: protein structure prediction with sparse NMR data. <i>Proteins: Structure, Function and Bioinformatics</i> , 2003 , 53, 290-306	4.2	35
136	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	16.4	35
135	Folding simulations and computer redesign of protein A three-helix bundle motifs. <i>Proteins: Structure, Function and Bioinformatics</i> , 1996 , 25, 286-299	4.2	35
134	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	3.4	34
133	A reduced model of short range interactions in polypeptide chains. <i>Journal of Chemical Physics</i> , 1995 , 103, 4312-4323	3.9	33
132	Monte Carlo studies on equilibrium globular protein folding. II. Beta-barrel globular protein models. <i>Biopolymers</i> , 1989 , 28, 1059-95	2.2	33
131	Protein-peptide molecular docking with large-scale conformational changes: the p53-MDM2 interaction. <i>Scientific Reports</i> , 2016 , 6, 37532	4.9	33
130	Modeling of loops in proteins: a multi-method approach. <i>BMC Structural Biology</i> , 2010 , 10, 5	2.7	32
129	Effect of double bonds on the dynamics of hydrocarbon chains. <i>Journal of Chemical Physics</i> , 1992 , 97, 1240-1249	3.9	32
128	Ab initio folding of proteins using restraints derived from evolutionary information. <i>Proteins: Structure, Function and Bioinformatics</i> , 1999 , 37, 177-185	4.2	32
127	Algorithm for rapid reconstruction of protein backbone from alpha carbon coordinates. <i>Journal of Computational Chemistry</i> , 1997 , 18, 80-85	3.5	31
126	Computer design of idealized motifs. <i>Journal of Chemical Physics</i> , 1995 , 103, 10286-10297	3.9	31
125	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, 2224-31	6.4	29
124	HCPM--program for hierarchical clustering of protein models. <i>Bioinformatics</i> , 2005 , 21, 3179-80	7.2	29
123	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	4.2	29

122	De novo simulations of the folding thermodynamics of the GCN4 leucine zipper. <i>Biophysical Journal</i> , 1999 , 77, 54-69	2.9	29
121	Monte Carlo study of local orientational order in a semiflexible polymer melt model. <i>Macromolecules</i> , 1986 , 19, 2550-2560	5.5	29
120	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, 7026-32	3.4	27
119	Optimization of protein models. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2012 , 2, 479-493	7.9	27
118	Type II restriction endonuclease R.Eco29ki is a member of the GIY-YIG nuclease superfamily. <i>BMC Structural Biology</i> , 2007 , 7, 48	2.7	27
117	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	3.9	27
116	A method for the prediction of surface α -turns and transglobular connections in small proteins 1997 , 27, 290-308		26
115	CABS-dock standalone: a toolbox for flexible protein-peptide docking. <i>Bioinformatics</i> , 2019 , 35, 4170-4172		25
114	ClusCo: clustering and comparison of protein models. <i>BMC Bioinformatics</i> , 2013 , 14, 62	3.6	25
113	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	24.3	25
112	Highly Flexible Protein-Peptide Docking Using CABS-Dock. <i>Methods in Molecular Biology</i> , 2017 , 1561, 69-94	1.4	24
111	Modeling of Disordered Protein Structures Using Monte Carlo Simulations and Knowledge-Based Statistical Force Fields. <i>International Journal of Molecular Sciences</i> , 2019 , 20,	6.3	24
110	Flexible docking of peptides to proteins using CABS-dock. <i>Protein Science</i> , 2020 , 29, 211-222	6.3	24
109	Computational reconstruction of atomistic protein structures from coarse-grained models. <i>Computational and Structural Biotechnology Journal</i> , 2020 , 18, 162-176	6.8	24
108	A lattice dynamics study of a Langmuir monolayer of monounsaturated fatty acids. <i>Journal of Chemical Physics</i> , 1993 , 98, 7581-7587	3.9	23
107	Order-disorder transitions in tetrahedral lattice polymer systems. <i>Macromolecules</i> , 1986 , 19, 2560-2567	5.5	23
106	Denatured proteins and early folding intermediates simulated in a reduced conformational space.. <i>Acta Biochimica Polonica</i> , 2019 , 53, 131-143	2	23
105	Collapse transitions in protein-like lattice polymers: The effect of sequence patterns. <i>Biopolymers</i> , 1997 , 42, 537-548	2.2	22

104	Protein structure prediction: combining de novo modeling with sparse experimental data. <i>Journal of Computational Chemistry</i> , 2007 , 28, 1668-76	3.5	22
103	Computer simulations of de novo designed helical proteins. <i>Biophysical Journal</i> , 1998 , 75, 92-105	2.9	22
102	Efficient scheme for optimization of parallel tempering Monte Carlo method. <i>Journal of Physics Condensed Matter</i> , 2007 , 19, 036225	1.8	21
101	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	1.4	20
100	Combining coarse-grained protein models with replica-exchange all-atom molecular dynamics. <i>International Journal of Molecular Sciences</i> , 2013 , 14, 9893-905	6.3	20
99	Method for predicting the state of association of discretized protein models. Application to leucine zippers. <i>Biochemistry</i> , 1996 , 35, 955-67	3.2	20
98	Dynamics of star branched polymers in a matrix of linear chains – Monte Carlo study. <i>Macromolecular Theory and Simulations</i> , 1994 , 3, 715-729	1.5	20
97	Coarse-grained modeling of mucus barrier properties. <i>Biophysical Journal</i> , 2012 , 102, 195-200	2.9	19
96	Exploring protein energy landscapes with hierarchical clustering. <i>International Journal of Quantum Chemistry</i> , 2005 , 105, 826-830	2.1	19
95	Structural features that predict real-value fluctuations of globular proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2012 , 80, 1425-35	4.2	18
94	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, 357-60	5.1	18
93	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		18
92	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	6.8	18
91	Determinants of secondary structure of polypeptide chains: Interplay between short range and burial interactions. <i>Journal of Chemical Physics</i> , 1997 , 107, 953-964	3.9	17
90	Hierarchical modeling of protein interactions. <i>Journal of Molecular Modeling</i> , 2007 , 13, 691-8	2	17
89	A simple lattice model that exhibits a protein-like cooperative all-or-none folding transition. <i>Biopolymers</i> , 2003 , 69, 399-405	2.2	17
88	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, 188-99	4.2	17
87	Neural network system for the evaluation of side-chain packing in protein structures. <i>Protein Engineering, Design and Selection</i> , 1995 , 8, 225-36	1.9	17

86	Dynamic Monte Carlo study of the conformational properties of long flexible polymers. <i>Macromolecules</i> , 1987 , 20, 438-440	5.5	17
85	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	3.6	17
84	Protein-peptide docking using CABS-dock and contact information. <i>Briefings in Bioinformatics</i> , 2019 , 20, 2299-2305	13.4	17
83	Preformed template fluctuations promote fibril formation: insights from lattice and all-atom models. <i>Journal of Chemical Physics</i> , 2015 , 142, 145104	3.9	16
82	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	3.9	16
81	Tertiary structure prediction of the KIX domain of CBP using Monte Carlo simulations driven by restraints derived from multiple sequence alignments. <i>Proteins: Structure, Function and Bioinformatics</i> , 1998 , 30, 287-94	4.2	16
80	Use of residual dipolar couplings as restraints in ab initio protein structure prediction. <i>Biopolymers</i> , 2003 , 70, 548-62	2.2	16
79	BioShell-Threading: versatile Monte Carlo package for protein 3D threading. <i>BMC Bioinformatics</i> , 2014 , 15, 22	3.6	15
78	Reduced protein models and their application to the protein folding problem. <i>Journal of Biomolecular Structure and Dynamics</i> , 1998 , 16, 381-96	3.6	15
77	Folding simulations and computer redesign of protein A three-helix bundle motifs. <i>Proteins: Structure, Function and Bioinformatics</i> , 1996 , 25, 286-99	4.2	15
76	Protein Folding: Flexible Lattice Models. <i>Progress of Theoretical Physics Supplement</i> , 2000 , 138, 292-300		14
75	Contact prediction in protein modeling: scoring, folding and refinement of coarse-grained models. <i>BMC Structural Biology</i> , 2008 , 8, 36	2.7	13
74	Comparative modeling without implicit sequence alignments. <i>Bioinformatics</i> , 2007 , 23, 2522-7	7.2	13
73	Role of Resultant Dipole Moment in Mechanical Dissociation of Biological Complexes. <i>Molecules</i> , 2018 , 23,	4.8	13
72	SURPASS Low-Resolution Coarse-Grained Protein Modeling. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 5766-5779	6.4	12
71	Modeling EphB4-EphrinB2 protein-protein interaction using flexible docking of a short linear motif. <i>BioMedical Engineering OnLine</i> , 2017 , 16, 71	4.1	12
70	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	6.1	12
69	A structure-based model fails to probe the mechanical unfolding pathways of the titin I27 domain. <i>Journal of Chemical Physics</i> , 2013 , 139, 065103	3.9	12

68	Analysis and optimization of interactions between peptides mimicking the GD2 ganglioside and the monoclonal antibody 14G2a. <i>International Journal of Molecular Medicine</i> , 2011 , 28, 47-57	4.4	12
67	Elastic network normal modes provide a basis for protein structure refinement. <i>Journal of Chemical Physics</i> , 2012 , 136, 195101	3.9	12
66	A minimal proteinlike lattice model: an alpha-helix motif. <i>Journal of Chemical Physics</i> , 2005 , 122, 214915	3.9	12
65	Numerical study of the entropy loss of dimerization and the folding thermodynamics of the GCN4 leucine zipper. <i>Biophysical Journal</i> , 2002 , 83, 2801-11	2.9	12
64	Helix-coil and beta sheet-coil transitions in a simplified, yet realistic protein model. <i>Macromolecular Theory and Simulations</i> , 2000 , 9, 523-533	1.5	12
63	Multiscale Approach to Protein Folding Dynamics 2011 , 281-293		11
62	Predicting the complex structure and functional motions of the outer membrane transporter and signal transducer FecA. <i>Biophysical Journal</i> , 2008 , 94, 2482-91	2.9	11
61	Ideal amino acid exchange forms for approximating substitution matrices. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007 , 69, 379-93	4.2	11
60	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, 717-21	1.9	11
59	Protocols for efficient simulations of long-time protein dynamics using coarse-grained CABS model. <i>Methods in Molecular Biology</i> , 2014 , 1137, 235-50	1.4	11
58	Coarse-Grained Modeling of Peptide Docking Associated with Large Conformation Transitions of the Binding Protein: Troponin I Fragment-Troponin C System. <i>Molecules</i> , 2015 , 20, 10763-80	4.8	10
57	CABS-NMR--De novo tool for rapid global fold determination from chemical shifts, residual dipolar couplings and sparse methyl-methyl NOEs. <i>Journal of Computational Chemistry</i> , 2011 , 32, 536-44	3.5	10
56	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		10
55	Denatured proteins and early folding intermediates simulated in a reduced conformational space. <i>Acta Biochimica Polonica</i> , 2006 , 53, 131-44	2	10
54	Coarse-grained Monte Carlo simulations of mucus: structure, dynamics, and thermodynamics. <i>Biophysical Journal</i> , 2010 , 99, 3507-16	2.9	9
53	Theoretical study of molecular mechanism of binding TRAP220 coactivator to Retinoid X Receptor alpha, activated by 9-cis retinoic acid. <i>Journal of Steroid Biochemistry and Molecular Biology</i> , 2010 , 121, 124-9	5.1	9
52	A simple technique to estimate partition functions and equilibrium constants from Monte Carlo simulations. <i>Journal of Chemical Physics</i> , 1995 , 102, 6189-6193	3.9	9
51	Switch from thermal to force-driven pathways of protein refolding. <i>Journal of Chemical Physics</i> , 2017 , 146, 135101	3.9	8

50	Improving thermal stability of thermophilic L-threonine aldolase from <i>Thermotoga maritima</i> . <i>Journal of Biotechnology</i> , 2015 , 199, 69-76	3.7	8
49	BioShell Threader: protein homology detection based on sequence profiles and secondary structure profiles. <i>Nucleic Acids Research</i> , 2012 , 40, W257-62	20.1	8
48	Improved method for prediction of protein backbone U-turn positions and major secondary structural elements between U-turns. <i>Proteins: Structure, Function and Bioinformatics</i> , 1997 , 29, 443-60	4.2	8
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