## Andrzej Kolinski

# List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

9,489 90 211 52 h-index g-index citations papers 6.53 10,521 5.2 223 L-index avg, IF ext. citations ext. papers

#	Paper	IF	Citations
211	Protein-Protein Docking with Large-Scale Backbone Flexibility Using Coarse-Grained Monte-Carlo Simulations. <i>International Journal of Molecular Sciences</i> , <b>2021</b> , 22,	6.3	2
<b>2</b> 10	Flexible docking of peptides to proteins using CABS-dock. <i>Protein Science</i> , <b>2020</b> , 29, 211-222	6.3	24
209	Computational reconstruction of atomistic protein structures from coarse-grained models. Computational and Structural Biotechnology Journal, <b>2020</b> , 18, 162-176	6.8	24
208	Protocols for All-Atom Reconstruction and High-Resolution Refinement of Protein-Peptide Complex Structures. <i>Methods in Molecular Biology</i> , <b>2020</b> , 2165, 273-287	1.4	4
207	Protocols for Fast Simulations of Protein Structure Flexibility Using CABS-Flex and SURPASS. <i>Methods in Molecular Biology</i> , <b>2020</b> , 2165, 337-353	1.4	4
206	CABS-dock standalone: a toolbox for flexible protein-peptide docking. <i>Bioinformatics</i> , <b>2019</b> , 35, 4170-41	172	25
205	Modeling of Disordered Protein Structures Using Monte Carlo Simulations and Knowledge-Based Statistical Force Fields. <i>International Journal of Molecular Sciences</i> , <b>2019</b> , 20,	6.3	24
204	CABS-flex standalone: a simulation environment for fast modeling of protein flexibility. <i>Bioinformatics</i> , <b>2019</b> , 35, 694-695	7.2	45
203	Protein modeling and structure prediction with a reduced representation <i>Acta Biochimica Polonica</i> , <b>2019</b> , 51, 349-371	2	221
202	Denatured proteins and early folding intermediates simulated in a reduced conformational space <i>Acta Biochimica Polonica</i> , <b>2019</b> , 53, 131-143	2	23
201	Protein Structure Prediction Using Coarse-Grained Models. <i>Springer Series on Bio- and Neurosystems</i> , <b>2019</b> , 27-59	0.5	2
200	Explicit-Solvent All-Atom Molecular Dynamics of Peptide Aggregation. <i>Springer Series on Bio- and Neurosystems</i> , <b>2019</b> , 541-558	0.5	
199	Protein Dynamics Simulations Using Coarse-Grained Models. <i>Springer Series on Bio- and Neurosystems</i> , <b>2019</b> , 61-87	0.5	1
198	Protein-peptide docking using CABS-dock and contact information. <i>Briefings in Bioinformatics</i> , <b>2019</b> , 20, 2299-2305	13.4	17
197	Explicit Solvent Molecular Dynamics Simulations of Self-Assembling Amyloidogenic Peptides. Biophysical Journal, <b>2018</b> , 114, 230a	2.9	
196	Coarse-Grained Modeling of the Interplay between Secondary Structure Propensities and Protein Fold Assembly. <i>Journal of Chemical Theory and Computation</i> , <b>2018</b> , 14, 2277-2287	6.4	5
195	Protein-peptide docking: opportunities and challenges. <i>Drug Discovery Today</i> , <b>2018</b> , 23, 1530-1537	8.8	118

### (2016-2018)

194	Kinetics and mechanical stability of the fibril state control fibril formation time of polypeptide chains: A computational study. <i>Journal of Chemical Physics</i> , <b>2018</b> , 148, 215106	3.9	16
193	Modeling of Protein Structural Flexibility and Large-Scale Dynamics: Coarse-Grained Simulations and Elastic Network Models. <i>International Journal of Molecular Sciences</i> , <b>2018</b> , 19,	6.3	37
192	Role of Resultant Dipole Moment in Mechanical Dissociation of Biological Complexes. <i>Molecules</i> , <b>2018</b> , 23,	4.8	13
191	CABS-flex 2.0: a web server for fast simulations of flexibility of protein structures. <i>Nucleic Acids Research</i> , <b>2018</b> , 46, W338-W343	20.1	118
190	Highly Flexible Protein-Peptide Docking Using CABS-Dock. <i>Methods in Molecular Biology</i> , <b>2017</b> , 1561, 69-94	1.4	24
189	Switch from thermal to force-driven pathways of protein refolding. <i>Journal of Chemical Physics</i> , <b>2017</b> , 146, 135101	3.9	8
188	SURPASS Low-Resolution Coarse-Grained Protein Modeling. <i>Journal of Chemical Theory and Computation</i> , <b>2017</b> , 13, 5766-5779	6.4	12
187	Modeling EphB4-EphrinB2 protein-protein interaction using flexible docking of a short linear motif. <i>BioMedical Engineering OnLine</i> , <b>2017</b> , 16, 71	4.1	12
186	A protocol for CABS-dock protein-peptide docking driven by side-chain contact information. <i>BioMedical Engineering OnLine</i> , <b>2017</b> , 16, 73	4.1	5
185	Toward more efficient simulations of slow processes in large biomolecular systems: Comment on "Ligand diffusion in proteins via enhanced sampling in molecular dynamics" by Jakub Rydzewski and Wieslaw Nowak. <i>Physics of Life Reviews</i> , <b>2017</b> , 22-23, 75-76	2.1	4
184	One-Dimensional Structural Properties of Proteins in the Coarse-Grained CABS Model. <i>Methods in Molecular Biology</i> , <b>2017</b> , 1484, 83-113	1.4	7
183	Predicting Real-Valued Protein Residue Fluctuation Using FlexPred. <i>Methods in Molecular Biology</i> , <b>2017</b> , 1484, 175-186	1.4	3
182	The GOR Method of Protein Secondary Structure Prediction and Its Application as a Protein Aggregation Prediction Tool. <i>Methods in Molecular Biology</i> , <b>2017</b> , 1484, 7-24	1.4	20
181	Coarse-Grained Simulations of Membrane Insertion and Folding of Small Helical Proteins Using the CABS Model. <i>Journal of Chemical Information and Modeling</i> , <b>2016</b> , 56, 2207-2215	6.1	12
180	Coarse-Grained Protein Models and Their Applications. <i>Chemical Reviews</i> , <b>2016</b> , 116, 7898-936	68.1	489
179	Modeling of protein-peptide interactions using the CABS-dock web server for binding site search and flexible docking. <i>Methods</i> , <b>2016</b> , 93, 72-83	4.6	104
178	Ensemble-based evaluation for protein structure models. <i>Bioinformatics</i> , <b>2016</b> , 32, i314-i321	7.2	5
177	Protein secondary structure prediction using a small training set (compact model) combined with a Complex-valued neural network approach. <i>BMC Bioinformatics</i> , <b>2016</b> , 17, 362	3.6	17

176	Protein-peptide molecular docking with large-scale conformational changes: the p53-MDM2 interaction. <i>Scientific Reports</i> , <b>2016</b> , 6, 37532	4.9	33
175	5-HT2 receptor affinity, docking studies and pharmacological evaluation of a series of 1,3-disubstituted thiourea derivatives. <i>European Journal of Medicinal Chemistry</i> , <b>2016</b> , 116, 173-186	6.8	18
174	Improving thermal stability of thermophilic L-threonine aldolase from Thermotoga maritima. <i>Journal of Biotechnology</i> , <b>2015</b> , 199, 69-76	3.7	8
173	Preformed template fluctuations promote fibril formation: insights from lattice and all-atom models. <i>Journal of Chemical Physics</i> , <b>2015</b> , 142, 145104	3.9	16
172	Coarse-Grained Modeling of Peptide Docking Associated with Large Conformation Transitions of the Binding Protein: Troponin I Fragment-Troponin C System. <i>Molecules</i> , <b>2015</b> , 20, 10763-80	4.8	10
171	CABS-dock web server for the flexible docking of peptides to proteins without prior knowledge of the binding site. <i>Nucleic Acids Research</i> , <b>2015</b> , 43, W419-24	20.1	237
170	Mechanism of Folding and Binding of an Intrinsically Disordered Protein As Revealed by ab Initio Simulations. <i>Journal of Chemical Theory and Computation</i> , <b>2014</b> , 10, 2224-31	6.4	29
169	CABS-flex predictions of protein flexibility compared with NMR ensembles. <i>Bioinformatics</i> , <b>2014</b> , 30, 2150-4	7.2	48
168	BioShell-Threading: versatile Monte Carlo package for protein 3D threading. <i>BMC Bioinformatics</i> , <b>2014</b> , 15, 22	3.6	15
167	Coarse-Grained Protein Models in Structure Prediction. <i>Springer Series in Bio-/neuroinformatics</i> , <b>2014</b> , 25-53		
166	Coarse-Grained Modeling of Protein Dynamics. Springer Series in Bio-/neuroinformatics, 2014, 55-79		7
165	Protocols for efficient simulations of long-time protein dynamics using coarse-grained CABS model. <i>Methods in Molecular Biology</i> , <b>2014</b> , 1137, 235-50	1.4	11
164	A structure-based model fails to probe the mechanical unfolding pathways of the titin I27 domain. Journal of Chemical Physics, <b>2013</b> , 139, 065103	3.9	12
163	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> , <b>2013</b> , 9, 119	-2 <del>5</del> 4	63
162	ClusCo: clustering and comparison of protein models. <i>BMC Bioinformatics</i> , <b>2013</b> , 14, 62	3.6	25
161	Combining coarse-grained protein models with replica-exchange all-atom molecular dynamics.  International Journal of Molecular Sciences, 2013, 14, 9893-905	6.3	20
160	CABS-flex: Server for fast simulation of protein structure fluctuations. <i>Nucleic Acids Research</i> , <b>2013</b> , 41, W427-31	20.1	98
159	CABS-fold: Server for the de novo and consensus-based prediction of protein structure. <i>Nucleic Acids Research</i> , <b>2013</b> , 41, W406-11	20.1	75

### (2010-2012)

158	Optimization of profile-to-profile alignment parameters for one-dimensional threading. <i>Journal of Computational Biology</i> , <b>2012</b> , 19, 879-86	1.7	4
157	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> , <b>2012</b> , 116, 7026-32	3.4	27
156	Coarse-grained modeling of mucus barrier properties. <i>Biophysical Journal</i> , <b>2012</b> , 102, 195-200	2.9	19
155	How noise in force fields can affect the structural refinement of protein models?. <i>Proteins:</i> Structure, Function and Bioinformatics, <b>2012</b> , 80, 335-41	4.2	6
154	Optimization of protein models. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , <b>2012</b> , 2, 479-493	7.9	27
153	Structural features that predict real-value fluctuations of globular proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2012</b> , 80, 1425-35	4.2	18
152	Elastic network normal modes provide a basis for protein structure refinement. <i>Journal of Chemical Physics</i> , <b>2012</b> , 136, 195101	3.9	12
151	BioShell Threader: protein homology detection based on sequence profiles and secondary structure profiles. <i>Nucleic Acids Research</i> , <b>2012</b> , 40, W257-62	20.1	8
150	Lattice Polymers and Protein Models <b>2011</b> , 1-20		
149	Multiscale Approach to Protein Folding Dynamics <b>2011</b> , 281-293		11
149	Multiscale Approach to Protein Folding Dynamics <b>2011</b> , 281-293  Analysis and optimization of interactions between peptides mimicking the GD2 ganglioside and the monoclonal antibody 14G2a. <i>International Journal of Molecular Medicine</i> , <b>2011</b> , 28, 47-57	4.4	11
	Analysis and optimization of interactions between peptides mimicking the GD2 ganglioside and the	4.4	
148	Analysis and optimization of interactions between peptides mimicking the GD2 ganglioside and the monoclonal antibody 14G2a. <i>International Journal of Molecular Medicine</i> , <b>2011</b> , 28, 47-57  Multibody coarse-grained potentials for native structure recognition and quality assessment of		12
148	Analysis and optimization of interactions between peptides mimicking the GD2 ganglioside and the monoclonal antibody 14G2a. <i>International Journal of Molecular Medicine</i> , <b>2011</b> , 28, 47-57  Multibody coarse-grained potentials for native structure recognition and quality assessment of protein models. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2011</b> , 79, 1923-9  CABS-NMRDe novo tool for rapid global fold determination from chemical shifts, residual dipolar	4.2	12 36 10
148 147 146	Analysis and optimization of interactions between peptides mimicking the GD2 ganglioside and the monoclonal antibody 14G2a. <i>International Journal of Molecular Medicine</i> , <b>2011</b> , 28, 47-57  Multibody coarse-grained potentials for native structure recognition and quality assessment of protein models. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2011</b> , 79, 1923-9  CABS-NMRDe novo tool for rapid global fold determination from chemical shifts, residual dipolar couplings and sparse methyl-methyl NOEs. <i>Journal of Computational Chemistry</i> , <b>2011</b> , 32, 536-44  Simulation of chaperonin effect on protein folding: a shift from nucleation-condensation to	4.2 3.5	12 36 10
148 147 146	Analysis and optimization of interactions between peptides mimicking the GD2 ganglioside and the monoclonal antibody 14G2a. <i>International Journal of Molecular Medicine</i> , <b>2011</b> , 28, 47-57  Multibody coarse-grained potentials for native structure recognition and quality assessment of protein models. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2011</b> , 79, 1923-9  CABS-NMRDe novo tool for rapid global fold determination from chemical shifts, residual dipolar couplings and sparse methyl-methyl NOEs. <i>Journal of Computational Chemistry</i> , <b>2011</b> , 32, 536-44  Simulation of chaperonin effect on protein folding: a shift from nucleation-condensation to framework mechanism. <i>Journal of the American Chemical Society</i> , <b>2011</b> , 133, 10283-9  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</i>	4.2 3.5 16.4	12 36 10 38
148 147 146 145	Analysis and optimization of interactions between peptides mimicking the GD2 ganglioside and the monoclonal antibody 14G2a. <i>International Journal of Molecular Medicine</i> , <b>2011</b> , 28, 47-57  Multibody coarse-grained potentials for native structure recognition and quality assessment of protein models. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2011</b> , 79, 1923-9  CABS-NMRDe novo tool for rapid global fold determination from chemical shifts, residual dipolar couplings and sparse methyl-methyl NOEs. <i>Journal of Computational Chemistry</i> , <b>2011</b> , 32, 536-44  Simulation of chaperonin effect on protein folding: a shift from nucleation-condensation to framework mechanism. <i>Journal of the American Chemical Society</i> , <b>2011</b> , 133, 10283-9  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> , <b>2011</b> , 108, 9443-8	4.2 3.5 16.4	12 36 10 38

140	Modeling of loops in proteins: a multi-method approach. BMC Structural Biology, 2010, 10, 5	2.7	32
139	TRACER. A new approach to comparative modeling that combines threading with free-space conformational sampling. <i>Acta Biochimica Polonica</i> , <b>2010</b> , 57, 125-33	2	3
138	Distance matrix-based approach to protein structure prediction. <i>Journal of Structural and Functional Genomics</i> , <b>2009</b> , 10, 67-81		36
137	Template-Free Predictions of Three-Dimensional Protein Structures: From First Principles to Knowledge-Based Potentials <b>2008</b> , 117-141		1
136	Predicting the complex structure and functional motions of the outer membrane transporter and signal transducer FecA. <i>Biophysical Journal</i> , <b>2008</b> , 94, 2482-91	2.9	11
135	Folding pathway of the b1 domain of protein G explored by multiscale modeling. <i>Biophysical Journal</i> , <b>2008</b> , 94, 726-36	2.9	85
134	Utility library for structural bioinformatics. <i>Bioinformatics</i> , <b>2008</b> , 24, 584-5	7.2	35
133	Uncharacterized DUF1574 leptospira proteins are SGNH hydrolases. <i>Cell Cycle</i> , <b>2008</b> , 7, 542-4	4.7	4
132	Fast and accurate methods for predicting short-range constraints in protein models. <i>Journal of Computer-Aided Molecular Design</i> , <b>2008</b> , 22, 783-8	4.2	
131	Contact prediction in protein modeling: scoring, folding and refinement of coarse-grained models. <i>BMC Structural Biology</i> , <b>2008</b> , 8, 36	2.7	13
130	AAindex: amino acid index database, progress report 2008. <i>Nucleic Acids Research</i> , <b>2008</b> , 36, D202-5	20.1	623
129	Why do proteins divide into domains? Insights from lattice model simulations. <i>Biomacromolecules</i> , <b>2007</b> , 8, 3519-24	6.9	2
128	Dynamics of Dense Polymer Systems: Computer Simulations and Analytic Theories. <i>Advances in Chemical Physics</i> , <b>2007</b> , 223-278		48
127	Backbone building from quadrilaterals: a fast and accurate algorithm for protein backbone reconstruction from alpha carbon coordinates. <i>Journal of Computational Chemistry</i> , <b>2007</b> , 28, 1593-159	7 <sup>3.5</sup>	90
126	Protein structure prediction: combining de novo modeling with sparse experimental data. <i>Journal of Computational Chemistry</i> , <b>2007</b> , 28, 1668-76	3.5	22
125	Towards the high-resolution protein structure prediction. Fast refinement of reduced models with all-atom force field. <i>BMC Structural Biology</i> , <b>2007</b> , 7, 43	2.7	44
124	Type II restriction endonuclease R.Eco29kI is a member of the GIY-YIG nuclease superfamily. <i>BMC Structural Biology</i> , <b>2007</b> , 7, 48	2.7	27
123	Ideal amino acid exchange forms for approximating substitution matrices. <i>Proteins: Structure,</i> Function and Bioinformatics, <b>2007</b> , 69, 379-93	4.2	11

122	Hierarchical modeling of protein interactions. <i>Journal of Molecular Modeling</i> , <b>2007</b> , 13, 691-8	2	17
121	Efficient scheme for optimization of parallel tempering Monte Carlo method. <i>Journal of Physics Condensed Matter</i> , <b>2007</b> , 19, 036225	1.8	21
120	Comparative modeling without implicit sequence alignments. <i>Bioinformatics</i> , <b>2007</b> , 23, 2522-7	7.2	13
119	Characterization of protein-folding pathways by reduced-space modeling. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2007</b> , 104, 12330-5	11.5	78
118	T-Pilea package for thermodynamic calculations for biomolecules. <i>Bioinformatics</i> , <b>2007</b> , 23, 1840-2	7.2	2
117	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> , <b>2007</b> , 103, 357-60	5.1	18
116	BioShella package of tools for structural biology computations. <i>Bioinformatics</i> , <b>2006</b> , 22, 621-2	7.2	42
115	Denatured proteins and early folding intermediates simulated in a reduced conformational space. <i>Acta Biochimica Polonica</i> , <b>2006</b> , 53, 131-44	2	10
114	Ab initio Modeling <b>2005</b> , 137-161		
113	Protein Folding with a Reduced Model and Inaccurate Short-Range Restraints. <i>Macromolecular Theory and Simulations</i> , <b>2005</b> , 14, 444-451	1.5	6
112	Protein structure prediction by tempering spatial constraints. <i>Journal of Computer-Aided Molecular Design</i> , <b>2005</b> , 19, 603-8	4.2	2
111	Exploring protein energy landscapes with hierarchical clustering. <i>International Journal of Quantum Chemistry</i> , <b>2005</b> , 105, 826-830	2.1	19
110	Inferring ideal amino acid interaction forms from statistical protein contact potentials. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2005</b> , 59, 49-57	4.2	55
109	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> , <b>2005</b> , 61 Suppl 7, 84-	9 <del>0</del> .2	92
108	DNA vaccine expressing the mimotope of GD2 ganglioside induces protective GD2 cross-reactive antibody responses. <i>Cancer Research</i> , <b>2005</b> , 65, 3410-8	10.1	53
107	HCPMprogram for hierarchical clustering of protein models. <i>Bioinformatics</i> , <b>2005</b> , 21, 3179-80	7.2	29
106	A minimal proteinlike lattice model: an alpha-helix motif. <i>Journal of Chemical Physics</i> , <b>2005</b> , 122, 21491	5 3.0	12
	Trimmind procentine tacase models an alpha field model. Southat of chemical rhysics, 2005, 122, 21151	- 5.9	

104	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> , <b>2005</b> , 102, 7835-40	11.5	47
103	Protein modeling with reduced representation: statistical potentials and protein folding mechanism <i>Acta Biochimica Polonica</i> , <b>2005</b> , 52, 741-748	2	5
102	Reduced models of proteins and their applications. <i>Polymer</i> , <b>2004</b> , 45, 511-524	3.9	159
101	Protein fragment reconstruction using various modeling techniques. <i>Journal of Computer-Aided Molecular Design</i> , <b>2003</b> , 17, 725-38	4.2	72
100	A simple lattice model that exhibits a protein-like cooperative all-or-none folding transition. <i>Biopolymers</i> , <b>2003</b> , 69, 399-405	2.2	17
99	Use of residual dipolar couplings as restraints in ab initio protein structure prediction. <i>Biopolymers</i> , <b>2003</b> , 70, 548-62	2.2	16
98	TOUCHSTONEX: protein structure prediction with sparse NMR data. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2003</b> , 53, 290-306	4.2	35
97	TOUCHSTONE: a unified approach to protein structure prediction. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2003</b> , 53 Suppl 6, 469-79	4.2	69
96	TOUCHSTONE II: a new approach to ab initio protein structure prediction. <i>Biophysical Journal</i> , <b>2003</b> , 85, 1145-64	2.9	223
95	Unfolding of globular proteins: monte carlo dynamics of a realistic reduced model. <i>Biophysical Journal</i> , <b>2003</b> , 85, 3271-8	2.9	8
94	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> , <b>2003</b> , 84, 1518-26	2.9	46
93	Ab initio protein structure prediction on a genomic scale: application to the Mycoplasma genitalium genome. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , <b>2002</b> , 99, 5993	3- <del>8</del> 1.5	39
92	Numerical study of the entropy loss of dimerization and the folding thermodynamics of the GCN4 leucine zipper. <i>Biophysical Journal</i> , <b>2002</b> , 83, 2801-11	2.9	12
91	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> , <b>2002</b> , 45, 3366-80	8.3	62
90	A Unified Approach to the Prediction of Protein Structure and Function. <i>Advances in Chemical Physics</i> , <b>2002</b> , 131-192		7
89	Computer simulations of protein folding with a small number of distance restraints <i>Acta Biochimica Polonica</i> , <b>2002</b> , 49, 683-692	2	2
88	Model of three-dimensional structure of vitamin D receptor and its binding mechanism with 1alpha,25-dihydroxyvitamin D(3). <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2001</b> , 44, 188-99	4.2	17
87	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> <b>2001</b> 14 717-21	1.9	11

86	A new combination of replica exchange Monte Carlo and histogram analysis for protein folding and thermodynamics. <i>Journal of Chemical Physics</i> , <b>2001</b> , 115, 1569-1574	3.9	27
85	Ab initio protein structure prediction via a combination of threading, lattice folding, clustering, and structure refinement. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2001</b> , Suppl 5, 149-56	4.2	58
84	Computer simulations of the properties of the 🛭, 🖺 C, and 🗓 D de novo designed helical proteins <b>2000</b> , 38, 17-28		6
83	Derivation of protein-specific pair potentials based on weak sequence fragment similarity <b>2000</b> , 38, 3-16	5	84
82	Accurate reconstruction of all-atom protein representations from side-chain-based low-resolution models. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2000</b> , 41, 86-97	4.2	8o
81	Helix-coil and beta sheet-coil transitions in a simplified, yet realistic protein model. <i>Macromolecular Theory and Simulations</i> , <b>2000</b> , 9, 523-533	1.5	12
80	Structural genomics and its importance for gene function analysis. <i>Nature Biotechnology</i> , <b>2000</b> , 18, 283-7	<b>7</b> 44.5	177
79	Protein Folding: Flexible Lattice Models. <i>Progress of Theoretical Physics Supplement</i> , <b>2000</b> , 138, 292-300		14
78	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> , <b>2000</b> , 113, 5065	3.9	62
77	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> , <b>2000</b> , 122, 8392-8402	16.4	35
76	De novo predictions of the quaternary structure of leucine zippers and other coiled coils. <i>International Journal of Quantum Chemistry</i> , <b>1999</b> , 75, 165-176	2.1	4
75	Ab initio folding of proteins using restraints derived from evolutionary information. <i>Proteins:</i> Structure, Function and Bioinformatics, <b>1999</b> , 37, 177-185	4.2	89
74	Correlation between knowledge-based and detailed atomic potentials: Application to the unfolding of the GCN4 leucine zipper. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>1999</b> , 35, 447-452	4.2	29
73	A method for the improvement of threading-based protein models. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>1999</b> , 37, 592-610	4.2	48
72	De novo simulations of the folding thermodynamics of the GCN4 leucine zipper. <i>Biophysical Journal</i> , <b>1999</b> , 77, 54-69	2.9	29
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