

Shoji Takada

List of Publications by Year in descending order

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Version: 2024-02-01

140
papers

6,315
citations

94269

37
h-index

74018

75
g-index

162
all docs

162
docs citations

162
times ranked

4717
citing authors

#	ARTICLE	IF	CITATIONS
1	Cooperation among c-subunits of FoF1-ATP synthase in rotation-coupled proton translocation. <i>ELife</i> , 2022, 11, .	2.8	4
2	Implementation of residue-level coarse-grained models in GENESIS for large-scale molecular dynamics simulations. <i>PLoS Computational Biology</i> , 2022, 18, e1009578.	1.5	27
3	Coarse-grained molecular dynamics simulations of base-pair mismatch recognition protein MutS sliding along DNA. <i>Biophysics and Physicobiology</i> , 2022, 19, .	0.5	2
4	Inferring Conformational State of Myosin Motor in an Atomic Force Microscopy Image via Flexible Fitting Molecular Simulations. <i>Frontiers in Molecular Biosciences</i> , 2022, 9, 882989.	1.6	4
5	Using incomplete Cholesky factorization to increase the time step in molecular dynamics simulations. <i>Journal of Computational and Applied Mathematics</i> , 2022, 415, 114519.	1.1	1
6	Coarse-grained Biomolecular Simulations. <i>Seibutsu Butsuri</i> , 2021, 61, 144-151.	0.0	0
7	Linker DNA Length is a Key to Tri-nucleosome Folding. <i>Journal of Molecular Biology</i> , 2021, 433, 166792.	2.0	8
8	Case Report: Bayesian Statistical Inference of Experimental Parameters via Biomolecular Simulations: Atomic Force Microscopy. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 636940.	1.6	10
9	Role of bacterial RNA polymerase gate opening dynamics in DNA loading and antibiotics inhibition elucidated by quasi-Markov State Model. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	30
10	Opening of cohesin's SMC ring is essential for timely DNA replication and DNA loop formation. <i>Cell Reports</i> , 2021, 35, 108999.	2.9	12
11	The kinetic landscape of nucleosome assembly: A coarse-grained molecular dynamics study. <i>PLoS Computational Biology</i> , 2021, 17, e1009253.	1.5	19
12	Rigid-body fitting to atomic force microscopy images for inferring probe shape and biomolecular structure. <i>PLoS Computational Biology</i> , 2021, 17, e1009215.	1.5	14
13	Modeling of DNA binding to the condensin hinge domain using molecular dynamics simulations guided by atomic force microscopy. <i>PLoS Computational Biology</i> , 2021, 17, e1009265.	1.5	4
14	The lane-switch mechanism for nucleosome repositioning by DNA translocase. <i>Nucleic Acids Research</i> , 2021, 49, 9066-9076.	6.5	5
15	Testing mechanisms of DNA sliding by architectural DNA-binding proteins: dynamics of single wild-type and mutant protein molecules <i>in vitro</i> and <i>in vivo</i> . <i>Nucleic Acids Research</i> , 2021, 49, 8642-8664.	6.5	11
16	Semi-Implicit Time Integration with Hessian Eigenvalue Corrections for a Larger Time Step in Molecular Dynamics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5792-5804.	2.3	2
17	Modeling lipid-protein interactions for coarse-grained lipid and $\text{C}\pm$ protein models. <i>Journal of Chemical Physics</i> , 2021, 155, 155101.	1.2	3
18	Modeling DNA Opening in the Eukaryotic Transcription Initiation Complexes via Coarse-Grained Models. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 772486.	1.6	4

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19	Nucleosomes as allosteric scaffolds for genetic regulation. <i>Current Opinion in Structural Biology</i> , 2020, 62, 93-101.	2.6	14
20	The HMGB chromatin protein Nhp6A can bypass obstacles when traveling on DNA. <i>Nucleic Acids Research</i> , 2020, 48, 10820-10831.	6.5	14
21	How Cytoplasmic Dynein Couples ATP Hydrolysis Cycle to Diverse Stepping Motions: Kinetic Modeling. <i>Biophysical Journal</i> , 2020, 118, 1930-1945.	0.2	4
22	Nucleosome allostery in pioneer transcription factor binding. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 20586-20596.	3.3	57
23	Resolving the data asynchronicity in high-speed atomic force microscopy measurement via the Kalman Smoother. <i>Scientific Reports</i> , 2020, 10, 18393.	1.6	9
24	Particle Filter Method to Integrate High-Speed Atomic Force Microscopy Measurements with Biomolecular Simulations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 6609-6619.	2.3	12
25	Molecular dynamics simulation of proton-transfer coupled rotations in ATP synthase FO motor. <i>Scientific Reports</i> , 2020, 10, 8225.	1.6	34
26	Flexible Fitting of Biomolecular Structures to Atomic Force Microscopy Images via Biased Molecular Simulations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 1349-1358.	2.3	38
27	Coarse-grained implicit solvent lipid force field with a compatible resolution to the C \pm protein representation. <i>Journal of Chemical Physics</i> , 2020, 153, 205101.	1.2	7
28	Overcoming the Bottleneck of the Enzymatic Cycle by Steric Frustration. <i>Physical Review Letters</i> , 2019, 122, 238102.	2.9	24
29	Nucleosome Crowding in Chromatin Slows the Diffusion but Can Promote Target Search of Proteins. <i>Biophysical Journal</i> , 2019, 116, 2285-2295.	0.2	17
30	GÅ•model revisited. <i>Biophysics and Physicobiology</i> , 2019, 16, 248-255.	0.5	40
31	DNA sliding in nucleosomes via twist defect propagation revealed by molecular simulations. <i>Nucleic Acids Research</i> , 2018, 46, 2788-2801.	6.5	77
32	Reconstruction of Atomistic Structures from Coarse-Grained Models for Proteinâ€“DNA Complexes. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1682-1694.	2.3	27
33	Interactions of HP1 Bound to H3K9me3 Dinucleosome by Molecular Simulations and Biochemical Assays. <i>Biophysical Journal</i> , 2018, 114, 2336-2351.	0.2	28
34	Chromatin remodelers couple inchworm motion with twist-defect formation to slide nucleosomal DNA. <i>PLoS Computational Biology</i> , 2018, 14, e1006512.	1.5	39
35	Dynamic and Structural Modeling of the Specificity in Proteinâ€“DNA Interactions Guided by Binding Assay and Structure Data. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3877-3889.	2.3	27
36	How one-dimensional diffusion of transcription factors are affected by obstacles: coarse-grained molecular dynamics study. <i>Molecular Simulation</i> , 2017, 43, 1315-1321.	0.9	7

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37	Allosteric conformational change cascade in cytoplasmic dynein revealed by structure-based molecular simulations. <i>PLoS Computational Biology</i> , 2017, 13, e1005748.	1.5	29
38	Sequence-dependent nucleosome sliding in rotation-coupled and uncoupled modes revealed by molecular simulations. <i>PLoS Computational Biology</i> , 2017, 13, e1005880.	1.5	50
39	The structural basis of a high affinity ATP binding $\hat{\mu}$ subunit from a bacterial ATP synthase. <i>PLoS ONE</i> , 2017, 12, e0177907.	1.1	13
40	Near-atomic structural model for bacterial DNA replication initiation complex and its functional insights. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, E8021-E8030.	3.3	56
41	Histone acetylation dependent energy landscapes in tri-nucleosome revealed by residue-resolved molecular simulations. <i>Scientific Reports</i> , 2016, 6, 34441.	1.6	31
42	Dynamic Coupling among Protein Binding, Sliding, and DNA Bending Revealed by Molecular Dynamics. <i>Journal of the American Chemical Society</i> , 2016, 138, 8512-8522.	6.6	63
43	On the ATP binding site of the $\hat{\mu}$ subunit from bacterial F-type ATP synthases. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2016, 1857, 332-340.	0.5	14
44	p53 dynamics upon response element recognition explored by molecular simulations. <i>Scientific Reports</i> , 2015, 5, 17107.	1.6	30
45	How Co-translational Folding of Multi-domain Protein Is Affected by Elongation Schedule: Molecular Simulations. <i>PLoS Computational Biology</i> , 2015, 11, e1004356.	1.5	22
46	Partial Unwrapping and Histone Tail Dynamics in Nucleosome Revealed by Coarse-Grained Molecular Simulations. <i>PLoS Computational Biology</i> , 2015, 11, e1004443.	1.5	73
47	On the Mg ²⁺ binding site of the $\hat{\mu}$ subunit from bacterial F-type ATP synthases. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2015, 1847, 1101-1112.	0.5	9
48	Dimer domain swapping versus monomer folding in apo-myoglobin studied by molecular simulations. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 5006-5013.	1.3	16
49	Couplings between hierarchical conformational dynamics from multi-time correlation functions and two-dimensional lifetime spectra: Application to adenylate kinase. <i>Journal of Chemical Physics</i> , 2015, 142, 212404.	1.2	17
50	Modeling Structural Dynamics of Biomolecular Complexes by Coarse-Grained Molecular Simulations. <i>Accounts of Chemical Research</i> , 2015, 48, 3026-3035.	7.6	134
51	Energy landscape views for interplays among folding, binding, and allostery of calmodulin domains. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 10550-10555.	3.3	150
52	Multi-scale Ensemble Modeling of Modular Proteins with Intrinsically Disordered Linker Regions: Application to p53. <i>Biophysical Journal</i> , 2014, 107, 721-729.	0.2	28
53	RESPAC: Method to Determine Partial Charges in Coarse-Grained Protein Model and Its Application to DNA-Binding Proteins. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 711-721.	2.3	39
54	1P148 Molecular mechanism of the epsilon subunit from F-type ATP synthases studied by Molecular Dynamics simulations(11. Molecular motor,Poster,The 52nd Annual Meeting of the Biophysical Society) Tj ETQq0 000rgBT /Overlock 10		

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55	3P276 Comprehensive analysis of protein folding energy landscape by multicanonical Go-model molecular dynamics simulation(24. Mathematical biology,Poster,The 52nd Annual Meeting of the Tj ETQq1 1 0.784314 rgBT/Overlock 10 Tf 50 462)	0.0	0
56	Protein-specific force field derived from the fragment molecular orbital method can improve protein-ligand binding interactions. Journal of Computational Chemistry, 2013, 34, 1251-1257.	1.5	15
57	Folding Coupled with Assembly in Split Green Fluorescent Proteins Studied by Structure-based Molecular Simulations. Journal of Physical Chemistry B, 2013, 117, 13212-13218.	1.2	9
58	Adenosine Triphosphate Hydrolysis Mechanism in Kinesin Studied by Combined Quantum-Mechanical/Molecular-Mechanical Metadynamics Simulations. Journal of the American Chemical Society, 2013, 135, 8908-8919.	6.6	56
59	Drug Uptake Pathways of Multidrug Transporter AcrB Studied by Molecular Simulations and Site-Directed Mutagenesis Experiments. Journal of the American Chemical Society, 2013, 135, 7474-7485.	6.6	53
60	Structure-based Molecular Simulations Reveal the Enhancement of Biased Brownian Motions in Single-headed Kinesin. PLoS Computational Biology, 2013, 9, e1002907.	1.5	15
61	1P149 The Mg ²⁺ binding site of the ATP synthase μ subunit from Bacillus subtilis derived by Molecular Dynamics simulations(11.Molecular motor,Poster,The 51st Annual Meeting of the Tj ETQq1 1 0.784314 rgBT/Overlock 10 Tf 50 462)	0.0	0
62	3P121 Poly-nucleosome structural dynamics by coarse-grained simulations(05A. Nucleic acid:) Tj ETQq0 0 0 rgBT/Overlock 10 Tf 50 462)	0.0	0
63	2SCP-03 Structure of model chromatin and dynamics of transcription factors studied by coarse-grained simulations(2SCP Functional dynamics of Nucleosome and Chromatin in Nuclear) Tj ETQq1 1 0.784314 rgBT/Overlock 10 Tf 50 462) Seibutsu Butsuri, 2013, 53, S98.	0.0	0
64	Molecular Dynamics Simulations of Biomolecules. Journal of the Society of Mechanical Engineers, 2013, 116, 78-80.	0.0	0
65	Bayesian Parameter Inference by Markov Chain Monte Carlo with Hybrid Fitness Measures: Theory and Test in Apoptosis Signal Transduction Network. PLoS ONE, 2013, 8, e74178.	1.1	5
66	Rigor of cell fate decision by variable p53 pulses and roles of cooperative gene expression by p53. Biophysics (Nagoya-shi, Japan), 2012, 8, 41-50.	0.4	4
67	3PT009 Mono- and poly-nucleosome structural dynamics by coarse-grained simulations(The 50th) Tj ETQq1 1 0.784314 rgBT/Overlock 10 Tf 50 462)	0.0	0
68	3PT011 Diffusion of TFIIIA zinc fingers along DNA studied by molecular simulations(The 50th Annual) Tj ETQq0 0 0 rgBT/Overlock 10 Tf 50 462)	0.0	0
69	Energy landscape and multiroute folding of topologically complex proteins adenylate kinase and 2ouf-knot. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 17789-17794.	3.3	134
70	p53 Searches on DNA by Rotation-Uncoupled Sliding at C-Terminal Tails and Restricted Hopping of Core Domains. Journal of the American Chemical Society, 2012, 134, 14555-14562.	6.6	89
71	Coarse-Grained Structure-Based Model for RNA-Protein Complexes Developed by Fluctuation Matching. Journal of Chemical Theory and Computation, 2012, 8, 3384-3394.	2.3	39
72	Coarse-grained molecular simulations of large biomolecules. Current Opinion in Structural Biology, 2012, 22, 130-137.	2.6	205

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73	Multiscale Ensemble Modeling of Intrinsically Disordered Proteins: p53 N-Terminal Domain. <i>Biophysical Journal</i> , 2011, 101, 1450-1458.	0.2	92
74	Frustration, specific sequence dependence, and nonlinearity in large-amplitude fluctuations of allosteric proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 3504-3509.	3.3	143
75	CafeMol: A Coarse-Grained Biomolecular Simulator for Simulating Proteins at Work. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1979-1989.	2.3	202
76	3A1112 Molecular dynamics simulation of pH-activated KcsA channel(3A Biol & Artifi memb 3:) <i>Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 Butsuri</i> , 2011, 51, S105.	0.0	0
77	1C1436 Coarse-grained simulations of multi-nucleosome systems(Nucleic acid,The 49th Annual Meeting) <i>Tj ETQq1 1 0.784314 rgBT /O</i>	0.0	0
78	1Q1324 Activation mechanism of rhodopsin elucidated by molecular dynamics simulations(Photobiology: Vision & Photoreception 1,The 49th Annual Meeting of the Biophysical) <i>Tj ETQq0 0 0 rgBT /Overlock 10</i>	0.0	0
79	Structural Comparison of F1-ATPase: Interplay among Enzyme Structures, Catalysis, and Rotations. <i>Structure</i> , 2011, 19, 588-598.	1.6	36
80	On easy implementation of a variant of the replica exchange with solute tempering in GROMACS. <i>Journal of Computational Chemistry</i> , 2011, 32, 1228-1234.	1.5	131
81	1P136 Coarse-grained simulation of protein-DNA complex : mechanical unzipping of nucleosome(Nucleic acid:Interaction & Complex formation,The 48th Annual Meeting of the Biophysical) <i>Tj ETQq1 1 0.784314 rgBT /O</i>	0.0	0
82	2P119 Functionally rotating mechanism of a multidrug transporter studied by coarse-grained simulation(The 48th Annual Meeting of the Biophysical Society of Japan). <i>Seibutsu Butsuri</i> , 2010, 50, S103.	0.0	0
83	3P309 Modeling Rhodopsin active conformation (Meta II) by molecular dynamics simulations(Mathematical biology,The 48th Annual Meeting of the Biophysical Society of Japan). <i>Seibutsu Butsuri</i> , 2010, 50, S200.	0.0	0
84	Drug export and allosteric coupling in a multidrug transporter revealed by molecular simulations. <i>Nature Communications</i> , 2010, 1, 117.	5.8	82
85	Characterizing Protein Energy Landscape by Self-Learning Multiscale Simulations: Application to a Designed β -Hairpin. <i>Biophysical Journal</i> , 2010, 99, 3029-3037.	0.2	17
86	35 Years of the Go Model. <i>Seibutsu Butsuri</i> , 2010, 50, 158-159.	0.0	1
87	Folding energy landscape and network dynamics of small globular proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 73-78.	3.3	68
88	Self-learning multiscale simulation for achieving high accuracy and high efficiency simultaneously. <i>Journal of Chemical Physics</i> , 2009, 130, 214108.	1.2	19
89	Bimodal protein solubility distribution revealed by an aggregation analysis of the entire ensemble of <i>Escherichia coli</i> proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 4201-4206.	3.3	253
90	Padding mechanism for the substrate translocation by AAA+ motor revealed by multiscale molecular simulations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009, 106, 18237-18242.	3.3	29

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91	3P-182 Functionally rotating mechanism of a multidrug transporter studied by coarse-grained simulation(Biol & Artifi memb.:Dynamics,Oral Presentations,The 47th Annual Meeting of the) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50	0.0	0
92	1TP5-07 Coarse-grained simulation of protein-DNA complex : dynamics of nucleosome(The 47th Annual) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	0.0	0
93	1P-099 Coarse-grained simulation of protein-DNA complex : dynamics of nucleosome(Nucleic) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 Seibutsu Butsuri, 2009, 49, S79.	0.0	0
94	2P-002 Folding simulations of chignolin by self-learning multiscale method(Protein:Structure, The) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	0.0	0
95	1TA4-02 Mechanism of unidirectional move of KIF1A motor studied by coarse-grained simulations(The) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50	0.0	0
96	2TP5-02 Folding simulations of chignolin by self-learning multiscale method(The 47th Annual Meeting) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	0.0	0
97	3TA3-02 Functionally rotating mechanism of a multidrug transporter studied by coarse-grained simulation(The 47th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2009, 49, S54-S55.	0.0	0
98	1P-129 Mechanism of unidirectional move of KIF1A motor studied by coarse-grained simulations(Molecular motor, The 47th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2009, 49, S83.	0.0	0
99	3P-183 Membrane morphology dynamics induced by proteins : Coarsegrained molecular simulations(Biol & Artifi memb.:Dynamics,The 47th Annual Meeting of the Biophysical Society of) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50	0.0	0
100	1P-098 Replica exchange simulations applied for coarse-grained models of giant protein-nucleic acid complex(Nucleic acid:Interaction & Complex formation, The 47th Annual Meeting of the) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 377	0.0	0
101	Molecular Mechanism of Allostery: MWC or KNF Model?-Approach by Theoretical Model Calculation. Seibutsu Butsuri, 2009, 49, 132-134.	0.0	1
102	Asymmetry in Membrane Protein Sequence and Structure: Glycine Outside Rule. Journal of Molecular Biology, 2008, 377, 74-82.	2.0	4
103	In Silico Chaperonin-Like Cycle Helps Folding of Proteins for Structure Prediction. Biophysical Journal, 2008, 94, 2558-2565.	0.2	3
104	Dynamic energy landscape view of coupled binding and protein conformational change: Induced-fit versus population-shift mechanisms. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 11182-11187.	3.3	297
105	1P-145 Simulation study on stepping mechanism of Conventional Kinesin by coarse-grained model(The) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50	0.0	0
106	1P-065 Simulating large-scale conformational change in a virus protein that mediates membrane fusion(The 46th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2008, 48, S31.	0.0	0
107	2S4-4 Structure change coupled with binding and its application to biomolecular systems(2S4 What) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 Seibutsu Butsuri, 2008, 48, S10.	0.0	0
108	S09A4 Rotary mechanisms of F1-ATPase revealed by molecular simulations(Mechanism of F_1-ATPase) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	0.0	0

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109	Protein Grabs a Ligand by Extending Anchor Residues: Molecular Simulation for Ca ²⁺ Binding to Calmodulin Loop. <i>Biophysical Journal</i> , 2006, 90, 3043-3051.	0.2	34
110	Secondary structure provides a template for the folding of nearby polypeptides. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 17765-17770.	3.3	31
111	Multiple-basin energy landscapes for large-amplitude conformational motions of proteins: Structure-based molecular dynamics simulations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 11844-11849.	3.3	286
112	Folding-based molecular simulations reveal mechanisms of the rotary motor F1-ATPase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 5367-5372.	3.3	116
113	SimFold energy function for de novo protein structure prediction: Consensus with Rosetta. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005, 62, 381-398.	1.5	46
114	Applying a grid technology to protein structure predictor "ROKKY". <i>Studies in Health Technology and Informatics</i> , 2005, 112, 27-36.	0.2	1
115	Roles of physical interactions in determining protein-folding mechanisms: Molecular simulation of protein G and λ spectrin SH3. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 55, 128-138.	1.5	16
116	Guiding the search for a protein's maximum rate of folding. <i>Chemical Physics</i> , 2004, 307, 99-109.	0.9	52
117	Protein folding mechanisms and energy landscape of src SH3 domain studied by a structure prediction toolbox. <i>Chemical Physics</i> , 2004, 307, 157-162.	0.9	18
118	De Novo Design of Foldable Proteins with Smooth Folding Funnel. <i>Structure</i> , 2003, 11, 581-590.	1.6	77
119	Optimizing physical energy functions for protein folding. <i>Proteins: Structure, Function and Bioinformatics</i> , 2003, 54, 88-103.	1.5	84
120	Competition between Protein Folding and Aggregation with Molecular Chaperones in Crowded Solutions: Insight from Mesoscopic Simulations. <i>Biophysical Journal</i> , 2003, 85, 3521-3531.	0.2	38
121	How protein thermodynamics and folding mechanisms are altered by the chaperonin cage: Molecular simulations. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2003, 100, 11367-11372.	3.3	204
122	A reversible fragment assembly method for de novo protein structure prediction. <i>Journal of Chemical Physics</i> , 2003, 119, 6895-6903.	1.2	46
123	On the Hamiltonian replica exchange method for efficient sampling of biomolecular systems: Application to protein structure prediction. <i>Journal of Chemical Physics</i> , 2002, 116, 9058-9067.	1.2	681
124	Roles of native topology and chain-length scaling in protein folding: A simulation study with a GÅ-like model 1 1 Edited by B. Honig. <i>Journal of Molecular Biology</i> , 2001, 313, 171-180.	2.0	344
125	Protein folding simulation with solvent-induced force field: Folding pathway ensemble of three-helix-bundle proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2001, 42, 85-98.	1.5	47
126	Microscopic theory of protein folding rates. II. Local reaction coordinates and chain dynamics. <i>Journal of Chemical Physics</i> , 2001, 114, 5082-5096.	1.2	164

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127	Microscopic theory of protein folding rates. I. Fine structure of the free energy profile and folding routes from a variational approach. <i>Journal of Chemical Physics</i> , 2001, 114, 5069-5081.	1.2	99
128	Simulating Folding of Helical Proteins with Coarse Grained Models. <i>Progress of Theoretical Physics Supplement</i> , 2000, 138, 366-371.	0.2	2
129	Folding dynamics with nonadditive forces: A simulation study of a designed helical protein and a random heteropolymer. <i>Journal of Chemical Physics</i> , 1999, 110, 11616-11629.	1.2	188
130	Microscopic theory of critical folding nuclei and reconfiguration activation barriers in folding proteins. <i>Journal of Chemical Physics</i> , 1997, 107, 9585-9598.	1.2	26
131	Statics, metastable states, and barriers in protein folding: A replica variational approach. <i>Physical Review E</i> , 1997, 55, 4562-4577.	0.8	30
132	Glassy Dynamics of Random Heteropolymers. <i>Progress of Theoretical Physics Supplement</i> , 1997, 126, 49-52.	0.2	2
133	Multidimensional tunneling in terms of complex classical mechanics: Wave functions, energy splittings, and decay rates in nonintegrable systems. <i>Journal of Chemical Physics</i> , 1996, 104, 3742-3759.	1.2	25
134	Effects of vibrational excitation on multidimensional tunneling: General study and proton tunneling in tropolone. <i>Journal of Chemical Physics</i> , 1995, 102, 3977-3992.	1.2	103
135	Transfer-matrix approach to tunneling between Kolmogorov-Arnold-Moser tori. <i>Physical Review A</i> , 1995, 52, 3546-3553.	1.0	13
136	Wentzel-Kramers-Brillouin theory of multidimensional tunneling: General theory for energy splitting. <i>Journal of Chemical Physics</i> , 1994, 100, 98-113.	1.2	83
137	Constant centrifugal potential approximation for atom-diatom chemical reaction dynamics. <i>Journal of Chemical Physics</i> , 1994, 100, 4284-4293.	1.2	7
138	WKB Theory of Tunneling between Tori. <i>Progress of Theoretical Physics Supplement</i> , 1994, 116, 295-301.	0.2	3
139	Reaction dynamics of $D+H_2^+\rightarrow DH+H$: Effects of potential energy surface topography and usefulness of the constant centrifugal potential approximation. <i>Journal of Chemical Physics</i> , 1992, 96, 339-348.	1.2	18
140	Rotational Mechanism of FO Motor in the F-Type ATP Synthase Driven by the Proton Motive Force. <i>Frontiers in Microbiology</i> , 0, 13, .	1.5	6