Shoji Takada

List of Publications by Year
in descending order

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	On the Hamiltonian replica exchange method for efficient sampling of biomolecular systems: Application to protein structure prediction. Journal of Chemical Physics, 2002, 116, 9058-9067.	1.2	681
2	Roles of native topology and chain-length scaling in protein folding: A simulation study with a GÅ•like model 1 1Edited by B. Honig. Journal of Molecular Biology, 2001, 313, 171-180.	2.0	344
3	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
4	Multiple-basin energy landscapes for large-amplitude conformational motions of proteins: Structure-based molecular dynamics simulations. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 11844-11849.	3.3	286
5	Bimodal protein solubility distribution revealed by an aggregation analysis of the entire ensemble of Escherichia coli proteins. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 4201-4206.	3.3	253
6	Coarse-grained molecular simulations of large biomolecules. Current Opinion in Structural Biology, 2012, 22, 130-137.	2.6	205
7	How protein thermodynamics and folding mechanisms are altered by the chaperonin cage: Molecular simulations. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 11367-11372.	3.3	204
8	CafeMol: A Coarse-Grained Biomolecular Simulator for Simulating Proteins at Work. Journal of Chemical Theory and Computation, 2011, 7, 1979-1989.	2.3	202
9	Folding dynamics with nonadditive forces: A simulation study of a designed helical protein and a random heteropolymer. Journal of Chemical Physics, 1999, 110, 11616-11629.	1.2	188
10	Microscopic theory of protein folding rates. II. Local reaction coordinates and chain dynamics. Journal of Chemical Physics, 2001, 114, 5082-5096.	1.2	164
11	Energy landscape views for interplays among folding, binding, and allostery of calmodulin domains. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 10550-10555.	3.3	150
12	Frustration, specific sequence dependence, and nonlinearity in large-amplitude fluctuations of allosteric proteins. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 3504-3509.	3.3	143
13	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
14	Modeling Structural Dynamics of Biomolecular Complexes by Coarse-Grained Molecular Simulations. Accounts of Chemical Research, 2015, 48, 3026-3035.	7.6	134
15	On easy implementation of a variant of the replica exchange with solute tempering in GROMACS. Journal of Computational Chemistry, 2011, 32, 1228-1234.	1.5	131
16	Folding-based molecular simulations reveal mechanisms of the rotary motor F1-ATPase. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 5367-5372.	3.3	116
17	Effects of vibrational excitation on multidimensional tunneling: General study and proton tunneling in tropolone. Journal of Chemical Physics, 1995, 102, 3977-3992.	1.2	103
18	Microscopic theory of protein folding rates. I. Fine structure of the free energy profile and folding routes from a variational approach. Journal of Chemical Physics, 2001, 114, 5069-5081.	1.2	99

#	Article	IF	Citations
19	Multiscale Ensemble Modeling of Intrinsically Disordered Proteins: p53 N-Terminal Domain. Biophysical Journal, 2011, 101, 1450-1458.	0.2	92
20	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
21	Optimizing physical energy functions for protein folding. Proteins: Structure, Function and Bioinformatics, 2003, 54, 88-103.	1.5	84
22	Wentzelâ€“Kramersâ€“Brillouin theory of multidimensional tunneling: General theory for energy splitting. Journal of Chemical Physics, 1994, 100, 98-113.	1.2	83
23	Drug export and allosteric coupling in a multidrug transporter revealed by molecular simulations. Nature Communications, 2010, 1, 117.	5.8	82
24	De Novo Design of Foldable Proteins with Smooth Folding Funnel. Structure, 2003, 11, 581-590.	1.6	77
25	DNA sliding in nucleosomes via twist defect propagation revealed by molecular simulations. Nucleic Acids Research, 2018, 46, 2788-2801.	6.5	77
26	Partial Unwrapping and Histone Tail Dynamics in Nucleosome Revealed by Coarse-Grained Molecular Simulations. PLoS Computational Biology, 2015, 11, e1004443.	1.5	73
27	Folding energy landscape and network dynamics of small globular proteins. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 73-78.	3.3	68
28	Dynamic Coupling among Protein Binding, Sliding, and DNA Bending Revealed by Molecular Dynamics. Journal of the American Chemical Society, 2016, 138, 8512-8522.	6.6	63
29	Nucleosome allostery in pioneer transcription factor binding. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 20586-20596.	3.3	57
30	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
31	Near-atomic structural model for bacterial DNA replication initiation complex and its functional insights. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E8021-E8030.	3.3	56
32	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
33	Guiding the search for a protein's maximum rate of folding. Chemical Physics, 2004, 307, 99-109.	0.9	52
34	Sequence-dependent nucleosome sliding in rotation-coupled and uncoupled modes revealed by molecular simulations. PLoS Computational Biology, 2017, 13, e1005880.	1.5	50
35	Protein folding simulation with solvent-induced force field: Folding pathway ensemble of three-helix-bundle proteins. Proteins: Structure, Function and Bioinformatics, 2001, 42, 85-98.	1.5	47
36	A reversible fragment assembly method for de novo protein structure prediction. Journal of Chemical Physics, 2003, 119, 6895-6903.	1.2	46

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37	SimFold energy function for de novo protein structure prediction: Consensus with Rosetta. Proteins: Structure, Function and Bioinformatics, 2005, 62, 381-398.	1.5	46
38	GÅ•model revisited. Biophysics and Physicobiology, 2019, 16, 248-255.	0.5	40
39	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
40	RESPAC: Method to Determine Partial Charges in Coarse-Grained Protein Model and Its Application to DNA-Binding Proteins. Journal of Chemical Theory and Computation, 2014, 10, 711-721.	2.3	39
41	Chromatin remodelers couple inchworm motion with twist-defect formation to slide nucleosomal DNA. PLoS Computational Biology, 2018, 14, e1006512.	1.5	39
42	Competition between Protein Folding and Aggregation with Molecular Chaperones in Crowded Solutions: Insight from Mesoscopic Simulations. Biophysical Journal, 2003, 85, 3521-3531.	0.2	38
43	Flexible Fitting of Biomolecular Structures to Atomic Force Microscopy Images via Biased Molecular Simulations. Journal of Chemical Theory and Computation, 2020, 16, 1349-1358.	2.3	38
44	Structural Comparison of F1-ATPase: Interplay among Enzyme Structures, Catalysis, and Rotations. Structure, 2011, 19, 588-598.	1.6	36
45	Protein Grabs a Ligand by Extending Anchor Residues: Molecular Simulation for Ca2+ Binding to Calmodulin Loop. Biophysical Journal, 2006, 90, 3043-3051.	0.2	34
46	Molecular dynamics simulation of proton-transfer coupled rotations in ATP synthase FO motor. Scientific Reports, 2020, 10, 8225.	1.6	34
47	Secondary structure provides a template for the folding of nearby polypeptides. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 17765-17770.	3.3	31
48	Histone acetylation dependent energy landscapes in tri-nucleosome revealed by residue-resolved molecular simulations. Scientific Reports, 2016, 6, 34441.	1.6	31
49	Statics, metastable states, and barriers in protein folding: A replica variational approach. Physical Review E, 1997, 55, 4562-4577.	0.8	30
50	p53 dynamics upon response element recognition explored by molecular simulations. Scientific Reports, 2015, 5, 17107.	1.6	30
51	Role of bacterial RNA polymerase gate opening dynamics in DNA loading and antibiotics inhibition elucidated by quasi-Markov State Model. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	30
52	Paddling mechanism for the substrate translocation by AAA+ motor revealed by multiscale molecular simulations. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 18237-18242.	3.3	29
53	Allosteric conformational change cascade in cytoplasmic dynein revealed by structure-based molecular simulations. PLoS Computational Biology, 2017, 13, e1005748.	1.5	29
54	Multi-scale Ensemble Modeling of Modular Proteins with Intrinsically Disordered Linker Regions: Application to p53. Biophysical Journal, 2014, 107, 721-729.	0.2	28

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55	Interactions of HP1 Bound to H3K9me3 Dinucleosome by Molecular Simulations andÂBiochemical Assays. Biophysical Journal, 2018, 114, 2336-2351.	0.2	28
56	Reconstruction of Atomistic Structures from Coarse-Grained Models for Proteinâ€“DNA Complexes. Journal of Chemical Theory and Computation, 2018, 14, 1682-1694.	2.3	27
57	Dynamic and Structural Modeling of the Specificity in Proteinâ€“DNA Interactions Guided by Binding Assay and Structure Data. Journal of Chemical Theory and Computation, 2018, 14, 3877-3889.	2.3	27
58	Implementation of residue-level coarse-grained models in GENESIS for large-scale molecular dynamics simulations. PLoS Computational Biology, 2022, 18, e1009578.	1.5	27
59	Microscopic theory of critical folding nuclei and reconfiguration activation barriers in folding proteins. Journal of Chemical Physics, 1997, 107, 9585-9598.	1.2	26
60	Multidimensional tunneling in terms of complex classical mechanics: Wave functions, energy splittings, and decay rates in nonintegrable systems. Journal of Chemical Physics, 1996, 104, 3742-3759.	1.2	25
61	Overcoming the Bottleneck of the Enzymatic Cycle by Steric Frustration. Physical Review Letters, 2019, 122, 238102.	2.9	24
62	How Co-translational Folding of Multi-domain Protein Is Affected by Elongation Schedule: Molecular Simulations. PLoS Computational Biology, 2015, 11, e1004356.	1.5	22
63	Self-learning multiscale simulation for achieving high accuracy and high efficiency simultaneously. Journal of Chemical Physics, 2009, 130, 214108.	1.2	19
64	The kinetic landscape of nucleosome assembly: A coarse-grained molecular dynamics study. PLoS Computational Biology, 2021, 17, e1009253.	1.5	19
65	Reaction dynamics of D+H2â†'DH+H: Effects of potential energy surface topography and usefulness of the constant centrifugal potential approximation. Journal of Chemical Physics, 1992, 96, 339-348.	1.2	18
66	Protein folding mechanisms and energy landscape of src SH3 domain studied by a structure prediction toolbox. Chemical Physics, 2004, 307, 157-162.	0.9	18
67	Characterizing Protein Energy Landscape by Self-Learning Multiscale Simulations: Application to a Designed Î²-Hairpin. Biophysical Journal, 2010, 99, 3029-3037.	0.2	17
68	Couplings between hierarchical conformational dynamics from multi-time correlation functions and two-dimensional lifetime spectra: Application to adenylate kinase. Journal of Chemical Physics, 2015, 142, 212404.	1.2	17
69	Nucleosome Crowding in Chromatin Slows the Diffusion but Can Promote Target Search of Proteins. Biophysical Journal, 2019, 116, 2285-2295.	0.2	17
70	Roles of physical interactions in determining protein-folding mechanisms: Molecular simulation of protein G and Î± spectrin SH3. Proteins: Structure, Function and Bioinformatics, 2004, 55, 128-138.	1.5	16
71	Dimer domain swapping versus monomer folding in apo-myoglobin studied by molecular simulations. Physical Chemistry Chemical Physics, 2015, 17, 5006-5013.	1.3	16
72	Proteinâ€specific force field derived from the fragment molecular orbital method can improve proteinâ€“ligand binding interactions. Journal of Computational Chemistry, 2013, 34, 1251-1257.	1.5	15

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73	Structure-based Molecular Simulations Reveal the Enhancement of Biased Brownian Motions in Single-headed Kinesin. PLoS Computational Biology, 2013, 9, e1002907.	1.5	15
74	On the ATP binding site of the Îµ subunit from bacterial F-type ATP synthases. Biochimica Et Biophysica Acta - Bioenergetics, 2016, 1857, 332-340.	0.5	14
75	Nucleosomes as allosteric scaffolds for genetic regulation. Current Opinion in Structural Biology, 2020, 62, 93-101.	2.6	14
76	The HMGB chromatin protein Nhp6A can bypass obstacles when traveling on DNA. Nucleic Acids Research, 2020, 48, 10820-10831.	6.5	14
77	Rigid-body fitting to atomic force microscopy images for inferring probe shape and biomolecular structure. PLoS Computational Biology, 2021, 17, e1009215.	1.5	14
78	Transfer-matrix approach to tunneling between Kolmogorov-Arnold-Moser tori. Physical Review A, 1995, 52, 3546-3553.	1.0	13
79	The structural basis of a high affinity ATP binding Îµ subunit from a bacterial ATP synthase. PLoS ONE, 2017, 12, e0177907.	1.1	13
80	Particle Filter Method to Integrate High-Speed Atomic Force Microscopy Measurements with Biomolecular Simulations. Journal of Chemical Theory and Computation, 2020, 16, 6609-6619.	2.3	12
81	Opening of cohesinâ€™s SMC ring is essential for timely DNA replication and DNA loop formation. Cell Reports, 2021, 35, 108999.	2.9	12
82	Testing mechanisms of DNA sliding by architectural DNA-binding proteins: dynamics of single wild-type and mutant protein molecules in vitro and in vivo. Nucleic Acids Research, 2021, 49, 8642-8664.	6.5	11
83	Case Report: Bayesian Statistical Inference of Experimental Parameters via Biomolecular Simulations: Atomic Force Microscopy. Frontiers in Molecular Biosciences, 2021, 8, 636940.	1.6	10
84	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
85	On the Mg2+ binding site of the Îµ subunit from bacterial F-type ATP synthases. Biochimica Et Biophysica Acta - Bioenergetics, 2015, 1847, 1101-1112.	0.5	9
86	Resolving the data asynchronicity in high-speed atomic force microscopy measurement via the Kalman Smoother. Scientific Reports, 2020, 10, 18393.	1.6	9
87	Linker DNA Length is a Key to Tri-nucleosome Folding. Journal of Molecular Biology, 2021, 433, 166792.	2.0	8
88	Constant centrifugal potential approximation for atomâ€“diatom chemical reaction dynamics. Journal of Chemical Physics, 1994, 100, 4284-4293.	1.2	7
89	How one-dimensional diffusion of transcription factors are affected by obstacles: coarse-grained molecular dynamics study. Molecular Simulation, 2017, 43, 1315-1321.	0.9	7
90	Coarse-grained implicit solvent lipid force field with a compatible resolution to the CÎ± protein representation. Journal of Chemical Physics, 2020, 153, 205101.	1.2	7

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91	Rotational Mechanism of FO Motor in the F-Type ATP Synthase Driven by the Proton Motive Force. Frontiers in Microbiology, 0, 13, .	1.5	6
92	The lane-switch mechanism for nucleosome repositioning by DNA translocase. Nucleic Acids Research, 2021, 49, 9066-9076.	6.5	5
93	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
94	Asymmetry in Membrane Protein Sequence and Structure: Glycine Outside Rule. Journal of Molecular Biology, 2008, 377, 74-82.	2.0	4
95	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
96	How Cytoplasmic Dynein Couples ATP Hydrolysis Cycle to Diverse Stepping Motions: Kinetic Modeling. Biophysical Journal, 2020, 118, 1930-1945.	0.2	4
97	Modeling of DNA binding to the condensin hinge domain using molecular dynamics simulations guided by atomic force microscopy. PLoS Computational Biology, 2021, 17, e1009265.	1.5	4
98	Modeling DNA Opening in the Eukaryotic Transcription Initiation Complexes via Coarse-Grained Models. Frontiers in Molecular Biosciences, 2021, 8, 772486.	1.6	4
99	Cooperation among c-subunits of FoF1-ATP synthase in rotation-coupled proton translocation. ELife, 2022, 11, .	2.8	4
100	Inferring Conformational State of Myosin Motor in an Atomic Force Microscopy Image via Flexible Fitting Molecular Simulations. Frontiers in Molecular Biosciences, 2022, 9, 882989.	1.6	4
101	In Silico Chaperonin-Like Cycle Helps Folding of Proteins for Structure Prediction. Biophysical Journal, 2008, 94, 2558-2565.	0.2	3
102	Modeling lipidâ€“protein interactions for coarse-grained lipid and CÎ± protein models. Journal of Chemical Physics, 2021, 155, 155101.	1.2	3
103	WKB Theory of Tunneling between Tori. Progress of Theoretical Physics Supplement, 1994, 116, 295-301.	0.2	3
104	Simulating Folding of Helical Proteins with Coarse Grained Models. Progress of Theoretical Physics Supplement, 2000, 138, 366-371.	0.2	2
105	Semi-Implicit Time Integration with Hessian Eigenvalue Corrections for a Larger Time Step in Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2021, 17, 5792-5804.	2.3	2
106	Glassy Dynamics of Random Heteropolymers. Progress of Theoretical Physics Supplement, 1997, 126, 49-52.	0.2	2
107	Coarse-grained molecular dynamics simulations of base-pair mismatch recognition protein MutS sliding along DNA. Biophysics and Physicobiology, 2022, 19, .	0.5	2
108	Molecular Mechanism of Allostery: MWC or KNF Model?-Approach by Theoretical Model Calculation. Seibutsu Butsuri, 2009, 49, 132-134.	0.0	1

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109	35 Years of the Go Model. Seibutsu Butsuri, 2010, 50, 158-159.	0.0	1
110	Applying a grid technology to protein structure predictor "ROKKY". Studies in Health Technology and Informatics, 2005, 112, 27-36.	0.2	1
111	Using incomplete Cholesky factorization to increase the time step in molecular dynamics simulations. Journal of Computational and Applied Mathematics, 2022, 415, 114519.	1.1	1
112	S09A4 Rotary mechanisms of F1-ATPase revealed by molecular simulations(Mechanism of F_1-ATPase) Tj ETQq0 0 0 rgBT /Overlock 10 T	0.0	0
113	1P-145 Simulation study on stepping mechanism of Conventional Kinesin by coarse-grained model(The) Tj ETQq1 1 0.784314 rgBT /Ov	0.0	0
114	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
115	2S4-4 Structure change coupled with binding and its application to biomolecular systems(2S4 What) Tj ETQq1 1 0.784314 rgBT /Ove Seibutsu Butsuri, 2008, 48, S10.	0.0	0
116	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 ETQq0 0 0 rgBT /Overlock 10 Tf 50 457	0.0	0
117	1TP5-07 Coarse-grained simulation of protein-DNA complex : dynamics of nucleosome(The 47th Annual) Tj ETQq1 1 0.784314 rgBT /Ov	0.0	0
118	1P-099 Coarse-grained simulation of protein-DNA complex : dynamics of nucleosome(Nucleic) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 387 Seibutsu Butsuri, 2009, 49, S79.	0.0	0
119	2P-002 Folding simulations of chignolin by self-learning multiscale method(Protein:Structure, The) Tj ETQq1 1 0.784314 rgBT /Overlock	0.0	0
120	1TA4-02 Mechanism of unidirectional move of KIF1A motor studied by coarse-grained simulations(The) Tj ETQq0 0 0 rgBT /Overlock 10 T	0.0	0
121	2TP5-02 Folding simulations of chignolin by self-learning multiscale method(The 47th Annual Meeting) Tj ETQq1 1 0.784314 rgBT /Over	0.0	0
122	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
123	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
124	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 ETQq0 0 0 rgBT /Overlock 10 T	0.0	0
125	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 ETQq1 1 0.784314 rgBT /Overlock 10 T	0.0	0
126	1P136 Coarse-grained simulation of protein-DNA complex : mechanical unzipping of nucleosome(Nucleic acid:Interaction & Complex formation,The 48th Annual Meeting of the Biophysical) Tj ETQq0 0 0 rgBT /Overlock 10	0.0	0

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127	2P119 Functionally rotating mechanism of a multidrug transporter studied by coarse-grained simulation(The 48th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2010, 50, S103.	0.0	0
128	3P309 Modeling Rhodopsin active conformation (Meta II) by molecular dynamics simulations(Mathematical biology,The 48th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2010, 50, S200.	0.0	0
129	3A1112 Molecular dynamics simulation of pH-activated KcsA channel(3A Biol & Artifi memb 3:) Tj ETQq1 1 0.784314 rgBT /Overloc Butsuri, 2011, 51, S105.	0.0	0
130	1C1436 Coarse-grained simulations of multi-nucleosome systems(Nucleic acid,The 49th Annual Meeting) Tj ETQq0 0 0 rgBT /Overlock 1	0.0	0
131	1Q1324 Activation mechanism of rhodopsin elucidated by molecular dynamics simulations(Photobiology: Vision & Photoreception 1,The 49th Annual Meeting of the Biophysical) Tj ETQq1 1 0.784314 rgBT /Ove	0.0	0
132	3PT009 Mono- and poly-nucleosome structural dynamics by coarse-grained simulations(The 50th) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	0.0	0
133	3PT011 Diffusion of TFIIIA zinc fingers along DNA studied by molecular simulations(The 50th Annual) Tj ETQq1 1 0.784314 rgBT /Overlo	0.0	0
134	1P149 The Mg^<2+> binding site of the ATP synthase Îµ subunit from Bacillus subtilis derived by Molecular Dynamics simulations(11.Molecular motor,Poster,The 51st Annual Meeting of the) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 457	0.0	0
135	3P121 Poly-nucleosome structural dynamics by coarse-grained simulations(05A. Nucleic acid:) Tj ETQq1 1 0.784314 rgBT /Overlock 10 T	0.0	0
136	2SCP-03 Structure of model chromatin and dynamics of transcription factors studied by coarse-grained simulations(2SCP Functional dynamics of Nucleosome and Chromathin in Nuclear) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 Seibutsu Butsuri, 2013, 53, S98.	0.0	0
137	Molecular Dynamics Simulations of Biomolecules. Journal of the Society of Mechanical Engineers, 2013, 116, 78-80.	0.0	0
138	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 0 0 rgBT /Overlock 10	0.0	0
139	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	0.0	0
140	Coarse-grained Biomolecular Simulations. Seibutsu Butsuri, 2021, 61, 144-151.	0.0	0