Yuko Okamoto

List of Publications by Year
in descending order

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248	12,855	44069	24982
papers	citations	48 h-index	109 g-index

251	251	251	7316
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Distribution and Structure Analysis of Fibril-Forming Peptides Focusing on Concentration Dependency. ACS Omega, 2022, 7, 10012-10021.	3.5	0
2	Combination of genetic algorithm and generalised-ensemble algorithms for biomolecular simulations. Frontiers of Nanoscience, 2022, , 93-109.	0.6	0
3	Calculation of the residual entropy of Ice Ih by Monte Carlo simulation with the combination of the replica-exchange Wangâ€“Landau algorithm and multicanonical replica-exchange method. Journal of Chemical Physics, 2021, 154, 044503.	3.0	5
4	Two-dimensional simulated tempering for the isobaricâ€“isothermal ensemble with fast on-the-fly weight determination. Molecular Physics, 2021, 119, .	1.7	0
5	Structural Characteristics of Monomeric AÎ²42 on Fibril in the Early Stage of Secondary Nucleation Process. ACS Chemical Neuroscience, 2020, 11, 2989-2998.	3.5	6
6	Analysis of liquids, gases, and supercritical fluids by a two-dimensional replica-exchange Monte Carlo method in temperature and chemical potential space. Journal of Chemical Physics, 2020, 152, 194108.	3.0	1
7	Molecular movie of nucleotide binding to a motor protein. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129654.	2.4	3
8	N+-C-HÂ·Â·Â·O Hydrogen bonds in protein-ligand complexes. Scientific Reports, 2019, 9, 767.	3.3	81
9	Conformational Change of Amyloid-Î² 40 in Association with Binding to GM1-Glycan Cluster. Scientific Reports, 2019, 9, 6853.	3.3	33
10	Structural Analysis of a Trimer of Î²2-Microgloblin Fragment by Molecular Dynamics Simulations. Biophysical Journal, 2019, 116, 781-790.	0.5	3
11	Determination of the structural ensemble of the molten globule state of a protein by computer simulations. Proteins: Structure, Function and Bioinformatics, 2019, 87, 635-645.	2.6	6
12	Protein structure predictions by enhanced conformational sampling methods. Biophysics and Physicobiology, 2019, 16, 344-366.	1.0	4
13	Efficient simulation protocol for determining the density of states: Combination of replica-exchange Wang-Landau method and multicanonical replica-exchange method. Physical Review E, 2019, 100, 043304.	2.1	6
14	Enhanced sampling method in molecular simulations using genetic algorithm for biomolecular systems. Journal of Computational Chemistry, 2019, 40, 475-481.	3.3	3
15	Two polyhedral frameworks of an M12L24 spherical complex revealed by replica-exchange molecular dynamics simulations. Chemical Physics Letters, 2019, 714, 185-189.	2.6	9
16	Optimizations of Protein Force Fields. Springer Series on Bio- and Neurosystems, 2019, , 203-256.	0.2	0
17	Computational analysis for selectivity of histone deacetylase inhibitor by replica-exchange umbrella sampling molecular dynamics simulations. Journal of Chemical Physics, 2018, 148, 125102.	3.0	7
18	Structureâ€“function insights into direct lipid transfer between membranes by Mmm1â€“Mdm12 of ERMES. Journal of Cell Biology, 2018, 217, 959-974.	5.2	116

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19	Implementation of replica-exchange umbrella sampling in GAMESS. Computer Physics Communications, 2018, 228, 152-162.	7.5	10
20	Conformational properties of an artificial GM1 glycan cluster based on a metal-ligand complex. Journal of Chemical Physics, 2018, 149, 135101.	3.0	8
21	Quantum chemical replica-exchange umbrella sampling molecular dynamics simulations reveal the formation mechanism of iron phthalocyanine from iron and phthalonitrile. Journal of Chemical Physics, 2018, 149, 072332.	3.0	1
22	10.1063/1.5045310.1. , 2018, , .		0
23	Conformational changes of ubiquitin under high pressure conditions: A pressure simulated tempering molecular dynamics study. Journal of Computational Chemistry, 2017, 38, 1167-1173.	3.3	10
24	Conformational effects of N-glycan core fucosylation of immunoglobulin G Fc region on its interaction with FcÎ³ receptor IIIa. Scientific Reports, 2017, 7, 13780.	3.3	57
25	Two major stable structures of amyloid-forming peptides: amorphous aggregates and amyloid fibrils. Molecular Simulation, 2017, 43, 1370-1376.	2.0	5
26	QM/MM free energy simulations: recent progress and challenges. Molecular Simulation, 2016, 42, 1056-1078.	2.0	89
27	Modeling 15N NMR chemical shift changes in protein backbone with pressure. Journal of Chemical Physics, 2016, 145, 085104.	3.0	7
28	Structural Studies of Fibril Formations of Tetrapeptides Using Replica Exchange Molecular Dynamics Simulations. Biophysical Journal, 2016, 110, 323a-324a.	0.5	0
29	Study of Ligand Binding Selectivity of Histone Deacetylases by Replica-Exchange Umbrella Sampling Molecular Dynamics Simulations. Biophysical Journal, 2016, 110, 544a-545a.	0.5	1
30	Implementation of replica-exchange umbrella sampling in the DFTB<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si6.gif" display="inline" overflow="scroll"><mml:mo>+</mml:mo></mml:math> semiempirical quantum chemistry package. Computer Physics Communications, 2016, 204, 1-10.	7.5	6
31	Structural Fluctuations of Proteins in Folding and Ligand Docking Studied by Replica-Exchange Simulations. , 2016, , 183-204.		0
32	Deterministic replica-exchange method without pseudo random numbers for simulations of complex systems. Computer Physics Communications, 2015, 197, 128-135.	7.5	2
33	Implementation of Replica-Exchange Umbrella Sampling to the DFTB+ Simulation Package. Biophysical Journal, 2015, 108, 159a.	0.5	0
34	Predictions of Tertiary Structures of Î±-Helical Membrane Proteins by Replica-Exchange Method with Consideration of Helix Deformations. Journal of the Physical Society of Japan, 2015, 84, 084802.	1.6	5
35	Observation of helix associations for insertion of a retinal molecule and distortions of helix structures in bacteriorhodopsin. Journal of Chemical Physics, 2015, 143, 235101.	3.0	4
36	New Implementations of Replica-exchange Method for Simulations of Complex Systems: Designed-walk and Deterministic Replica-exchange Methods. Physics Procedia, 2015, 68, 100-104.	1.2	0

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37	Molecular Dynamics Simulations to Clarify the Concentration Dependency of Protein Aggregation. , 2015, , .		1
38	Replica-exchange molecular dynamics simulation for understanding the initial process of amyloid peptide aggregation. Molecular Simulation, 2015, 41, 1041-1044.	2.0	7
39	Conformational Dynamics of Oligosaccharides Characterized by Paramagnetism-Assisted NMR Spectroscopy in Conjunction with Molecular Dynamics Simulation. Advances in Experimental Medicine and Biology, 2015, 842, 217-230.	1.6	16
40	Designed-walk replica-exchange method for simulations of complex systems. Computer Physics Communications, 2015, 196, 380-383.	7.5	5
41	Conformational search simulations of Trp-cage using genetic crossover. Molecular Simulation, 2015, 41, 1045-1049.	2.0	3
42	Equilibrium Molecular Thermodynamics from Kirkwood Sampling. Journal of Physical Chemistry B, 2015, 119, 6155-6169.	2.6	1
43	A Conformational Search Method for Protein Systems Using Genetic Crossover and Metropolis Criterion. Journal of Physics: Conference Series, 2014, 487, 012003.	0.4	8
44	Computer Simulations for Predicting Membrane Protein Structures with the Replica-Exchange Methods and Implicit Membrane Model of a Restricted Configurational Space. Biophysical Journal, 2014, 106, 655a.	0.5	0
45	Salt effects on hydrophobicâ€core formation in folding of a helical miniprotein studied by molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2014, 82, 933-943.	2.6	3
46	Exploration of Conformational Spaces of Highâ€Mannoseâ€Type Oligosaccharides by an NMRâ€Validated Simulation. Angewandte Chemie - International Edition, 2014, 53, 10941-10944.	13.8	60
47	Prediction of Ligand Binding Affinity by the Combination of Replica-Exchange Method and Double-Decoupling Method. Journal of Chemical Theory and Computation, 2014, 10, 3563-3569.	5.3	12
48	Salt Effects on Folding of a Helical Mini Protein Villin Headpiece Subdomain HP36 Studied by Generalized-Ensemble Simulations. Biophysical Journal, 2014, 106, 672a.	0.5	0
49	2P008 Parameter dependency of an optimized force field for each amino acid(01A.) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 267 Seibutsu Butsuri, 2014, 54, S196.	0.1	0
50	Protein Folding Simulations by Generalized-Ensemble Algorithms. Advances in Experimental Medicine and Biology, 2014, 805, 1-27.	1.6	7
51	Optimizations of Protein Force Fields. Springer Series in Bio-/neuroinformatics, 2014, , 195-247.	0.1	1
52	Prediction of Proteinâ€“Ligand Binding Structures by Replica-Exchange Umbrella Sampling Simulations: Application to Kinase Systems. Journal of Chemical Theory and Computation, 2013, 9, 4660-4671.	5.3	28
53	Twoâ€dimensional replicaâ€exchange method for predicting proteinâ€“ligand binding structures. Journal of Computational Chemistry, 2013, 34, 2601-2614.	3.3	35
54	Free-energy analyses of a proton transfer reaction by simulated-tempering umbrella sampling and first-principles molecular dynamics simulations. Physical Review E, 2013, 87, 023301.	2.1	11

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55	Enhanced Sampling Algorithms. Methods in Molecular Biology, 2013, 924, 153-195.	0.9	59
56	A Proposal for Amino Acid Dependent Main-Chain Torsion-Energy Terms for Protein Force Fields. Biophysical Journal, 2013, 104, 507a.	0.5	0
57	Application of simulated tempering and magnetizing to a two-dimensional Potts model. Journal of Statistical Mechanics: Theory and Experiment, 2013, 2013, P02039.	2.3	4
58	Ligand Docking Simulations by Generalized-Ensemble Algorithms. Advances in Protein Chemistry and Structural Biology, 2013, 92, 63-91.	2.3	6
59	Communication: Simulated tempering with fast on-the-fly weight determination. Journal of Chemical Physics, 2013, 138, 061102.	3.0	43
60	Amino-acid-dependent main-chain torsion-energy terms for protein systems. Journal of Chemical Physics, 2013, 138, 064103.	3.0	5
61	Improvement of the backbone-torsion-energy term in the force field for protein systems by the double Fourier series expansion. Molecular Simulation, 2013, 39, 85-93.	2.0	2
62	2P016 Optimization of force-field parameters for protein systems by an energy-based reweighting approach(01A. Protein: Structure,Poster). Seibutsu Butsuri, 2013, 53, S161.	0.1	0
63	1P128 Calculation of proton transfer in malonaldehyde using DFTB and REUS(06.Electronic) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf S127.	0.1	0
64	Phase Behavior of a Lipid Bilayer System Studied by a Replica-Exchange Molecular Dynamics Simulation. Journal of the Physical Society of Japan, 2012, 81, 024002.	1.6	16
65	Simulated tempering and magnetizing: Application of two-dimensional simulated tempering to the two-dimensional Ising model and its crossover. Physical Review E, 2012, 86, 056705.	2.1	9
66	3PT224 First principles molecular simulation with a generalized-ensemble algorithm for studying chemical reactions of biomolecular systems(The 50th Annual Meeting of the Biophysical Society of) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	0	
67	1PT132 Development of a force field of backbone dihedral angles for each amino acid using Protein Data Bank(The 50th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2012, 52, S91.	0.1	0
68	Molecular simulations in generalised ensemble. Molecular Simulation, 2012, 38, 1282-1296.	2.0	4
69	Pressure-Induced Denaturation of Proteins Studied by Generalized-Ensemble Molecular Simulations. Biophysical Journal, 2012, 102, 736a.	0.5	0
70	Replica-exchange molecular dynamics simulation of a lipid bilayer system with a coarse-grained model. Molecular Simulation, 2012, 38, 437-441.	2.0	13
71	Simulated Tempering and Magnetizing Simulations of the Ising Model. Physics Procedia, 2012, 34, 100-104.	1.2	1
72	Protein Force Field Improved by using a New Backbone-Torsion-Energy Term. Biophysical Journal, 2012, 102, 171a.	0.5	1

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73	Residual entropy of ordinary ice calculated from multicanonical Monte Carlo simulations. Molecular Simulation, 2012, 38, 856-860.	2.0	11
74	Generalized-Ensemble Algorithms for Protein Folding and Unfolding. Current Physical Chemistry, 2012, 2, 92-106.	0.2	0
75	Generalised-ensemble algorithms for studying temperature and pressure dependence of complex systems. Molecular Simulation, 2012, 38, 452-457.	2.0	2
76	Generalized-Ensemble Algorithms for Simulations of Complex Molecular Systems. , 2012, , 69-101.		6
77	Recent Applications of Replica-Exchange Molecular Dynamics Simulations of Biomolecules. Current Physical Chemistry, 2012, 2, 401-412.	0.2	4
78	Folding Simulation of a Mini Protein with a Hydrophobic Core and .ALPHA.-helices. Seibutsu Butsuri, 2012, 52, 022-023.	0.1	0
79	3G1346 Protein Structure Predictions by Simulated Annealing Molecular Dynamics Using Genetic Crossover(3G Protein: Structure 4,The 49th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2011, 51, S131.	0.1	0
80	1H1336 Conformations of ubiquitin at high pressure studied by isobaric-isothermal simulated tempering simulations(Protein: Property 2,The 49th Annual Meeting of the Biophysical Society of) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	0.1	0
81	1A1412 Phase Transition Behavior of Lipid Bilayer Studied by REMD with a Coarse-Grained Model(Biol &) Tj ETQq1 1 0.784314 rgBT /Ov	0.1	0
82	Drug Design by Generalized-Ensemble Simulations. Current Pharmaceutical Design, 2011, 17, 1758-1772.	1.9	2
83	Protein structure predictions by parallel simulated annealing molecular dynamics using genetic crossover. Journal of Computational Chemistry, 2011, 32, 1353-1360.	3.3	16
84	Ab Initio prediction of proteinâ€“ligand binding structures by replicaâ€exchange umbrella sampling simulations. Journal of Computational Chemistry, 2011, 32, 2810-2821.	3.3	53
85	Dynamic structure of the polytheonamide B channel studied by normal mode analysis. Molecular Simulation, 2011, 37, 975-985.	2.0	13
86	Replica-Exchange Molecular Dynamics Simulations for Various Constant Temperature Algorithms. Journal of the Physical Society of Japan, 2010, 79, 074001.	1.6	23
87	1P235 1I1325 Phase behavior of DPPC bilayer studied by REMD with coarse-grained model(Biol & Artifi) Tj ETQq1 1 0.784314 rgBT /Ov	0.1	0
88	3P018 A Simulated Annealing Molecular Dynamics Using Genetic Crossover with Knot Theory(Protein:) Tj ETQq0 0 0 rgBT /Overlock 10 T S148.	0.1	0
89	3P075 Pressure dependence of protein conformations studied by generalized simulated tempering molecular dynamics simulations(Protein: Property,The 48th Annual Meeting of the Biophysical Society) Tj ETQq1 1 0.784314 rgBT /Ov		
90	Dependency of ligand free energy landscapes on charge parameters and solvent models. Journal of Computer-Aided Molecular Design, 2010, 24, 699-712.	2.9	6

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91	Multi-dimensional multicanonical algorithm, simulated tempering, replica-exchange method, and all that. Physics Procedia, 2010, 4, 89-105.	1.2	6
92	Replica-exchange method in van der Waals radius space: Overcoming steric restrictions for biomolecules. Journal of Chemical Physics, 2010, 132, 134105.	3.0	46
93	Optimisation of OPLSâ€“UA force-field parameters for protein systems using protein data bank. Molecular Simulation, 2010, 36, 1148-1156.	2.0	10
94	Controlling the secondary-structure-forming tendencies of proteins by a backbone torsion-energy term. Molecular Simulation, 2010, 36, 138-158.	2.0	9
95	Determination method of the balance of the secondary-structure-forming tendencies of force fields. Molecular Simulation, 2010, 36, 159-165.	2.0	4
96	Folding simulations of three proteins having all Î±-helix, all Î²-strand and Î±/Î²-structures. Molecular Simulation, 2010, 36, 302-310.	2.0	8
97	Hydrophobic Core Formation and Dehydration in Protein Folding Studied by Generalized-Ensemble Simulations. Biophysical Journal, 2010, 99, 1637-1644.	0.5	40
98	Generalized-Ensemble Algorithms for the Isobaricâ€“Isothermal Ensemble. Journal of the Physical Society of Japan, 2010, 79, 074003.	1.6	32
99	Helix-Hairpin Transitions of a Designed Peptide Studied by a Generalized-Ensemble Simulation. Journal of Chemical Theory and Computation, 2010, 6, 979-983.	5.3	9
100	From multidimensional replica-exchange method to multidimensional multicanonical algorithm and simulated tempering. Physical Review E, 2009, 79, 047701.	2.1	35
101	Multidimensional generalized-ensemble algorithms for complex systems. Journal of Chemical Physics, 2009, 130, 214105.	3.0	52
102	Thermodynamic Perspective on the Dockâ"Lock Growth Mechanism of Amyloid Fibrils. Journal of Physical Chemistry B, 2009, 113, 14421-14430.	2.6	88
103	Analysis of Helix-Helix Interactions of Bacteriorhodopsin by Replica-Exchange Simulations. Biophysical Journal, 2009, 96, 765-776.	0.5	12
104	Folding simulations of gramicidin A into the Î²-helix conformations: Simulated annealing molecular dynamics study. Journal of Chemical Physics, 2009, 131, 165103.	3.0	11
105	3P-056 A simulated annealing molecular dynamics simulation with a genetic crossover for protein systems(Protein:Property,The 47th Annual Meeting of the Biophysical Society of Japan). Seibutsu Butsuri, 2009, 49, S160.	0.1	0
106	3P-054 Molecular dynamics study of temperature and pressure effects on a biomolecule with generalized-ensemble algorithms(Protein:Property,The 47th Annual Meeting of the Biophysical Society) Tj ETQq0 0 0 rgBT /Overlock 10		
107	Electrostatic effects on the Î±-helix and Î²-strand formation of BPTI(16-36) studied by Monte Carlo simulated annealing. Chemical Biology and Drug Design, 2008, 54, 230-236.	1.1	8
108	Generalized-Ensemble Algorithms for Protein Folding Simulations. , 2008, , 369-407.		8

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109	Amyloid-Î²(29â^'42) Dimer Formations Studied by a Multicanonicalâ^'Multioverlap Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2008, 112, 2767-2770.	2.6	47
110	Temperature and Pressure Dependence of Alanine Dipeptide Studied by Multibaricâ^'Multithermal Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2008, 112, 12038-12049.	2.6	55
111	Thermodynamics of two lattice ice models in three dimensions. Physical Review E, 2008, 78, 041113.	2.1	2
112	Monte Carlo simulation in the isobaric-multithermal ensemble of a bulk Lennard-Jones fluid system: Thermodynamic quantities for pressure fromPâ^—=2.42to 7.25. Physical Review E, 2008, 77, 051201.	2.1	2
113	Monte Carlo Study of First-Order Phase Transitions of a Bulk Lennardâ€"Jones Fluid System in the Isobaricâ€"Multithermal Ensemble. Bulletin of the Chemical Society of Japan, 2008, 81, 697-702.	3.2	3
114	Explicit symplectic integrators of molecular dynamics algorithms for rigid-body molecules in the canonical, isobaric-isothermal, and related ensembles. Journal of Chemical Physics, 2007, 126, 084103.	3.0	88
115	Multibaricâ€"multithermal molecular dynamics simulation: generalized NosÃ©â€"PoincarÃ©â€"Andersen method. Molecular Simulation, 2007, 33, 91-96.	2.0	0
116	Residual entropy of ordinary ice from multicanonical simulations. Physical Review B, 2007, 75, .	3.2	41
117	Effective sampling in the configurational space of a small peptide by the multicanonical-multioverlap algorithm. Physical Review E, 2007, 76, 026705.	2.1	23
118	Multibaricâ€"Multithermal Molecular Dynamics Simulation of Alanine Dipeptide in Explicit Water. Bulletin of the Chemical Society of Japan, 2007, 80, 1114-1123.	3.2	37
119	2P113 Simulated Annealing Molecular Dynamics Simulations of Gramicidin A in the Low-Dielectric Environment(Proteins-stability, folding, and other physicochemical properties,Poster Presentations). Seibutsu Butsuri, 2007, 47, S141.	0.1	0
120	3P043 Role of Glycines on Amyloidogenesis of Alzheimer's Amyloid-Beta Peptide Fragments(Proteins-stability, folding, and other physicochemical properties,Poster Presentations). Seibutsu Butsuri, 2007, 47, S213.	0.1	0
121	Generalized-ensemble algorithms for molecular dynamics simulations. Molecular Simulation, 2007, 33, 47-56.	2.0	33
122	Normal Mode Analysis of Polytheonamide B. Journal of the Physical Society of Japan, 2007, 76, 094801.	1.6	4
123	Theoretical studies of transition states by the multioverlap molecular dynamics methods. Journal of Chemical Physics, 2006, 124, 104103.	3.0	29
124	Replica-exchange methods and predictions of helix configurations of membrane proteins. Molecular Simulation, 2006, 32, 791-801.	2.0	9
125	1P584 Amyloid Î²-peptides studied by the multicanonical-multioverlap algorithm(27. Molecular dynamics) Tj ETQq1 1 0.784314 rgBT /O S292.	0.1	0
126	1P585 Explicit Symplectic Molecular Dynamics Simulation for Rigid-Body Molecules in the Canonical Ensemble(27. Molecular dynamics simulation,Poster Session,Abstract,Meeting Program of EABS &) Tj ETQq0 0 0 rgBT /Overlock 10	0.1	0

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127	Cooperative folding mechanism of a Î²-hairpin peptide studied by a multicanonical replica-exchange molecular dynamics simulation. Proteins: Structure, Function and Bioinformatics, 2006, 66, 846-859.	2.6	56
128	Multibaric-multithermal ensemble molecular dynamics simulations. Journal of Computational Chemistry, 2006, 27, 379-395.	3.3	53
129	Secondary-Structure Design of Proteins by a Backbone Torsion Energy. Journal of the Physical Society of Japan, 2006, 75, 054802.	1.6	14
130	Multibaricâ€“multithermal ensemble simulations for fluid systems. Physica A: Statistical Mechanics and Its Applications, 2005, 350, 150-158.	2.6	0
131	Molecular simulations in the multibaric-multithermal ensembles. Computer Physics Communications, 2005, 169, 317-321.	7.5	1
132	Replica-exchange molecular dynamics simulation of small peptide in water and in ethanol. Chemical Physics Letters, 2005, 412, 280-284.	2.6	16
133	Effects of the fixed end in single-molecule imaging techniques: A replica-exchange molecular dynamics simulation study. Chemical Physics Letters, 2005, 414, 449-455.	2.6	8
134	MOLECULAR DYNAMICS SIMULATIONS OF DNA DIMERS BASED ON REPLICA-EXCHANGE UMBRELLA SAMPLING II: FREE ENERGY ANALYSIS. Journal of Theoretical and Computational Chemistry, 2005, 04, 433-448.	1.8	3
135	MOLECULAR DYNAMICS SIMULATIONS OF DNA DIMERS BASED ON REPLICA-EXCHANGE UMBRELLA SAMPLING I: TEST OF SAMPLING EFFICIENCY. Journal of Theoretical and Computational Chemistry, 2005, 04, 411-432.	1.8	7
136	Structures of a peptide fragment of Î²2-microglobulin studied by replica-exchange molecular dynamics simulations - Towards the understanding of the mechanism of amyloid formation. FEBS Letters, 2005, 579, 5425-5429.	2.8	26
137	Molecular Mechanism for Stabilizing a Short Helical Peptide Studied by Generalized-Ensemble Simulations with Explicit Solvent. Biophysical Journal, 2005, 88, 3180-3190.	0.5	31
138	Mega Process Genetic Algorithm Using Grid MP. Lecture Notes in Computer Science, 2005, , 152-170.	1.3	3
139	Optimizations of Protein Force-Field Parameters with Protein Data Bank. Seibutsu Butsuri, 2005, 45, 145-148.	0.1	0
140	Free energy calculations of the stacked and unstacked states for DNA dimers by replica-exchange umbrella sampling. AIP Conference Proceedings, 2004, , .	0.4	0
141	Generalized-Ensemble Monte Carlo Algorithms for Simulations of Proteins. AIP Conference Proceedings, 2004, , .	0.4	0
142	Monte Carlo simulations in generalized isobaric-isothermal ensembles. Physical Review E, 2004, 70, 026702.	2.1	54
143	New approach to the first-order phase transition of Lennard-Jones fluids. Journal of Chemical Physics, 2004, 120, 7557-7563.	3.0	12
144	Prediction of membrane protein structures by replica-exchange Monte Carlo simulations: Case of two helices. Journal of Chemical Physics, 2004, 120, 10837-10847.	3.0	35

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145	Replica-exchange extensions of simulated tempering method. Journal of Chemical Physics, 2004, 121, 2491.	3.0	53
146	PROTEIN FORCE-FIELD PARAMETERS OPTIMIZED WITH THE PROTEIN DATA BANK II: COMPARISONS OF FORCE FIELDS BY FOLDING SIMULATIONS OF SHORT PEPTIDES. Journal of Theoretical and Computational Chemistry, 2004, 03, 359-378.	1.8	20
147	PROTEIN FORCE-FIELD PARAMETERS OPTIMIZED WITH THE PROTEIN DATA BANK I: FORCE-FIELD OPTIMIZATIONS. Journal of Theoretical and Computational Chemistry, 2004, 03, 339-358.	1.8	18
148	Multibaricâ€“Multithermal Ensemble Simulation for Simple Liquids. Molecular Simulation, 2004, 30, 847-852.	2.0	0
149	Free energy calculations for DNA base stacking by replica-exchange umbrella sampling. Chemical Physics Letters, 2004, 385, 1-7.	2.6	61
150	Generalized-ensemble algorithms: enhanced sampling techniques for Monte Carlo and molecular dynamics simulations. Journal of Molecular Graphics and Modelling, 2004, 22, 425-439.	2.4	307
151	Secondary-structure preferences of force fields for proteins evaluated by generalized-ensemble simulations. Chemical Physics, 2004, 307, 269-283.	1.9	85
152	Monte Carlo simulations in multibaricâ€“multithermal ensemble. Chemical Physics Letters, 2004, 383, 391-396.	2.6	57
153	Prediction of transmembrane helix configurations by replica-exchange simulations. Chemical Physics Letters, 2004, 383, 397-402.	2.6	26
154	Comparisons of force fields for proteins by generalized-ensemble simulations. Chemical Physics Letters, 2004, 386, 460-467.	2.6	151
155	Molecular dynamics simulations in the multibaricâ€“multithermal ensemble. Chemical Physics Letters, 2004, 391, 248-253.	2.6	54
156	Self-assembly of transmembrane helices of bacteriorhodopsin by a replica-exchange Monte Carlo simulation. Chemical Physics Letters, 2004, 392, 168-175.	2.6	25
157	Multi-overlap molecular dynamics methods for biomolecular systems. Chemical Physics Letters, 2004, 400, 308-313.	2.6	36
158	Combination of the Replica-Exchange Monte Carlo Method and the Reference Interaction Site Model Theory for Simulating a Peptide Molecule in Aqueous Solution. Journal of Physical Chemistry B, 2004, 108, 19002-19012.	2.6	30
159	Liquidâ€“Gas Phase Transitions Studied by Multibaricâ€“Multithermal Monte Carlo Simulations. Journal of the Physical Society of Japan, 2004, 73, 3304-3311.	1.6	28
160	Classification and Prediction of Low-Energy Membrane Protein Helix Configurations by Replica-Exchange Monte Carlo Method. Journal of the Physical Society of Japan, 2004, 73, 2571-2585.	1.6	9
161	Molecular dynamics of C-peptide of ribonuclease A studied by replica-exchange Monte Carlo method and diffusion theory. Chemical Physics Letters, 2003, 380, 609-619.	2.6	18
162	Optimization of protein force-field parameters with the Protein Data Bank. Chemical Physics Letters, 2003, 382, 626-636.	2.6	31

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163	Replica-exchange multicanonical and multicanonical replica-exchange Monte Carlo simulations of peptides. II. Application to a more complex system. Journal of Chemical Physics, 2003, 118, 6676-6688.	3.0	79
164	Replica-exchange multicanonical and multicanonical replica-exchange Monte Carlo simulations of peptides. I. Formulation and benchmark test. Journal of Chemical Physics, 2003, 118, 6664-6675.	3.0	133
165	Multioverlap simulations for transitions between reference configurations. Physical Review E, 2003, 68, 036126.	2.1	49
166	Metropolis Algorithms in Generalized Ensemble. AIP Conference Proceedings, 2003, , .	0.4	4
167	A pH-dependent variation in ?-helix structure of the S-peptide of ribonuclease A studied by Monte Carlo simulated annealing. Biopolymers, 2002, 63, 273-279.	2.4	3
168	Generalized-ensemble simulations of spin systems and protein systems. Computer Physics Communications, 2002, 146, 69-76.	7.5	8
169	Free-Energy Calculations in Protein Folding by Generalized-Ensemble Algorithms. Lecture Notes in Computational Science and Engineering, 2002, , 304-332.	0.3	22
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