Yuji Sugita

List of Publications by Year in descending order

232 papers	13,069 citations	50276 46 h-index	25787 108 g-index
249 all docs	249 docs citations	249 times ranked	10985 citing authors

#	Article	IF	Citations
1	Weight average approaches for predicting dynamical properties of biomolecules. Current Opinion in Structural Biology, 2022, 72, 88-94.	5.7	3
2	Unraveling SARS-CoV-2 spike protein activation pathway reveals unprecedented cryptic pockets. Biophysical Journal, 2022, 121, 457a.	0.5	0
3	The inherent flexibility of receptor binding domains in SARS-CoV-2 spike protein. ELife, 2022, 11, .	6.0	40
4	Implementation of residue-level coarse-grained models in GENESIS for large-scale molecular dynamics simulations. PLoS Computational Biology, 2022, 18, e1009578.	3.2	27
5	Protein assembly and crowding simulations. Current Opinion in Structural Biology, 2022, 73, 102340.	5.7	18
6	Computational Analysis on the Allostery of Tryptophan Synthase: Relationship between Î±/Î²-Ligand Binding and Distal Domain Closure. Journal of Physical Chemistry B, 2022, 126, 3300-3308.	2.6	5
7	Practical Protocols for Efficient Sampling of Kinase-Inhibitor Binding Pathways Using Two-Dimensional Replica-Exchange Molecular Dynamics. Frontiers in Molecular Biosciences, 2022, 9, 878830.	3.5	3
8	Modified Hamiltonian in FEP Calculations for Reducing the Computational Cost of Electrostatic Interactions. Journal of Chemical Information and Modeling, 2022, 62, 2846-2856.	5.4	4
9	New parallel computing algorithm of molecular dynamics for extremely huge scale biological systems. Journal of Computational Chemistry, 2021, 42, 231-241.	3.3	40
10	Mutations of N1 Riboswitch Affect its Dynamics and Recognition by Neomycin Through Conformational Selection. Frontiers in Molecular Biosciences, 2021, 8, 633130.	3.5	9
11	Unraveling the Coupling between Conformational Changes and Ligand Binding in Ribose Binding Protein Using Multiscale Molecular Dynamics and Free-Energy Calculations. Journal of Physical Chemistry B, 2021, 125, 2898-2909.	2.6	7
12	Multi-Scale Flexible Fitting of Proteins to Cryo-EM Density Maps at Medium Resolution. Frontiers in Molecular Biosciences, 2021, 8, 631854.	3.5	13
13	Elucidation of interactions regulating conformational stability and dynamics of SARS-CoV-2 S-protein. Biophysical Journal, 2021, 120, 1060-1071.	0.5	57
14	Exploring the Minimum-Energy Pathways and Free-Energy Profiles of Enzymatic Reactions with QM/MM Calculations. Journal of Physical Chemistry B, 2021, 125, 4701-4713.	2.6	21
15	Coarse-Grained Modeling of Multiple Pathways in Conformational Transitions of Multi-Domain Proteins. Journal of Chemical Information and Modeling, 2021, 61, 2427-2443.	5.4	6
16	Efficient Flexible Fitting Refinement with Automatic Error Fixing for De Novo Structure Modeling from Cryo-EM Density Maps. Journal of Chemical Information and Modeling, 2021, 61, 3516-3528.	5.4	11
17	Anharmonic Vibrational Calculations Based on Group-Localized Coordinates: Applications to Internal Water Molecules in Bacteriorhodopsin. Journal of Chemical Theory and Computation, 2021, 17, 5007-5020.	5.3	8
18	Optimized Hydrogen Mass Repartitioning Scheme Combined with Accurate Temperature/Pressure Evaluations for Thermodynamic and Kinetic Properties of Biological Systems. Journal of Chemical Theory and Computation, 2021, 17, 5312-5321.	5.3	15

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19	Reduced efficacy of a Src kinase inhibitor in crowded protein solution. Nature Communications, 2021, 12, 4099.	12.8	22
20	Molecular Basis for Two Stereoselective Dielsâ€“Alderases that Produce Decalin Skeletons**. Angewandte Chemie, 2021, 133, 22575-22584.	2.0	0
21	Molecular Basis for Two Stereoselective Dielsâ€“Alderases that Produce Decalin Skeletons**. Angewandte Chemie - International Edition, 2021, 60, 22401-22410.	13.8	10
22	Innentitelbild: Molecular Basis for Two Stereoselective Dielsâ€“Alderases that Produce Decalin Skeletons (Angew. Chem. 41/2021). Angewandte Chemie, 2021, 133, 22258-22258.	2.0	0
23	Structural and energetic analysis of metastable intermediate states in the E1Pâ€“E2P transition of Ca ²⁺ -ATPase. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	13
24	Exploring Large Domain Motions in Proteins Using Atomistic Molecular Dynamics with Enhanced Conformational Sampling. International Journal of Molecular Sciences, 2021, 22, 270.	4.1	11
25	Role of the Nâ€Terminal Transmembrane Helix Contacts in the Activation of FGFR3. Journal of Computational Chemistry, 2020, 41, 561-572.	3.3	4
26	Amide A band is a fingerprint for water dynamics in reverse osmosis polyamide membranes. Journal of Membrane Science, 2020, 596, 117705.	8.2	15
27	Implicit Micelle Model for Membrane Proteins Using Superellipsoid Approximation. Journal of Chemical Theory and Computation, 2020, 16, 711-724.	5.3	10
28	Building a Macro-mixing Dual-basin Go Model using the Multistate Bennett Acceptance Ratio. Biophysical Journal, 2020, 118, 179a.	0.5	0
29	A singularity-free torsion angle potential for coarse-grained molecular dynamics simulations. Journal of Chemical Physics, 2020, 153, 044110.	3.0	5
30	Prediction of Proteinâ€“Ligand Binding Pose and Affinity Using the gREST+FEP Method. Journal of Chemical Information and Modeling, 2020, 60, 5382-5394.	5.4	26
31	Atg9 is a lipid scramblase that mediates autophagosomal membrane expansion. Nature Structural and Molecular Biology, 2020, 27, 1185-1193.	8.2	253
32	CHARMM-GUI Free Energy Calculator for Absolute and Relative Ligand Solvation and Binding Free Energy Simulations. Journal of Chemical Theory and Computation, 2020, 16, 7207-7218.	5.3	57
33	All-Atom Molecular Dynamics Simulation of the Altered Protein-Protein Interaction with Metabolites and Ions in the Cytoplasm. Biophysical Journal, 2020, 118, 217a.	0.5	0
34	Faces of Contemporary CryoEM Information and Modeling. Journal of Chemical Information and Modeling, 2020, 60, 2407-2409.	5.4	1
35	Mosaic Cooperativity in Slow Polypeptide Topological Isomerization Revealed by Residue-Specific NMR Thermodynamic Analysis. Journal of Physical Chemistry Letters, 2020, 11, 1934-1939.	4.6	8
36	Use of single-molecule time-series data for refining conformational dynamics in molecular simulations. Current Opinion in Structural Biology, 2020, 61, 153-159.	5.7	14

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37	Short disordered protein segment regulates cross-species transmission of a yeast prion. Nature Chemical Biology, 2020, 16, 756-765.	8.0	12
38	Free Energy Analysis of a Conformational Change of Heme ABC Transporter BhuUV-T. Journal of Physical Chemistry Letters, 2020, 11, 2824-2829.	4.6	9
39	Group-based evaluation of temperature and pressure for molecular dynamics simulation with a large time step. Journal of Chemical Physics, 2020, 153, 234115.	3.0	8
40	Molecular Dynamics Simulation of Glycans. Trends in Glycoscience and Glycotechnology, 2020, 32, E113-E118.	0.1	4
41	ALGORITHMS FOR BROWNIAN DYNAMICS SIMULATION. , 2020, , .		0
42	Molecular Dynamics Simulation of Glycans. Trends in Glycoscience and Glycotechnology, 2020, 32, J93-J98.	0.1	0
43	Replica-Exchange Methods for Biomolecular Simulations. Methods in Molecular Biology, 2019, 2022, 155-177.	0.9	16
44	De Novo Prediction of Binders and Nonbinders for T4 Lysozyme by gREST Simulations. Journal of Chemical Information and Modeling, 2019, 59, 3879-3888.	5.4	23
45	Whole-Cell Models and Simulations in Molecular Detail. Annual Review of Cell and Developmental Biology, 2019, 35, 191-211.	9.4	47
46	Chemo-Mechanical Coupling in the Transport Cycle of a Heme ABC Transporter. Journal of Physical Chemistry B, 2019, 123, 7270-7281.	2.6	6
47	Structural Mechanisms Underlying Activity Changes in an AMPA-type Glutamate Receptor Induced by Substitutions in Its Ligand-Binding Domain. Structure, 2019, 27, 1698-1709.e5.	3.3	3
48	Structural and Functional Basis for LILRB Immune Checkpoint Receptor Recognition of HLA-G Isoforms. Journal of Immunology, 2019, 203, 3386-3394.	0.8	33
49	Encounter complexes and hidden poses of kinase-inhibitor binding on the free-energy landscape. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 18404-18409.	7.1	41
50	Replica-Exchange Umbrella Sampling Combined with Gaussian Accelerated Molecular Dynamics for Free-Energy Calculation of Biomolecules. Journal of Chemical Theory and Computation, 2019, 15, 5199-5208.	5.3	64
51	Effect of proteinâ€“protein interactions and solvent viscosity on the rotational diffusion of proteins in crowded environments. Physical Chemistry Chemical Physics, 2019, 21, 876-883.	2.8	39
52	Frontiers in CryoEM Modeling. Journal of Chemical Information and Modeling, 2019, 59, 3091-3093.	5.4	2
53	Optimal Temperature and Pressure Evaluations in Molecular Dynamics Simulations with a Large Time Step. Biophysical Journal, 2019, 116, 141a.	0.5	0
54	Conformational Fluctuations and Changes of Sr-Ca2+-ATPase on the E1/E2 Transition. Biophysical Journal, 2019, 116, 435a.	0.5	0

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55	Integrative Modeling of Protein Dynamics from Time-Series Data of Single-Molecule Experiments and Molecular Dynamics Simulations. Biophysical Journal, 2019, 116, 343a.	0.5	1
56	Scaling molecular dynamics beyond 100,000 processor cores for largeâ€scale biophysical simulations. Journal of Computational Chemistry, 2019, 40, 1919-1930.	3.3	79
57	Anharmonic Vibrational Analysis of Biomolecules and Solvated Molecules Using Hybrid QM/MM Computations. Journal of Chemical Theory and Computation, 2019, 15, 1924-1938.	5.3	30
58	Clustering and dynamics of crowded proteins near membranes and their influence on membrane bending. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 24562-24567.	7.1	52
59	Population Shift Mechanism for Partial Agonism of AMPA Receptor. Biophysical Journal, 2019, 116, 57-68.	0.5	3
60	Optimal Temperature Evaluation in Molecular Dynamics Simulations with a Large Time Step. Journal of Chemical Theory and Computation, 2019, 15, 84-94.	5.3	14
61	Acceleration of cryo-EM Flexible Fitting for Large Biomolecular Systems by Efficient Space Partitioning. Structure, 2019, 27, 161-174.e3.	3.3	16
62	Building a macro-mixing dualâ€'basin GÅ•model using the Multistate Bennett Acceptance Ratio. Biophysics and Physicobiology, 2019, 16, 310-321.	1.0	4
63	Molecular Dynamics Simulations of a Riboswitch Binding Aminoglycoside Antibiotics. Biophysical Journal, 2018, 114, 433a.	0.5	0
64	Dynamics and Interactions of Proteins and Metabolites in Cellular Crowding Environments: All-Atom Molecular Dynamics Study of Proteins and Metabolites in Cellular Crowding Environments: All-atom Molecular Dynamics Study. Biophysical Journal, 2018, 114, 190a.	0.5	0
65	Characterization of Conformational Ensembles of Protonated N-glycans in the Gas-Phase. Scientific Reports, 2018, 8, 1644.	3.3	15
66	Protein Diffusion in a Dense Solution Studied by All-Atom Molecular Dynamics Simulations. Biophysical Journal, 2018, 114, 233a-234a.	0.5	0
67	Refining Markov state models for conformational dynamics using ensemble-averaged data and time-series trajectories. Journal of Chemical Physics, 2018, 148, 241731.	3.0	11
68	Structure of APP-C991â€“99 and implications for role of extra-membrane domains in function and oligomerization. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 1698-1708.	2.6	38
69	Effects of T686A Mutation on the Structural Stability of the AMPA Receptor Ligand-Binding Domain. Biophysical Journal, 2018, 114, 125a.	0.5	0
70	High-Performance Data Analysis on the Big Trajectory Data of Cellular Scale All-atom Molecular Dynamics Simulations. Journal of Physics: Conference Series, 2018, 1036, 012009.	0.4	6
71	Challenges and opportunities in connecting simulations with experiments via molecular dynamics of cellular environments. Journal of Physics: Conference Series, 2018, 1036, 012010.	0.4	20
72	Molecular Dynamics Simulations for Conformational Changes on a Reaction Step of SR-Ca2+-ATPase. Biophysical Journal, 2018, 114, 341a.	0.5	0

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73	Molecular mechanisms for dynamic regulation of N1 riboswitch by aminoglycosides. Nucleic Acids Research, 2018, 46, 9960-9970.	14.5	5
74	Flexible Choice of Solute in Replica Exchange with Solute Tempering Can Improve Performance of Conformation Search for Small Proteins. Biophysical Journal, 2018, 114, 676a.	0.5	0
75	Kinetic energy definition in velocity Verlet integration for accurate pressure evaluation. Journal of Chemical Physics, 2018, 148, 164109.	3.0	12
76	Flexible selection of the solute region in replica exchange with solute tempering: Application to protein-folding simulations. Journal of Chemical Physics, 2018, 149, 072304.	3.0	75
77	Linking time-series of single-molecule experiments with molecular dynamics simulations by machine learning. ELife, 2018, 7, .	6.0	40
78	Influence of protein crowder size on hydration structure and dynamics in macromolecular crowding. Chemical Physics Letters, 2017, 671, 63-70.	2.6	41
79	Enhanced Conformational Sampling of N-Glycans in Solution with Replica State Exchange Metadynamics. Journal of Chemical Theory and Computation, 2017, 13, 1934-1942.	5.3	16
80	Neural Network and Nearest Neighbor Algorithms for Enhancing Sampling of Molecular Dynamics. Journal of Chemical Theory and Computation, 2017, 13, 2489-2500.	5.3	51
81	Tunnel Formation Inferred from the I-Form Structures of the Proton-Driven Protein Secretion Motor SecDF. Cell Reports, 2017, 19, 895-901.	6.4	38
82	Weight-Averaged Anharmonic Vibrational Analysis of Hydration Structures of Polyamide 6. Journal of Physical Chemistry B, 2017, 121, 6050-6063.	2.6	11
83	Flexible fitting to cryoâ€EM density map using ensemble molecular dynamics simulations. Journal of Computational Chemistry, 2017, 38, 1447-1461.	3.3	46
84	Protein Diffusion Around Bacterial Nucleoid. Biophysical Journal, 2017, 112, 217a-218a.	0.5	0
85	Dynamics of nitric oxide controlled by protein complex in bacterial system. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 9888-9893.	7.1	35
86	GENESIS 1.1: A hybridâ€parallel molecular dynamics simulator with enhanced sampling algorithms on multiple computational platforms. Journal of Computational Chemistry, 2017, 38, 2193-2206.	3.3	133
87	Slow-Down in Diffusion in Crowded Protein Solutions Correlates with Transient Cluster Formation. Journal of Physical Chemistry B, 2017, 121, 11072-11084.	2.6	93
88	Crowding in Cellular Environments at an Atomistic Level from Computer Simulations. Journal of Physical Chemistry B, 2017, 121, 8009-8025.	2.6	136
89	Multiple program/multiple data molecular dynamics method with multiple time step integrator for large biological systems. Journal of Computational Chemistry, 2017, 38, 1410-1418.	3.3	6
90	Molecular Dynamics Simulations of Biomolecules in Cellular Environments. Molecular Science, 2017, 11, A0094.	0.2	2

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91	Dimensionality of Collective Variables for Describing Conformational Changes of a Multi-Domain Protein. Journal of Physical Chemistry Letters, 2016, 7, 1446-1451.	4.6	26
92	Detection of Sphingomyelin Clusters by Raman Spectroscopy. Biophysical Journal, 2016, 111, 999-1007.	0.5	35
93	Water Orientation at Ceramide/Water Interfaces Studied by Heterodyne-Detected Vibrational Sum Frequency Generation Spectroscopy and Molecular Dynamics Simulation. Journal of Physical Chemistry C, 2016, 120, 23692-23697.	3.1	12
94	Graphics Processing Unit Acceleration and Parallelization of GENESIS for Large-Scale Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2016, 12, 4947-4958.	5.3	24
95	Anharmonic Vibrational Analyses of Pentapeptide Conformations Explored with Enhanced Sampling Simulations. Journal of Physical Chemistry B, 2016, 120, 10199-10213.	2.6	11
96	Thermodynamics of Macromolecular Association in Heterogeneous Crowding Environments: Theoretical and Simulation Studies with a Simplified Model. Journal of Physical Chemistry B, 2016, 120, 11856-11865.	2.6	23
97	Exploring N-Glycan Conformers: Assessment of Enhanced Sampling Algorithms. Biophysical Journal, 2016, 110, 643a.	0.5	0
98	Mechanisms for Two-Step Proton Transfer Reactions in the Outward-Facing Form of MATE Transporter. Biophysical Journal, 2016, 110, 1346-1354.	0.5	16
99	Rational design of crystal contactâ€free space in protein crystals for analyzing spatial distribution of motions within protein molecules. Protein Science, 2016, 25, 754-768.	7.6	10
100	Parallel implementation of 3D FFT with volumetric decomposition schemes for efficient molecular dynamics simulations. Computer Physics Communications, 2016, 200, 57-65.	7.5	20
101	Dynamics and Interactions of OmpF and LPS: Influence on Pore Accessibility and Ion Permeability. Biophysical Journal, 2016, 110, 930-938.	0.5	64
102	Molecular dynamics simulations of biological membranes and membrane proteins using enhanced conformational sampling algorithms. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1635-1651.	2.6	111
103	Biomolecular interactions modulate macromolecular structure and dynamics in atomistic model of a bacterial cytoplasm. ELife, 2016, 5, .	6.0	238
104	Crystal Structures of SecYEG in Lipidic Cubic Phase Elucidate a Precise Resting and a Peptide-Bound State. Cell Reports, 2015, 13, 1561-1568.	6.4	58
105	GENESIS: a hybridâ€parallel and multiâ€scale molecular dynamics simulator with enhanced sampling algorithms for biomolecular and cellular simulations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 310-323.	14.6	166
106	Replica state exchange metadynamics for improving the convergence of free energy estimates. Journal of Computational Chemistry, 2015, 36, 1446-1455.	3.3	18
107	Hierarchical domainâ€motion analysis of conformational changes in sarcoplasmic reticulum Ca²⁺â€ATPase. Proteins: Structure, Function and Bioinformatics, 2015, 83, 746-756.	2.6	7
108	Complete atomistic model of a bacterial cytoplasm for integrating physics, biochemistry, and systems biology. Journal of Molecular Graphics and Modelling, 2015, 58, 1-9.	2.4	71

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109	A weight averaged approach for predicting amide vibrational bands of a sphingomyelin bilayer. Physical Chemistry Chemical Physics, 2015, 17, 29113-29123.	2.8	13
110	REIN: Replicaâ€exchange INterface for simulating protein dynamics and function. International Journal of Quantum Chemistry, 2015, 115, 325-332.	2.0	3
111	Sequential data assimilation for single-molecule FRET photon-counting data. Journal of Chemical Physics, 2015, 142, 214115.	3.0	12
112	Domain Motion Enhanced (DoME) Model for Efficient Conformational Sampling of Multidomain Proteins. Journal of Physical Chemistry B, 2015, 119, 14584-14593.	2.6	14
113	Mosaic of Water Orientation Structures at a Neutral Zwitterionic Lipid/Water Interface Revealed by Molecular Dynamics Simulations. Journal of Physical Chemistry Letters, 2014, 5, 4343-4348.	4.6	59
114	Midpoint cell method for hybrid (MPI+OpenMP) parallelization of molecular dynamics simulations. Journal of Computational Chemistry, 2014, 35, 1064-1072.	3.3	22
115	Structural basis of Sec-independent membrane protein insertion by YidC. Nature, 2014, 509, 516-520.	27.8	203
116	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
117	CHARMM Force-Fields with Modified Polyphosphate Parameters Allow Stable Simulation of the ATP-Bound Structure of Ca²⁺-ATPase. Journal of Chemical Theory and Computation, 2014, 10, 4133-4142.	5.3	14
118	Multidimensional umbrella sampling and replicaâ€exchange molecular dynamics simulations for structure prediction of transmembrane helix dimers. Journal of Computational Chemistry, 2014, 35, 300-308.	3.3	32
119	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
120	Surface-Tension Replica-Exchange Molecular Dynamics Method for Efficient Conformational Sampling of Biological Membrane Systems. Biophysical Journal, 2014, 106, 704a.	0.5	1
121	Drug Extrusion Process of Mate Multidrug Efflux Transporter Revealed by Molecular Dynamics Simulations. Biophysical Journal, 2014, 106, 801a.	0.5	1
122	1P204 Structure and orientation of hydrating water molecules at phospholipid/water interface revealed by molecular dynamics simulation(13A. Biological & Artificial membrane: Structure &) Tj ETQq0 0 0 rgBT /Overlock 10 Butsuri, 2014, 54, S174.	0.1	0
123	1P105 Molecular dynamics simulations of ATP/ADP bound forms of SR Ca^<2+>-ATPase using CHARMM force field with modified polyphosphate parameters(03. Membrane proteins,Poster,The 52nd Annual) Tj ETQq1 1 0.784314 rgBT /Ove	0.1	0
124	1P216 Surface-tension replica-exchange molecular dynamics simulations of biological membrane systems(13B. Biological & Artificial membrane: Dynamics,Poster,The 52nd Annual Meeting of the) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	0.1	0
125	1P129 Free-energy analysis of the effect of ions on protein structure(07. Water & Hydration &) Tj ETQq1 1 0.784314 rgBT /Ov Butsuri, 2014, 54, S162.	0.1	0
126	3P058 Dynamics and Interactions of Macromolecules in the Bacterial Cytoplasm : All-atom Molecular Dynamics Study(01C. Protein: Property,Poster,The 52nd Annual Meeting of the Biophysical Society of) Tj ETQq0 0 0 rgBT /Overlock 10 T	0.1	0

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127	Protein Folding Simulations by Generalized-Ensemble Algorithms. Advances in Experimental Medicine and Biology, 2014, 805, 1-27.	1.6	7
128	Decoupling Architecture for All-to-all Computation. , 2014, , .		0
129	Conformational Diversity of N-Glycans in Solution Studied by REMD Simulations. Biophysical Journal, 2013, 104, 170a.	0.5	0
130	Different Scale Conformational Changes of SERCA Analyzed with Motion Tree Method. Biophysical Journal, 2013, 104, 665a.	0.5	0
131	Improved Constrained Optimization Method for Reaction-Path Determination in Quantum Mechanical/Molecular Mechanical Calculations. Biophysical Journal, 2013, 104, 511a.	0.5	0
132	Reaching new levels of realism in modeling biological macromolecules in cellular environments. Journal of Molecular Graphics and Modelling, 2013, 45, 144-156.	2.4	58
133	Multiple Conformers and their Spectroscopic Properties of N-Glycan Predicted using Replica-Exchange Simulations. Biophysical Journal, 2013, 104, 665a.	0.5	0
134	Stability of Proteins in Cellular Environments. Biophysical Journal, 2013, 104, 566a.	0.5	0
135	Free Energy Analysis on the Tom20-Presequence Complex in Solution for Understanding a Dynamic-Equilibrium Model. Biophysical Journal, 2013, 104, 665a.	0.5	0
136	Efficient Parallel Implementations of QM/MM-REMD (Quantum Mechanical/Molecular) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 387 Td (Me Journal of Physical Chemistry B, 2013, 117, 7996-8002.	2.6	26
137	Reduced Native State Stability in Crowded Cellular Environment Due to Proteinâ€“Protein Interactions. Journal of the American Chemical Society, 2013, 135, 3696-3701.	13.7	145
138	Interionic Hydration Structures of NaCl in Aqueous Solution: A Combined Study of Quantum Mechanical Cluster Calculations and QM/EFP-MD Simulations. Journal of Physical Chemistry B, 2013, 117, 289-295.	2.6	47
139	Solvent Electronic Polarization Effects on Na⁺â€“Na⁺ and Cl^{â€“}â€“Cl^{â€“} Pair Associations in Aqueous Solution. Journal of Physical Chemistry B, 2013, 117, 9273-9279.	2.6	24
140	Energetics of the Presequence-Binding Poses in Mitochondrial Protein Import Through Tom20. Journal of Physical Chemistry B, 2013, 117, 2864-2871.	2.6	11
141	Surface-Tension Replica-Exchange Molecular Dynamics Method for Enhanced Sampling of Biological Membrane Systems. Journal of Chemical Theory and Computation, 2013, 9, 5629-5640.	5.3	37
142	Improved constrained optimization method for reaction-path determination in the generalized hybrid orbital quantum mechanical/molecular mechanical calculations. Journal of Chemical Physics, 2013, 138, 044106.	3.0	8
143	Efficient lookup table using a linear function of inverse distance squared. Journal of Computational Chemistry, 2013, 34, 2412-2420.	3.3	21
144	Structural basis for dynamic mechanism of proton-coupled symport by the peptide transporter POT. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 11343-11348.	7.1	197

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145	3P112 Interaction between cholesterol and transmembrane region of Amyloid Precursor Protein(03.) Tj ETQq1 1 0.784314 rgBT /Ove	0.1	0
146	Crystal structure of Î±5Î²1 integrin ectodomain: Atomic details of the fibronectin receptor. Journal of Cell Biology, 2012, 197, 131-140.	5.2	193
147	The Intertransmembrane Region of Kaposi's Sarcoma-Associated Herpesvirus Modulator of Immune Recognition 2 Contributes to B7-2 Downregulation. Journal of Virology, 2012, 86, 5288-5296.	3.4	13
148	2PT139 Molecular dynamics simulations of SR Ca2+-pump in the ATP bound forms(The 50th Annual) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	0.1	0
149	Effect of Bisecting GlcNAc and Core Fucosylation on Conformational Properties of Biantennary Complex-Type N-Glycans in Solution. Journal of Physical Chemistry B, 2012, 116, 8504-8512.	2.6	79
150	Confident identification of isomeric Nâ€glycan structures by combined ion mobility mass spectrometry and hydrophilic interaction liquid chromatography. Rapid Communications in Mass Spectrometry, 2012, 26, 2877-2884.	1.5	50
151	Protein-Protein Interactions in Crowded Cellular Environments. Biophysical Journal, 2012, 102, 473a.	0.5	0
152	Quantum mechanical/effective fragment potential molecular dynamics (QM/EFP-MD) study on intra-molecular proton transfer of glycine in water. Chemical Physics Letters, 2012, 539-540, 218-221.	2.6	28
153	Analysis of the Area Per Lipid in Protein-Membrane Systems. Biophysical Journal, 2012, 102, 81a.	0.5	0
154	Conformational flexibility of N-glycans in solution studied by REMD simulations. Biophysical Reviews, 2012, 4, 179-187.	3.2	40
155	In silico mutants of nitric oxide reductases provide insights into development of proton pathways in the heme-copper oxidase superfamily. Biochimica Et Biophysica Acta - Bioenergetics, 2012, 1817, S150.	1.0	0
156	Crystal structure of quinol-dependent nitric oxide reductase from Geobacillus stearothermophilus. Nature Structural and Molecular Biology, 2012, 19, 238-245.	8.2	106
157	Variable Interactions between Protein Crowders and Biomolecular Solutes Are Important in Understanding Cellular Crowding. Journal of Physical Chemistry B, 2012, 116, 599-605.	2.6	127
158	Protein Crowding Affects Hydration Structure and Dynamics. Journal of the American Chemical Society, 2012, 134, 4842-4849.	13.7	189
159	Rapid flip-flop motions of diacylglycerol and ceramide in phospholipid bilayers. Chemical Physics Letters, 2012, 522, 96-102.	2.6	52
160	Analysis of lipid surface area in proteinâ€“membrane systems combining voronoi tessellation and monte carlo integration methods. Journal of Computational Chemistry, 2012, 33, 286-293.	3.3	32
161	Molecular Dynamics Simulations Reveal Proton Transfer Pathways in Cytochrome C-Dependent Nitric Oxide Reductase. PLoS Computational Biology, 2012, 8, e1002674.	3.2	27
162	Folding Simulation of a Mini Protein with a Hydrophobic Core and .ALPHA.-helices. Seibutsu Butsuri, 2012, 52, 022-023.	0.1	0

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163	Recent Applications of Replica-Exchange Molecular Dynamics Simulations of Biomolecules. Current Physical Chemistry, 2012, 2, 401-412.	0.2	1
164	Functionality Mapping on Internal Surfaces of Multidrug Transporter AcrB Based on Molecular Theory of Solvation: Implications for Drug Efflux Pathway. Journal of Physical Chemistry B, 2011, 115, 8288-8295.	2.6	45
165	Theoretical Study of Magnesium Fluoride in Aqueous Solution. Journal of Physical Chemistry B, 2011, 115, 10553-10559.	2.6	13
166	Structural Diversity and Changes in Conformational Equilibria of Biantennary Complex-Type N-Glycans in Water Revealed by Replica-Exchange Molecular Dynamics Simulation. Biophysical Journal, 2011, 101, L44-L46.	0.5	42
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