

Qiang Shao

List of Publications by Year in descending order

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Version: 2024-02-01

66
papers

1,841
citations

279798

23
h-index

289244

40
g-index

70
all docs

70
docs citations

70
times ranked

2368
citing authors

#	ARTICLE	IF	CITATIONS
1	Enhanced sampling in molecular dynamics. <i>Journal of Chemical Physics</i> , 2019, 151, 070902.	3.0	243
2	Identification of pyrogallol as a warhead in design of covalent inhibitors for the SARS-CoV-2 3CL protease. <i>Nature Communications</i> , 2021, 12, 3623.	12.8	111
3	Methanol Strengthens Hydrogen Bonds and Weakens Hydrophobic Interactions in Proteins – A Combined Molecular Dynamics and NMR study. <i>Journal of Physical Chemistry B</i> , 2011, 115, 6653-6660.	2.6	80
4	What coronavirus 3C-like protease tells us: From structure, substrate selectivity, to inhibitor design. <i>Medicinal Research Reviews</i> , 2021, 41, 1965-1998.	10.5	73
5	From Thermodynamics to Kinetics: Enhanced Sampling of Rare Events. <i>Accounts of Chemical Research</i> , 2015, 48, 947-955.	15.6	66
6	On the influence of hydrated imidazolium-based ionic liquid on protein structure stability: A molecular dynamics simulation study. <i>Journal of Chemical Physics</i> , 2013, 139, 115102.	3.0	58
7	Exploring Transition Pathway and Free-Energy Profile of Large-Scale Protein Conformational Change by Combining Normal Mode Analysis and Umbrella Sampling Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , 2014, 118, 134-143.	2.6	58
8	Thermodynamics and Folding Pathways of Trpzip2: An Accelerated Molecular Dynamics Simulation Study. <i>Journal of Physical Chemistry B</i> , 2009, 113, 803-808.	2.6	56
9	Force fields and scoring functions for carbohydrate simulation. <i>Carbohydrate Research</i> , 2015, 401, 73-81.	2.3	49
10	On the hand-over-hand mechanism of kinesin. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 8072-8077.	7.1	48
11	Structural basis for DNA recognition by STAT6. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, 13015-13020.	7.1	46
12	From protein denaturant to protectant: Comparative molecular dynamics study of alcohol/protein interactions. <i>Journal of Chemical Physics</i> , 2012, 136, 115101.	3.0	44
13	Comparison between integrated and parallel tempering methods in enhanced sampling simulations. <i>Journal of Chemical Physics</i> , 2009, 130, 124111.	3.0	43
14	Thermodynamics and kinetics simulations of multi-time-scale processes for complex systems. <i>International Reviews in Physical Chemistry</i> , 2008, 27, 201-227.	2.3	40
15	Enhanced sampling molecular dynamics simulation captures experimentally suggested intermediate and unfolded states in the folding pathway of Trp-cage miniprotein. <i>Journal of Chemical Physics</i> , 2012, 137, 125103.	3.0	40
16	Effects of drug-resistant mutations on the dynamic properties of HIV-1 protease and inhibition by Amprenavir and Darunavir. <i>Scientific Reports</i> , 2015, 5, 10517.	3.3	39
17	The effects of organic solvents on the folding pathway and associated thermodynamics of proteins: a microscopic view. <i>Scientific Reports</i> , 2016, 6, 19500.	3.3	39
18	Effects of Turn Stability and Side-Chain Hydrophobicity on the Folding of β^2 -Structures. <i>Journal of Molecular Biology</i> , 2010, 402, 595-609.	4.2	37

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19	Assessing AMBER force fields for protein folding in an implicit solvent. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 7206-7216.	2.8	35
20	The Stabilization Effect of Dielectric Constant and Acidic Amino Acids on Arginine-Arginine (Arg-Arg) Pairings: Database Survey and Computational Studies. <i>Journal of Physical Chemistry B</i> , 2013, 117, 4827-4835.	2.6	33
21	Temperature Dependence of Hydrogen-Bond Stability in β^2 -Hairpin Structures. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3750-3760.	5.3	32
22	A Combined Theoretical and Experimental Study of the Ammonia Tunnel in Carbamoyl Phosphate Synthetase. <i>Journal of the American Chemical Society</i> , 2009, 131, 10211-10219.	13.7	30
23	Thermodynamics calculation of protein-ligand interactions by QM/MM polarizable charge parameters. <i>Journal of Biomolecular Structure and Dynamics</i> , 2016, 34, 163-176.	3.5	26
24	Molecular Dynamics and Ion Mobility Spectrometry Study of Model β^2 -Hairpin Peptide, Trpzip1. <i>Journal of Physical Chemistry A</i> , 2011, 115, 4427-4435.	2.5	23
25	A test of implicit solvent models on the folding simulation of the GB1 peptide. <i>Journal of Chemical Physics</i> , 2009, 130, 195104.	3.0	22
26	The relative helix and hydrogen bond stability in the B domain of protein A as revealed by integrated tempering sampling molecular dynamics simulation. <i>Journal of Chemical Physics</i> , 2011, 135, 135102.	3.0	22
27	Exploring the Ligand Binding/Unbinding Pathway by Selectively Enhanced Sampling of Ligand in a Protein-Ligand Complex. <i>Journal of Physical Chemistry B</i> , 2019, 123, 7974-7983.	2.6	21
28	Exploring Conformational Change of Adenylate Kinase by Replica Exchange Molecular Dynamic Simulation. <i>Biophysical Journal</i> , 2020, 118, 1009-1018.	0.5	21
29	Structure change of β^2 -hairpin induced by turn optimization: An enhanced sampling molecular dynamics simulation study. <i>Journal of Chemical Physics</i> , 2011, 135, 235104.	3.0	20
30	Ammonium Transport Proteins with Changes in One of the Conserved Pore Histidines Have Different Performance in Ammonia and Methylamine Conduction. <i>PLoS ONE</i> , 2013, 8, e62745.	2.5	20
31	Determining Protein Folding Pathway and Associated Energetics through Partitioned Integrated-Tempering-Sampling Simulation. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1229-1243.	5.3	20
32	Direct Observation of the Uptake of Outer Membrane Proteins by the Periplasmic Chaperone Skp. <i>PLoS ONE</i> , 2012, 7, e46068.	2.5	19
33	How Do Distance and Solvent Affect Halogen Bonding Involving Negatively Charged Donors?. <i>Journal of Physical Chemistry B</i> , 2016, 120, 8784-8793.	2.6	19
34	Enhanced conformational sampling technique provides an energy landscape view of large-scale protein conformational transitions. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 29170-29182.	2.8	17
35	Energetics and structural characterization of the α -DFG-flip-conformational transition of B-RAF kinase: a SITS molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 1257-1267.	2.8	17
36	The effects of side chain hydrophobicity on the denaturation of simple β^2 -hairpins. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 9292.	2.8	16

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37	Mapping Central α -Helix Linker Mediated Conformational Transition Pathway of Calmodulin via Simple Computational Approach. <i>Journal of Physical Chemistry B</i> , 2014, 118, 9677-9685.	2.6	16
38	Design, Synthesis, and Pharmacological Evaluation of Fused β -Homophenylalanine Derivatives as Potent DPP-4 Inhibitors. <i>ACS Medicinal Chemistry Letters</i> , 2015, 6, 602-606.	2.8	16
39	Structural insights into HIV-1 protease flap opening processes and key intermediates. <i>RSC Advances</i> , 2017, 7, 45121-45128.	3.6	16
40	In silico screening-based discovery of novel covalent inhibitors of the SARS-CoV-2 3CL protease. <i>European Journal of Medicinal Chemistry</i> , 2022, 231, 114130.	5.5	16
41	How Well Can Implicit Solvent Simulations Explore Folding Pathways? A Quantitative Analysis of α -Helix Bundle Proteins. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 6177-6190.	5.3	15
42	Probing Sequence Dependence of Folding Pathway of α -Helix Bundle Proteins through Free Energy Landscape Analysis. <i>Journal of Physical Chemistry B</i> , 2014, 118, 5891-5900.	2.6	14
43	Carbamate Transport in Carbamoyl Phosphate Synthetase: A Theoretical and Experimental Investigation. <i>Journal of the American Chemical Society</i> , 2010, 132, 3870-3878.	13.7	13
44	Improving the accuracy of predicting protein-ligand binding-free energy with semiempirical quantum chemistry charge. <i>Future Medicinal Chemistry</i> , 2019, 11, 303-321.	2.3	13
45	Counterion Effects on the Denaturing Activity of Guanidinium Cation to Protein. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 4364-4373.	5.3	12
46	Robustness in Protein Folding Revealed by Thermodynamics Calculations. <i>Journal of Physical Chemistry B</i> , 2012, 116, 13848-13856.	2.6	11
47	Molecular dynamics simulation indicating cold denaturation of β -hairpins. <i>Journal of Chemical Physics</i> , 2013, 138, 085102.	3.0	10
48	The addition of 2,2,2-trifluoroethanol prevents the aggregation of guanidinium around protein and impairs its denaturation ability: A molecular dynamics simulation study. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 944-953.	2.6	10
49	Methanol Concentration Dependent Protein Denaturing Ability of Guanidinium/Methanol Mixed Solution. <i>Journal of Physical Chemistry B</i> , 2014, 118, 6175-6185.	2.6	10
50	Folding or Misfolding: The Choice of β -Hairpin. <i>Journal of Physical Chemistry B</i> , 2015, 119, 3893-3900.	2.6	10
51	The universality of β -hairpin misfolding indicated by molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2013, 139, 165103.	3.0	9
52	Water plays an important role in osmolyte-induced hairpin structure change: A molecular dynamics simulation study. <i>Journal of Chemical Physics</i> , 2012, 137, 145101.	3.0	8
53	Design, Synthesis, and Pharmacological Evaluation of Highly Potent and Selective Dipeptidyl Peptidase-4 Inhibitors. <i>Archiv Der Pharmazie</i> , 2015, 348, 399-407.	4.1	7
54	Nonnative contact effects in protein folding. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 11924-11936.	2.8	7

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55	Ligand binding effects on the activation of the EGFR extracellular domain. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 8141-8151.	2.8	7
56	Modeling the Thermal Unfolding 2DIR Spectra of a β^2 -Hairpin Peptide Based on the Implicit Solvent MD Simulation. <i>Journal of Physical Chemistry A</i> , 2013, 117, 6256-6263.	2.5	6
57	Selective enhanced sampling in dihedral energy facilitates overcoming the dihedral energy increase in protein folding and accelerates the searching for protein native structure. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 10423-10435.	2.8	6
58	Asymmetry in Kinesin Walking. <i>Biochemistry</i> , 2007, 46, 9098-9106.	2.5	5
59	Effective Conformational Sampling in Explicit Solvent with Gaussian Biased Accelerated Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 4240-4252.	5.3	5
60	Increasing the sampling efficiency of protein conformational transition using velocity-scaling optimized hybrid explicit/implicit solvent REMD simulation. <i>Journal of Chemical Physics</i> , 2015, 142, 125105.	3.0	4
61	Important roles of hydrophobic interactions in folding and charge interactions in misfolding of β -helix bundle protein. <i>RSC Advances</i> , 2015, 5, 4191-4199.	3.6	3
62	The effects of implicit modeling of nonpolar solvation on protein folding simulations. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 18410-18419.	2.8	3
63	On the influence of the mixture of denaturants on protein structure stability: A molecular dynamics study. <i>Chemical Physics</i> , 2014, 441, 38-46.	1.9	2
64	The Protein Folding Mechanism Revealed by the Folding Free Energy Landscape Analysis and Denaturation Simulations. <i>Current Physical Chemistry</i> , 2012, 2, 33-44.	0.2	1
65	Conformational Dynamics, Intramolecular Domain Conformation Signaling, and Activation of Apo-FimD Revealed by Single-Molecule Fluorescence Resonance Energy Transfer Studies. <i>Biochemistry</i> , 2019, 58, 1931-1941.	2.5	1
66	Front Cover Image, Volume 41, Issue 4. <i>Medicinal Research Reviews</i> , 2021, 41, i.	10.5	0