Qiang Shao

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/698550/publications.pdf

Version: 2024-02-01

66	1,841	279798	289244
papers	citations	23 h-index	40 g-index

70	70	70	2368
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	In silico screening-based discovery of novel covalent inhibitors of the SARS-CoV-2 3CL protease. European Journal of Medicinal Chemistry, 2022, 231, 114130.	5.5	16
2	What coronavirus 3Câ€like protease tells us: From structure, substrate selectivity, to inhibitor design. Medicinal Research Reviews, 2021, 41, 1965-1998.	10.5	73
3	Front Cover Image, Volume 41, Issue 4. Medicinal Research Reviews, 2021, 41, i.	10.5	0
4	Identification of pyrogallol as a warhead in design of covalent inhibitors for the SARS-CoV-2 3CL protease. Nature Communications, 2021, 12, 3623.	12.8	111
5	Exploring Conformational Change of Adenylate Kinase by Replica Exchange Molecular Dynamic Simulation. Biophysical Journal, 2020, 118, 1009-1018.	0.5	21
6	Enhanced sampling in molecular dynamics. Journal of Chemical Physics, 2019, 151, 070902.	3.0	243
7	Exploring the Ligand Binding/Unbinding Pathway by Selectively Enhanced Sampling of Ligand in a Proteinâ€“Ligand Complex. Journal of Physical Chemistry B, 2019, 123, 7974-7983.	2.6	21
8	Nonnative contact effects in protein folding. Physical Chemistry Chemical Physics, 2019, 21, 11924-11936.	2.8	7
9	Conformational Dynamics, Intramolecular Domain Conformation Signaling, and Activation of Apo-FimD Revealed by Single-Molecule Fluorescence Resonance Energy Transfer Studies. Biochemistry, 2019, 58, 1931-1941.	2.5	1
10	Ligand binding effects on the activation of the EGFR extracellular domain. Physical Chemistry Chemical Physics, 2019, 21, 8141-8151.	2.8	7
11	Selective enhanced sampling in dihedral energy facilitates overcoming the dihedral energy increase in protein folding and accelerates the searching for protein native structure. Physical Chemistry Chemical Physics, 2019, 21, 10423-10435.	2.8	6
12	Improving the accuracy of predicting proteinâ€“ligand binding-free energy with semiempirical quantum chemistry charge. Future Medicinal Chemistry, 2019, 11, 303-321.	2.3	13
13	Assessing AMBER force fields for protein folding in an implicit solvent. Physical Chemistry Chemical Physics, 2018, 20, 7206-7216.	2.8	35
14	The effects of implicit modeling of nonpolar solvation on protein folding simulations. Physical Chemistry Chemical Physics, 2018, 20, 18410-18419.	2.8	3
15	Determining Protein Folding Pathway and Associated Energetics through Partitioned Integrated-Tempering-Sampling Simulation. Journal of Chemical Theory and Computation, 2017, 13, 1229-1243.	5.3	20
16	Energetics and structural characterization of the â€œDFG-flipâ€•conformational transition of B-RAF kinase: a SITS molecular dynamics study. Physical Chemistry Chemical Physics, 2017, 19, 1257-1267.	2.8	17
17	Structural insights into HIV-1 protease flap opening processes and key intermediates. RSC Advances, 2017, 7, 45121-45128.	3.6	16
18	Effective Conformational Sampling in Explicit Solvent with Gaussian Biased Accelerated Molecular Dynamics. Journal of Chemical Theory and Computation, 2017, 13, 4240-4252.	5.3	5

#	Article	IF	Citations
19	How Well Can Implicit Solvent Simulations Explore Folding Pathways? A Quantitative Analysis of Î±-Helix Bundle Proteins. Journal of Chemical Theory and Computation, 2017, 13, 6177-6190.	5.3	15
20	The effects of organic solvents on the folding pathway and associated thermodynamics of proteins: a microscopic view. Scientific Reports, 2016, 6, 19500.	3.3	39
21	Enhanced conformational sampling technique provides an energy landscape view of large-scale protein conformational transitions. Physical Chemistry Chemical Physics, 2016, 18, 29170-29182.	2.8	17
22	How Do Distance and Solvent Affect Halogen Bonding Involving Negatively Charged Donors?. Journal of Physical Chemistry B, 2016, 120, 8784-8793.	2.6	19
23	Structural basis for DNA recognition by STAT6. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 13015-13020.	7.1	46
24	Thermodynamics calculation of proteinâ€“ligand interactions by QM/MM polarizable charge parameters. Journal of Biomolecular Structure and Dynamics, 2016, 34, 163-176.	3.5	26
25	Folding or Misfolding: The Choice of Î²-Hairpin. Journal of Physical Chemistry B, 2015, 119, 3893-3900.	2.6	10
26	Effects of drug-resistant mutations on the dynamic properties of HIV-1 protease and inhibition by Amprenavir and Darunavir. Scientific Reports, 2015, 5, 10517.	3.3	39
27	From Thermodynamics to Kinetics: Enhanced Sampling of Rare Events. Accounts of Chemical Research, 2015, 48, 947-955.	15.6	66
28	Design, Synthesis, and Pharmacological Evaluation of Highly Potent and Selective Dipeptidyl Peptidaseâ€4 Inhibitors. Archiv Der Pharmazie, 2015, 348, 399-407.	4.1	7
29	Design, Synthesis, and Pharmacological Evaluation of Fused Î²-Homophenylalanine Derivatives as Potent DPP-4 Inhibitors. ACS Medicinal Chemistry Letters, 2015, 6, 602-606.	2.8	16
30	Increasing the sampling efficiency of protein conformational transition using velocity-scaling optimized hybrid explicit/implicit solvent REMD simulation. Journal of Chemical Physics, 2015, 142, 125105.	3.0	4
31	Important roles of hydrophobic interactions in folding and charge interactions in misfolding of Î±-helix bundle protein. RSC Advances, 2015, 5, 4191-4199.	3.6	3
32	Force fields and scoring functions for carbohydrate simulation. Carbohydrate Research, 2015, 401, 73-81.	2.3	49
33	The addition of 2,2,2â€trifluoroethanol prevents the aggregation of guanidinium around protein and impairs its denaturation ability: A molecular dynamics simulation study. Proteins: Structure, Function and Bioinformatics, 2014, 82, 944-953.	2.6	10
34	Exploring Transition Pathway and Free-Energy Profile of Large-Scale Protein Conformational Change by Combining Normal Mode Analysis and Umbrella Sampling Molecular Dynamics. Journal of Physical Chemistry B, 2014, 118, 134-143.	2.6	58
35	Methanol Concentration Dependent Protein Denaturing Ability of Guanidinium/Methanol Mixed Solution. Journal of Physical Chemistry B, 2014, 118, 6175-6185.	2.6	10
36	Mapping Central Î±-Helix Linker Mediated Conformational Transition Pathway of Calmodulin via Simple Computational Approach. Journal of Physical Chemistry B, 2014, 118, 9677-9685.	2.6	16

#	Article	IF	Citations
37	On the influence of the mixture of denaturants on protein structure stability: A molecular dynamics study. Chemical Physics, 2014, 441, 38-46.	1.9	2
38	Probing Sequence Dependence of Folding Pathway of Î±-Helix Bundle Proteins through Free Energy Landscape Analysis. Journal of Physical Chemistry B, 2014, 118, 5891-5900.	2.6	14
39	On the influence of hydrated imidazolium-based ionic liquid on protein structure stability: A molecular dynamics simulation study. Journal of Chemical Physics, 2013, 139, 115102.	3.0	58
40	Molecular dynamics simulation indicating cold denaturation of Î²-hairpins. Journal of Chemical Physics, 2013, 138, 085102.	3.0	10
41	The universality of Î²-hairpin misfolding indicated by molecular dynamics simulations. Journal of Chemical Physics, 2013, 139, 165103.	3.0	9
42	The Stabilization Effect of Dielectric Constant and Acidic Amino Acids on Arginineâ€“Arginine (Argâ€“Arg) Pairings: Database Survey and Computational Studies. Journal of Physical Chemistry B, 2013, 117, 4827-4835.	2.6	33
43	Modeling the Thermal Unfolding 2DIR Spectra of a Î²-Hairpin Peptide Based on the Implicit Solvent MD Simulation. Journal of Physical Chemistry A, 2013, 117, 6256-6263.	2.5	6
44	Ammonium Transport Proteins with Changes in One of the Conserved Pore Histidines Have Different Performance in Ammonia and Methylamine Conduction. PLoS ONE, 2013, 8, e62745.	2.5	20
45	Water plays an important role in osmolyte-induced hairpin structure change: A molecular dynamics simulation study. Journal of Chemical Physics, 2012, 137, 145101.	3.0	8
46	From protein denaturant to protectant: Comparative molecular dynamics study of alcohol/protein interactions. Journal of Chemical Physics, 2012, 136, 115101.	3.0	44
47	Counterion Effects on the Denaturing Activity of Guanidinium Cation to Protein. Journal of Chemical Theory and Computation, 2012, 8, 4364-4373.	5.3	12
48	Robustness in Protein Folding Revealed by Thermodynamics Calculations. Journal of Physical Chemistry B, 2012, 116, 13848-13856.	2.6	11
49	Enhanced sampling molecular dynamics simulation captures experimentally suggested intermediate and unfolded states in the folding pathway of Trp-cage miniprotein. Journal of Chemical Physics, 2012, 137, 125103.	3.0	40
50	Direct Observation of the Uptake of Outer Membrane Proteins by the Periplasmic Chaperone Skp. PLoS ONE, 2012, 7, e46068.	2.5	19
51	The Protein Folding Mechanism Revealed by the Folding Free Energy Landscape Analysis and Denaturation Simulations. Current Physical Chemistry, 2012, 2, 33-44.	0.2	1
52	Methanol Strengthens Hydrogen Bonds and Weakens Hydrophobic Interactions in Proteins â€“ A Combined Molecular Dynamics and NMR study. Journal of Physical Chemistry B, 2011, 115, 6653-6660.	2.6	80
53	Molecular Dynamics and Ion Mobility Spectrometry Study of Model Î²-Hairpin Peptide, Trpzip1. Journal of Physical Chemistry A, 2011, 115, 4427-4435.	2.5	23
54	The relative helix and hydrogen bond stability in the B domain of protein A as revealed by integrated tempering sampling molecular dynamics simulation. Journal of Chemical Physics, 2011, 135, 135102.	3.0	22

#	Article	IF	Citations
55	Structure change of Î²-hairpin induced by turn optimization: An enhanced sampling molecular dynamics simulation study. Journal of Chemical Physics, 2011, 135, 235104.	3.0	20
56	Carbamate Transport in Carbamoyl Phosphate Synthetase: A Theoretical and Experimental Investigation. Journal of the American Chemical Society, 2010, 132, 3870-3878.	13.7	13
57	Temperature Dependence of Hydrogen-Bond Stability in Î²-Hairpin Structures. Journal of Chemical Theory and Computation, 2010, 6, 3750-3760.	5.3	32
58	Effects of Turn Stability and Side-Chain Hydrophobicity on the Folding of Î²-Structures. Journal of Molecular Biology, 2010, 402, 595-609.	4.2	37
59	The effects of side chain hydrophobicity on the denaturation of simple Î²-hairpins. Physical Chemistry Chemical Physics, 2010, 12, 9292.	2.8	16
60	Comparison between integrated and parallel tempering methods in enhanced sampling simulations. Journal of Chemical Physics, 2009, 130, 124111.	3.0	43
61	A test of implicit solvent models on the folding simulation of the GB1 peptide. Journal of Chemical Physics, 2009, 130, 195104.	3.0	22
62	Thermodynamics and Folding Pathways of Trpzip2: An Accelerated Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2009, 113, 803-808.	2.6	56
63	A Combined Theoretical and Experimental Study of the Ammonia Tunnel in Carbamoyl Phosphate Synthetase. Journal of the American Chemical Society, 2009, 131, 10211-10219.	13.7	30
64	Thermodynamics and kinetics simulations of multi-time-scale processes for complex systems. International Reviews in Physical Chemistry, 2008, 27, 201-227.	2.3	40
65	Asymmetry in Kinesin Walking. Biochemistry, 2007, 46, 9098-9106.	2.5	5
66	On the hand-over-hand mechanism of kinesin. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 8072-8077.	7.1	48