Fangqiang Zhu

List of Publications by Year
in descending order

32 papers	1,739 citations	516710 16 h-index	454955 30 g-index
32 all docs	32 docs citations	32 times ranked	2112 citing authors

#	Article	IF	Citations
1	Discovery of Small-Molecule Inhibitors of SARS-CoV-2 Proteins Using a Computational and Experimental Pipeline. Frontiers in Molecular Biosciences, 2021, 8, 678701.	3.5	22
2	Toward Convergence in Free Energy Calculations for Protein Conformational Changes: A Case Study on the Thin Gate of Mhp1 Transporter. Journal of Chemical Theory and Computation, 2021, 17, 6583-6596.	5.3	3
3	High-throughput virtual screening of small molecule inhibitors for SARS-CoV-2 protein targets with deep fusion models. , 2021, , .		7
4	Assessing the Perturbing Effects of Drugs on Lipid Bilayers Using Gramicidin Channel-Based In Silico and In Vitro Assays. Journal of Medicinal Chemistry, 2020, 63, 11809-11818.	6.4	10
5	Binding Affinity Prediction by Pairwise Function Based on Neural Network. Journal of Chemical Information and Modeling, 2020, 60, 2766-2772.	5.4	39
6	Calculating Single-Channel Permeability and Conductance from Transition Paths. Journal of Chemical Information and Modeling, 2019, 59, 777-785.	5.4	10
7	Kinetic mechanism for water in vibrating carbon nanotubes. Physical Review E, 2018, 98, .	2.1	5
8	Vitamin E Has Reduced Affinity for a Polyunsaturated Phospholipid: An Umbrella Sampling Molecular Dynamics Simulations Study. Journal of Physical Chemistry B, 2018, 122, 8351-8358.	2.6	9
9	Structural Model of the Tubular Assembly of the Rous Sarcoma Virus Capsid Protein. Journal of the American Chemical Society, 2017, 139, 2006-2013.	13.7	10
10	Parameter Optimization for Interaction between C-Terminal Domains of HIV-1 Capsid Protein. Journal of Chemical Information and Modeling, 2017, 57, 1134-1141.	5.4	3
11	Calculating transition rates from durations of transition paths. Journal of Chemical Physics, 2017, 146, 124128.	3.0	5
12	Thermodynamics of Protein Folding Studied by Umbrella Sampling along a Reaction Coordinate of Native Contacts. Journal of Chemical Theory and Computation, 2017, 13, 2086-2097.	5.3	20
13	Finite Temperature String Method with Umbrella Sampling: Application on a Side Chain Flipping in Mhp1 Transporter. Journal of Physical Chemistry B, 2017, 121, 3376-3386.	2.6	14
14	Construction of a novel coarse grain model for simulations of HIV capsid assembly to capture the backbone structure and inter-domain motions in solution. Data in Brief, 2015, 5, 506-512.	1.0	9
15	Conformational Changes in Two Inter-Helical Loops of Mhp1 Membrane Transporter. PLoS ONE, 2015, 10, e0133388.	2.5	11
16	Mechanism of polymorphism and curvature of HIV capsid assemblies probed by 3D simulations with a novel coarse grain model. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 2353-2367.	2.4	32
17	Interface dipole enhancement effect and enhanced Rayleigh scattering. Nano Research, 2015, 8, 303-319.	10.4	12
18	True-color real-time imaging and spectroscopy of carbon nanotubes on substrates using enhanced Rayleigh scattering. Nano Research, 2015, 8, 2721-2732.	10.4	34

#	ARTICLE	IF	CITATIONS
19	Monte Carlo Simulations of HIV Capsid Protein Homodimer. Journal of Chemical Information and Modeling, 2015, 55, 1361-1368.	5.4	11
20	Evaluating membrane affinity by integrating protein orientations. Journal of Molecular Graphics and Modelling, 2014, 54, 141-147.	2.4	0
21	How does Water Pass through a Sugar Transporter?. Biophysical Journal, 2014, 106, 1229-1230.	0.5	4
22	Collective Diffusion Model for Ion Conduction through Microscopic Channels. Biophysical Journal, 2013, 104, 368-376.	0.5	18
23	Conformational Dynamics of a Ligand-Free Adenylate Kinase. PLoS ONE, 2013, 8, e68023.	2.5	27
24	Drying Transition in the Hydrophobic Gate of the GLIC Channel Blocks Ion Conduction. Biophysical Journal, 2012, 103, 219-227.	0.5	94
25	Theory and Simulation of Ion Conduction in the Pentameric GLIC Channel. Journal of Chemical Theory and Computation, 2012, 8, 3759-3768.	5.3	62
26	Convergence and error estimation in free energy calculations using the weighted histogram analysis method. Journal of Computational Chemistry, 2012, 33, 453-465.	3.3	187
27	Water Transport through Nanotubes with Varying Interaction Strength between Tube Wall and Water. Journal of Physical Chemistry Letters, 2011, 2, 2978-2983.	4.6	90
28	Pore opening and closing of a pentameric ligand-gated ion channel. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 19814-19819.	7.1	145
29	Gating Transition of Pentameric Ligand-Gated Ion Channels. Biophysical Journal, 2009, 97, 2456-2463.	0.5	35
30	Collective Diffusion Model for Water Permeation through Microscopic Channels. Physical Review Letters, 2004, 93, 224501.	7.8	204
31	Theory and Simulation of Water Permeation in Aquaporin-1. Biophysical Journal, 2004, 86, 50-57.	0.5	332
32	Water and Proton Conduction through Carbon Nanotubes as Models for Biological Channels. Biophysical Journal, 2003, 85, 236-244.	0.5	275