Yi Wang

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4394676/publications.pdf

Version: 2024-02-01

45 papers	4,854 citations	196777 29 h-index	274796 44 g-index
47 all docs	47 docs citations	47 times ranked	7055 citing authors

#	Article	IF	Citations
1	Enhanced mechanosensing of cells in synthetic 3D matrix with controlled biophysical dynamics. Nature Communications, 2021, 12, 3514.	5.8	92
2	Scalable molecular dynamics on CPU and GPU architectures with NAMD. Journal of Chemical Physics, 2020, 153, 044130.	1.2	1,548
3	Pore formation induced by nanoparticles binding to a lipid membrane. Nanoscale, 2020, 12, 7902-7913.	2.8	7
4	Accelerating Membrane Simulations with Hydrogen Mass Repartitioning. Journal of Chemical Theory and Computation, 2019, 15, 4673-4686.	2.3	85
5	Affordable Membrane Permeability Calculations: Permeation of Short-Chain Alcohols through Pure-Lipid Bilayers and a Mammalian Cell Membrane. Journal of Chemical Theory and Computation, 2019, 15, 2913-2924.	2.3	27
6	Mechanistic basis for the evolution of chalcone synthase catalytic cysteine reactivity in land plants. Journal of Biological Chemistry, 2018, 293, 18601-18612.	1.6	38
7	Structural and dynamic basis of substrate permissiveness in hydroxycinnamoyltransferase (HCT). PLoS Computational Biology, 2018, 14, e1006511.	1.5	25
8	Selective Permeability of Carboxysome Shell Pores to Anionic Molecules. Journal of Physical Chemistry B, 2018, 122, 9110-9118.	1.2	54
9	Link between Membrane Composition and Permeability to Drugs. Journal of Chemical Theory and Computation, 2018, 14, 2895-2909.	2.3	35
10	Reverse Binding Mode of Phosphotyrosine Peptides with SH2 Protein. Biochemistry, 2018, 57, 5257-5269.	1.2	6
11	Gaussian Accelerated Molecular Dynamics in NAMD. Journal of Chemical Theory and Computation, 2017, 13, 9-19.	2.3	117
12	A Rationally Designed, General Strategy for Membrane Orientation of Photoinduced Electron Transfer-Based Voltage-Sensitive Dyes. ACS Chemical Biology, 2017, 12, 407-413.	1.6	40
13	Anchored but not internalized: shape dependent endocytosis of nanodiamond. Scientific Reports, 2017, 7, 46462.	1.6	31
14	Estimation of Nanodiamond Surface Charge Density from Zeta Potential and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2017, 121, 3394-3402.	1.2	39
15	Virtual substitution scan via singleâ€step free energy perturbation. Biopolymers, 2016, 105, 324-336.	1.2	3
16	The role of intramolecular nonbonded interaction and angle sampling in single-step free energy perturbation. Journal of Chemical Physics, 2016, 145, 234109.	1.2	1
17	Simulation-Based Approaches for Determining Membrane Permeability of Small Compounds. Journal of Chemical Information and Modeling, 2016, 56, 721-733.	2.5	174
18	Antimicrobial Peptide Simulations and the Influence of Force Field on the Free Energy for Pore Formation in Lipid Bilayers. Journal of Chemical Theory and Computation, 2016, 12, 4524-4533.	2.3	78

#	Article	IF	Citations
19	Dynamic Conformational States Dictate Selectivity toward the Native Substrate in a Substrate-Permissive Acyltransferase. Biochemistry, 2016, 55, 6314-6326.	1.2	57
20	Investigation of the conformational dynamics of the apo A_{2A} adenosine receptor. Protein Science, 2015, 24, 1004-1012.	3.1	11
21	Free Energy Calculation of Nanodiamond-Membrane Associationâ€"The Effect of Shape and Surface Functionalization. Journal of Chemical Theory and Computation, 2014, 10, 2751-2758.	2.3	24
22	Microsecond Molecular Dynamics Simulations of Lipid Mixing. Langmuir, 2014, 30, 11993-12001.	1.6	101
23	Effects of histidine protonation and rotameric states on virtual screening of M. tuberculosis RmlC. Journal of Computer-Aided Molecular Design, 2013, 27, 235-246.	1.3	42
24	Structureâ€based network analysis of an evolved G proteinâ€coupled receptor homodimer interface. Protein Science, 2013, 22, 745-754.	3.1	11
25	Introduction to Molecular Dynamics: Theory and Applications in Biomolecular Modeling. Biological and Medical Physics Series, 2012, , 3-30.	0.3	4
26	Accelerated molecular dynamics: Theory, implementation and applications. , 2012, , .		4
27	Comparative molecular dynamics simulations of the antimicrobial peptide CM15 in model lipid bilayers. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 1402-1409.	1.4	81
28	Spectroscopic and Computational Study of Melittin, Cecropin A, and the Hybrid Peptide CM15. Journal of Physical Chemistry B, 2012, 116, 10600-10608.	1.2	37
29	Independent-Trajectory Thermodynamic Integration: A Practical Guide to Protein-Drug Binding Free Energy Calculations Using Distributed Computing. Methods in Molecular Biology, 2012, 819, 469-486.	0.4	10
30	Enhanced Lipid Diffusion and Mixing in Accelerated Molecular Dynamics. Journal of Chemical Theory and Computation, 2011, 7, 3199-3207.	2.3	62
31	Implementation of accelerated molecular dynamics in NAMD. Computational Science & Discovery, 2011, 4, 015002.	1.5	124
32	Effects of Biomolecular Flexibility on Alchemical Calculations of Absolute Binding Free Energies. Journal of Chemical Theory and Computation, 2011, 7, 2224-2232.	2.3	18
33	Novel inhibitors of Mycobacterium tuberculosis dTDP-6-deoxy-l-lyxo-4-hexulose reductase (RmlD) identified by virtual screening. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 7064-7067.	1.0	23
34	Nitric oxide conduction by the brain aquaporin AQP4. Proteins: Structure, Function and Bioinformatics, 2010, 78, 661-670.	1.5	84
35	Identification of triazinoindol-benzimidazolones as nanomolar inhibitors of the Mycobacterium tuberculosis enzyme TDP-6-deoxy-d-xylo-4-hexopyranosid-4-ulose 3,5-epimerase (RmlC). Bioorganic and Medicinal Chemistry, 2010, 18, 896-908.	1.4	79
36	Tyrosine phosphorylation by Src within the cavity of the adenine nucleotide translocase 1 regulates ADP/ATP exchange in mitochondria. American Journal of Physiology - Cell Physiology, 2010, 298, C740-C748.	2.1	55

#	Article	IF	Citations
37	Exploring Transmembrane Diffusion Pathways With Molecular Dynamics. Physiology, 2010, 25, 142-154.	1.6	42
38	Structural and Functional Analysis of SoPIP2;1 Mutants Adds Insight into Plant Aquaporin Gating. Journal of Molecular Biology, 2009, 387, 653-668.	2.0	95
39	Electrostatic funneling of substrate in mitochondrial inner membrane carriers. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 9598-9603.	3.3	133
40	Chapter 12 Gas Conduction of Lipid Bilayers and Membrane Channels. Current Topics in Membranes, 2008, 60, 343-367.	0.5	12
41	Exploring gas permeability of cellular membranes and membrane channels with molecular dynamics. Journal of Structural Biology, 2007, 157, 534-544.	1.3	184
42	Molecular Mechanisms of Conduction and Selectivity in Aquaporin Water Channels. Journal of Nutrition, 2007, 137, 1509S-1515S.	1.3	68
43	Structural mechanism of plant aquaporin gating. Nature, 2006, 439, 688-694.	13.7	752
44	What Makes an Aquaporin a Glycerol Channel? A Comparative Study of AqpZ and GlpF. Structure, 2005, 13, 1107-1118.	1.6	159
45	Molecular dynamics simulations of proteins in lipid bilayers. Current Opinion in Structural Biology, 2005, 15, 423-431.	2.6	180