

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

172457

29
h-index

243625

44
g-index

47
all docs

47
docs citations

47
times ranked

6282
citing authors

#	ARTICLE	IF	CITATIONS
1	Enhanced mechanosensing of cells in synthetic 3D matrix with controlled biophysical dynamics. <i>Nature Communications</i> , 2021, 12, 3514.	12.8	92
2	Scalable molecular dynamics on CPU and GPU architectures with NAMD. <i>Journal of Chemical Physics</i> , 2020, 153, 044130.	3.0	1,548
3	Pore formation induced by nanoparticles binding to a lipid membrane. <i>Nanoscale</i> , 2020, 12, 7902-7913.	5.6	7
4	Accelerating Membrane Simulations with Hydrogen Mass Repartitioning. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4673-4686.	5.3	85
5	Affordable Membrane Permeability Calculations: Permeation of Short-Chain Alcohols through Pure-Lipid Bilayers and a Mammalian Cell Membrane. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2913-2924.	5.3	27
6	Mechanistic basis for the evolution of chalcone synthase catalytic cysteine reactivity in land plants. <i>Journal of Biological Chemistry</i> , 2018, 293, 18601-18612.	3.4	38
7	Structural and dynamic basis of substrate permissiveness in hydroxycinnamoyltransferase (HCT). <i>PLoS Computational Biology</i> , 2018, 14, e1006511.	3.2	25
8	Selective Permeability of Carboxysome Shell Pores to Anionic Molecules. <i>Journal of Physical Chemistry B</i> , 2018, 122, 9110-9118.	2.6	54
9	Link between Membrane Composition and Permeability to Drugs. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2895-2909.	5.3	35
10	Reverse Binding Mode of Phosphotyrosine Peptides with SH2 Protein. <i>Biochemistry</i> , 2018, 57, 5257-5269.	2.5	6
11	Gaussian Accelerated Molecular Dynamics in NAMD. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 9-19.	5.3	117
12	A Rationally Designed, General Strategy for Membrane Orientation of Photoinduced Electron Transfer-Based Voltage-Sensitive Dyes. <i>ACS Chemical Biology</i> , 2017, 12, 407-413.	3.4	40
13	Anchored but not internalized: shape dependent endocytosis of nanodiamond. <i>Scientific Reports</i> , 2017, 7, 46462.	3.3	31
14	Estimation of Nanodiamond Surface Charge Density from Zeta Potential and Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3394-3402.	2.6	39
15	Virtual substitution scan via single-step free energy perturbation. <i>Biopolymers</i> , 2016, 105, 324-336.	2.4	3
16	The role of intramolecular nonbonded interaction and angle sampling in single-step free energy perturbation. <i>Journal of Chemical Physics</i> , 2016, 145, 234109.	3.0	1
17	Simulation-Based Approaches for Determining Membrane Permeability of Small Compounds. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 721-733.	5.4	174
18	Antimicrobial Peptide Simulations and the Influence of Force Field on the Free Energy for Pore Formation in Lipid Bilayers. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 4524-4533.	5.3	78

#	ARTICLE	IF	CITATIONS
19	Dynamic Conformational States Dictate Selectivity toward the Native Substrate in a Substrate-Permissive Acyltransferase. <i>Biochemistry</i> , 2016, 55, 6314-6326.	2.5	57
20	Investigation of the conformational dynamics of the apo A _{2A} adenosine receptor. <i>Protein Science</i> , 2015, 24, 1004-1012.	7.6	11
21	Free Energy Calculation of Nanodiamond-Membrane Association—The Effect of Shape and Surface Functionalization. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2751-2758.	5.3	24
22	Microsecond Molecular Dynamics Simulations of Lipid Mixing. <i>Langmuir</i> , 2014, 30, 11993-12001.	3.5	101
23	Effects of histidine protonation and rotameric states on virtual screening of <i>M. tuberculosis</i> RmlC. <i>Journal of Computer-Aided Molecular Design</i> , 2013, 27, 235-246.	2.9	42
24	Structure-based network analysis of an evolved G protein-coupled receptor homodimer interface. <i>Protein Science</i> , 2013, 22, 745-754.	7.6	11
25	Introduction to Molecular Dynamics: Theory and Applications in Biomolecular Modeling. <i>Biological and Medical Physics Series</i> , 2012, , 3-30.	0.4	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. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2012, 1818, 1402-1409.	2.6	81
28	Spectroscopic and Computational Study of Melittin, Cecropin A, and the Hybrid Peptide CM15. <i>Journal of Physical Chemistry B</i> , 2012, 116, 10600-10608.	2.6	37
29	Independent-Trajectory Thermodynamic Integration: A Practical Guide to Protein-Drug Binding Free Energy Calculations Using Distributed Computing. <i>Methods in Molecular Biology</i> , 2012, 819, 469-486.	0.9	10
30	Enhanced Lipid Diffusion and Mixing in Accelerated Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 3199-3207.	5.3	62
31	Implementation of accelerated molecular dynamics in NAMD. <i>Computational Science & Discovery</i> , 2011, 4, 015002.	1.5	124
32	Effects of Biomolecular Flexibility on Alchemical Calculations of Absolute Binding Free Energies. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 2224-2232.	5.3	18
33	Novel inhibitors of <i>Mycobacterium tuberculosis</i> dTDP-6-deoxy-l-xylo-4-hexulose reductase (RmlD) identified by virtual screening. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2011, 21, 7064-7067.	2.2	23
34	Nitric oxide conduction by the brain aquaporin AQP4. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 661-670.	2.6	84
35	Identification of triazinoindol-benzimidazolones as nanomolar inhibitors of the <i>Mycobacterium tuberculosis</i> enzyme TDP-6-deoxy-d-xylo-4-hexopyranosid-4-ulose 3,5-epimerase (RmlC). <i>Bioorganic and Medicinal Chemistry</i> , 2010, 18, 896-908.	3.0	79
36	Tyrosine phosphorylation by Src within the cavity of the adenine nucleotide translocase 1 regulates ADP/ATP exchange in mitochondria. <i>American Journal of Physiology - Cell Physiology</i> , 2010, 298, C740-C748.	4.6	55

#	ARTICLE	IF	CITATIONS
37	Exploring Transmembrane Diffusion Pathways With Molecular Dynamics. <i>Physiology</i> , 2010, 25, 142-154.	3.1	42
38	Structural and Functional Analysis of SoPIP2;1 Mutants Adds Insight into Plant Aquaporin Gating. <i>Journal of Molecular Biology</i> , 2009, 387, 653-668.	4.2	95
39	Electrostatic funneling of substrate in mitochondrial inner membrane carriers. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 9598-9603.	7.1	133
40	Chapter 12 Gas Conduction of Lipid Bilayers and Membrane Channels. <i>Current Topics in Membranes</i> , 2008, 60, 343-367.	0.9	12
41	Exploring gas permeability of cellular membranes and membrane channels with molecular dynamics. <i>Journal of Structural Biology</i> , 2007, 157, 534-544.	2.8	184
42	Molecular Mechanisms of Conduction and Selectivity in Aquaporin Water Channels. <i>Journal of Nutrition</i> , 2007, 137, 1509S-1515S.	2.9	68
43	Structural mechanism of plant aquaporin gating. <i>Nature</i> , 2006, 439, 688-694.	27.8	752
44	What Makes an Aquaporin a Glycerol Channel? A Comparative Study of AqpZ and GlpF. <i>Structure</i> , 2005, 13, 1107-1118.	3.3	159
45	Molecular dynamics simulations of proteins in lipid bilayers. <i>Current Opinion in Structural Biology</i> , 2005, 15, 423-431.	5.7	180