Song Wang

List of Publications by Year
in descending order

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40 papers	320 citations	840776 11 h-index	996975 15 g-index
40 all docs	40 docs citations	40 times ranked	435 citing authors

#	Article	IF	Citations
1	In silico study to predict potential precursors of human dipeptidyl peptidase-IV inhibitors from hazelnut. Journal of Biomolecular Structure and Dynamics, 2022, 40, 11664-11675.	3.5	4
2	Exploration of the Interactions between Maltaseâ€“Glucoamylase and Its Potential Peptide Inhibitors by Molecular Dynamics Simulation. Catalysts, 2022, 12, 522.	3.5	0
3	The study on the inhibitory mechanism of JTZ-951 and its analogue against prolyl hydroxylase-2 to mediate the response to hypoxia in the process of sports. Molecular Physics, 2021, 119, .	1.7	0
4	Structural basis of different surface-modified fullerene derivatives as novel thrombin inhibitors: insight into the inhibitory mechanism through molecular modelling studies. Molecular Physics, 2021, 119, .	1.7	0
5	Penicillin biosensor based on rhombusâ€shaped porous carbon/hematoxylin/penicillinase. Journal of Food Science, 2021, 86, 3505-3516.	3.1	8
6	Targeting N-Terminal Human Maltase-Glucoamylase to Unravel Possible Inhibitors Using Molecular Docking, Molecular Dynamics Simulations, and Adaptive Steered Molecular Dynamics Simulations. Frontiers in Chemistry, 2021, 9, 711242.	3.6	7
7	Structural basis of fullerene derivatives as novel potent inhibitors of protein acetylcholinesterase without catalytic active site interaction: insight into the inhibitory mechanism through molecular modeling studies. Journal of Biomolecular Structure and Dynamics, 2020, 38, 410-425.	3.5	13
8	A novel HIV-1 inhibitor that blocks viral replication and rescues APOBEC3s by interrupting vif/CBFÎ² interaction. Journal of Biological Chemistry, 2020, 295, 14592-14605.	3.4	12
9	The C-terminal domain of feline and bovine SAMHD1 proteins has a crucial role in lentiviral restriction. Journal of Biological Chemistry, 2020, 295, 4252-4264.	3.4	6
10	Exploration of Binding Mechanism of a Potential Streptococcus pneumoniae Neuraminidase Inhibitor from Herbaceous Plants by Molecular Simulation. International Journal of Molecular Sciences, 2020, 21, 1003.	4.1	6
11	How Different Substitution Positions of F, Cl Atoms in Benzene Ring of 5-Methylpyrimidine Pyridine Derivatives Affect the Inhibition Ability of EGFRL858R/T790M/C797S Inhibitors: A Molecular Dynamics Simulation Study. Molecules, 2020, 25, 895.	3.8	9
12	Insight into the process of product expulsion in cellobiohydrolase Cel6A from Trichoderma reesei by computational modeling. Journal of Biomolecular Structure and Dynamics, 2019, 37, 1360-1374.	3.5	2
13	A novel small molecule displays two different binding modes during inhibiting H1N1 influenza A virus neuraminidases. Journal of Structural Biology, 2018, 202, 142-149.	2.8	4
14	Effects of Tyr555 and Trp678 on the processivity of cellobiohydrolase A from Ruminiclostridium thermocellum: A simulation study. Biopolymers, 2018, 109, e23238.	2.4	2
15	Why Is a High Temperature Needed by Thermus thermophilus Argonaute During mRNA Silencing: A Theoretical Study. Frontiers in Chemistry, 2018, 6, 223.	3.6	9
16	Binding modes of phosphotriesterase-like lactonase complexed with Î´-nonanoic lactone and paraoxon using molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2017, 35, 273-286.	3.5	10
17	Theoretical prediction on the synthesis of 2,3â€dihydropyridines through Co(III)â€catalysed reaction of unsaturated oximes with alkenes. International Journal of Quantum Chemistry, 2017, 117, e25353.	2.0	1
18	Understanding the Phosphorylation Mechanism by Using Quantum Chemical Calculations and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2017, 121, 3565-3573.	2.6	12

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19	Exploration of binding and inhibition mechanism of a small molecule inhibitor of influenza virus H1N1 hemagglutinin by molecular dynamics simulation. Scientific Reports, 2017, 7, 3786.	3.3	28
20	Theoretical Insights into the Synthesis of 2,3â€Dihydropyridines from Unsaturated Oximes by Rh‹sup›III‹/sup›â€Catalyzed Câ€“H Activation â€“ A DFT Study. European Journal of Organic Chemistry, 2017, 2017, 397-408.	2.4	1
21	Investigation of an â€œalternate water supply systemâ€•in enzymatic hydrolysis in the processive endocellulase Cel7A from ‹scp›‹i›R‹/i›‹/scp›‹i›asamsonia emersonii‹/i› by molecular dynamics simulation. Biopolymers, 2017, 107, 46-60.	2.4	2
22	Structural and molecular basis of cellulase Cel48F by computational modeling: Insight into catalytic and product release mechanism. Journal of Structural Biology, 2016, 194, 347-356.	2.8	15
23	Structural Basis of Fullerene Derivatives as Novel Potent Inhibitors of Protein Tyrosine Phosphatase 1B: Insight into the Inhibitory Mechanism through Molecular Modeling Studies. Journal of Chemical Information and Modeling, 2016, 56, 2024-2034.	5.4	26
24	Insight into the interactive residues between two domains of human somatic Angiotensin-converting enzyme and Angiotensin II by MM-PBSA calculation and steered molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2016, 34, 15-28.	3.5	21
25	A novel antimicrobial peptide derived from membrane-proximal external region of human immunodeficiency virus type 1. Biochimie, 2016, 123, 110-116.	2.6	3
26	Conserved stem fragment from H3 influenza hemagglutinin elicits cross-clade neutralizing antibodies through stalk-targeted blocking of conformational change during membrane fusion. Immunology Letters, 2016, 172, 11-20.	2.5	11
27	Stereoselectivity of phosphotriesterase with paraoxon derivatives: a computational study. Journal of Biomolecular Structure and Dynamics, 2016, 34, 600-611.	3.5	9
28	Elicitation of HIV-1 neutralizing antibodies by presentation of 4E10 and 10E8 epitopes on Norovirus P particles. Immunology Letters, 2015, 168, 271-278.	2.5	12
29	Changes in the phase morphology of miktoarm PS-b-PMMA copolymer induced by a monolayer surface. Colloid and Polymer Science, 2015, 293, 2831-2844.	2.1	8
30	Conformational changes in MetNI: steered molecular dynamic studies of the methionine ABC transporter with and without substrates. Molecular Simulation, 2015, 41, 613-621.	2.0	1
31	Narrow bandgap covalentâ€“organic frameworks with strong optical response in the visible and infrared. Journal of Materials Chemistry C, 2015, 3, 2244-2254.	5.5	18
32	MesoDyn simulation study on the phase morphologies of miktoarm PSâ€‹i›b‹/i›â€PMMA copolymer doped by nanoparticles. Journal of Applied Polymer Science, 2013, 127, 1561-1568.	2.6	8
33	Insights into the specific binding site of adenosine to the Stx2, the protein toxin from‹i›Escherichia coli‹/i›O157:H7 using molecular dynamics simulations and free energy calculations. Molecular Simulation, 2013, 39, 199-205.	2.0	5
34	MesoDyn simulation study on the phase morphologies of miktoarm PEO-b-PMMA copolymer induced by surfaces. Journal of Polymer Research, 2012, 19, 1.	2.4	6
35	Mesoscopic simulation of the surface inducing effects on the compatibility of PSâ€‹i›b‹/i›â€PMMA copolymers. Journal of Applied Polymer Science, 2012, 124, 879-889.	2.6	4
36	Computer modelling study on the compatibility of PEOâ€“PMMA block copolymers. Molecular Simulation, 2011, 37, 90-99.	2.0	0

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37	A density functional investigation of the reaction mechanism of H₂O + HCNO. International Journal of Quantum Chemistry, 2011, 111, 165-173.	2.0	4
38	Computer modeling study on the phase morphology of PSâ€bâ€PMMA copolymers. Journal of Applied Polymer Science, 2011, 119, 265-274.	2.6	6
39	Modeling and analysis of the compatibility of poly(ethylene oxide)/poly(methyl methacrylate) blends with surface and shear inducing effects. Journal of Applied Polymer Science, 2011, 122, 64-75.	2.6	13
40	Theoretical study on the mechanism of OHÂ+ÂHCNO reaction. Theoretical Chemistry Accounts, 2007, 118, 337-345.	1.4	14