Jinyu Li

List of Publications by Year in descending order

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48 papers	929 citations	516710 16 h-index	501196 28 g-index
50 all docs	50 docs citations	50 times ranked	1326 citing authors

#	Article	IF	Citations
1	Bispecific Aptamer Induced Artificial Protein-Pairing: A Strategy for Selective Inhibition of Receptor Function. Journal of the American Chemical Society, 2019, 141, 12673-12681.	13.7	102
2	Selfâ€Assembled and Sizeâ€Controllable Oligonucleotide Nanospheres for Effective Antisense Gene Delivery through an Endocytosisâ€Independent Pathway. Angewandte Chemie - International Edition, 2019, 58, 5236-5240.	13.8	97
3	Water desalination across multilayer graphitic carbon nitride membrane: Insights from non-equilibrium molecular dynamics simulations. Carbon, 2018, 140, 131-138.	10.3	75
4	Exploration of the mechanism for LPFFD inhibiting the formation of Î²-sheet conformation of AÎ²(1â€“42) in water. Journal of Molecular Modeling, 2010, 16, 813-821.	1.8	48
5	Characterization of the binding of angiotensin II receptor blockers to human serum albumin using docking and molecular dynamics simulation. Journal of Molecular Modeling, 2010, 16, 789-798.	1.8	39
6	A novel tumor and mitochondria dual-targeted photosensitizer showing ultra-efficient photodynamic anticancer activities. Chemical Communications, 2019, 55, 866-869.	4.1	39
7	The effect of solvents on the conformations of Amyloid Î²-peptide (1â€“42) studied by molecular dynamics simulation. Computational and Theoretical Chemistry, 2009, 895, 1-8.	1.5	36
8	Proton Dynamics in Protein Mass Spectrometry. Journal of Physical Chemistry Letters, 2017, 8, 1105-1112.	4.6	34
9	Smart Photosensitizer: Tumor-Triggered Oncotherapy by Self-Assembly Photodynamic Nanodots. ACS Applied Materials & Interfaces, 2018, 10, 15369-15380.	8.0	34
10	Nucleolar-nucleoplasmic shuttling of TARG1 and its control by DNA damage-induced poly-ADP-ribosylation and by nucleolar transcription. Scientific Reports, 2018, 8, 6748.	3.3	32
11	Mechanistic investigation of the cis/trans isomerization of 2-butene on Pt(111): DFT study of the influence of the hydrogen coverage. Journal of Catalysis, 2014, 311, 190-198.	6.2	23
12	Selfâ€Assembled and Sizeâ€Controllable Oligonucleotide Nanospheres for Effective Antisense Gene Delivery through an Endocytosisâ€Independent Pathway. Angewandte Chemie, 2019, 131, 5290-5294.	2.0	23
13	Molecular basis of rutin inhibition of protein disulfide isomerase (PDI) by combinedin silicoand experimental methods. RSC Advances, 2018, 8, 18480-18491.	3.6	22
14	Structural basis of sequence-specific Holliday junction cleavage by MOC1. Nature Chemical Biology, 2019, 15, 1241-1248.	8.0	21
15	Cryo-electron Microscopy Structure of the Swine Acute Diarrhea Syndrome Coronavirus Spike Glycoprotein Provides Insights into Evolution of Unique Coronavirus Spike Proteins. Journal of Virology, 2020, 94, .	3.4	17
16	Enhanced Sampling Approach to the Induced-Fit Docking Problem in Proteinâ€“Ligand Binding: The Case of Mono-ADP-Ribosylation Hydrolase Inhibitors. Journal of Chemical Theory and Computation, 2021, 17, 7899-7911.	5.3	17
17	Erlotinib Analogueâ€substituted Zinc(II) Phthalocyanines for Small Molecular Targetâ€based Photodynamic Cancer Therapy. Chinese Journal of Chemistry, 2016, 34, 983-988.	4.9	16
18	Noncovalent Indocyanine Green Conjugate of C-Phycocyanin: Preparation and Tumor-Associated Macrophages-Targeted Photothermal Therapeutics. Bioconjugate Chemistry, 2020, 31, 1438-1448.	3.6	15

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19	Specifically targeting cancer proliferation and metastasis processes: the development of matriptase inhibitors. Cancer and Metastasis Reviews, 2019, 38, 507-524.	5.9	14
20	Probing the interactions of phthalocyanine-based photosensitizers with model phospholipid bilayer by molecular dynamics simulations. Journal of Porphyrins and Phthalocyanines, 2018, 22, 764-770.	0.8	13
21	Assessment of Intracellular Auto-Modification Levels of ARTD10 Using Mono-ADP-Ribose-Specific Macrodomains 2 and 3 of Murine Artd8. Methods in Molecular Biology, 2018, 1813, 41-63.	0.9	13
22	siRNA-Based Carrier-Free System for Synergistic Chemo/Chemodynamic/RNAi Therapy of Drug-Resistant Tumors. ACS Applied Materials & Interfaces, 2022, 14, 361-372.	8.0	13
23	Exploration of the binding of proton pump inhibitors to human P450 2C9 based on docking and molecular dynamics simulation. Journal of Molecular Modeling, 2011, 17, 1941-1951.	1.8	12
24	Insights into the binding mechanism of BODIPY-based photosensitizers to human serum albumin: A combined experimental and computational study. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 203, 158-165.	3.9	12
25	Halogen bonding for the design of inhibitors by targeting the S1 pocket of serine proteases. RSC Advances, 2018, 8, 28189-28197.	3.6	12
26	Suppression of Tumor Growth and Metastases by Targeted Intervention in Urokinase Activity with Cyclic Peptides. Journal of Medicinal Chemistry, 2019, 62, 2172-2183.	6.4	12
27	The search for inhibitors of macrodomains for targeting the readers and erasers of mono-ADP-ribosylation. Drug Discovery Today, 2021, 26, 2547-2558.	6.4	12
28	Intramolecular hydrophobic interactions are critical mediators of STAT5 dimerization. Scientific Reports, 2016, 6, 35454.	3.3	11
29	Computational studies of the binding mechanisms of fullerenes to human serum albumin. Journal of Molecular Modeling, 2015, 21, 177.	1.8	10
30	Exploration of the binding of benzimidazole-biphenyl derivatives to hemoglobin using docking and molecular dynamics simulation. International Journal of Biological Macromolecules, 2011, 48, 20-26.	7.5	9
31	Using porphyrins as albumin-binding molecules to enhance antitumor efficacies and reduce systemic toxicities of antimicrobial peptides. European Journal of Medicinal Chemistry, 2021, 217, 113382.	5.5	9
32	Unveiling the molecular mechanism of pH-dependent interactions of human serum albumin with chemotherapeutic agent doxorubicin: A combined spectroscopic and constant-pH molecular dynamics study. Journal of Molecular Liquids, 2021, 333, 115949.	4.9	9
33	Discovery of a novel Aurora B inhibitor GSK650394 with potent anticancer and anti-aspergillus fumigatus dual efficacies inÂvitro. Journal of Enzyme Inhibition and Medicinal Chemistry, 2022, 37, 109-117.	5.2	9
34	Switch in Relative Stability between cis and trans 2-Butene on Pt(111) as a Function of Experimental Conditions: A Density Functional Theory Study. ACS Catalysis, 2018, 8, 3067-3075.	11.2	8
35	tPA Point Mutation at Autolysis Loop Enhances Resistance to PAI-1 Inhibition and Catalytic Activity. Thrombosis and Haemostasis, 2019, 119, 077-086.	3.4	8
36	Flavonoids as Protein Disulfide Isomerase Inhibitors: Key Molecular and Structural Features for the Interaction. Journal of Agricultural and Food Chemistry, 2022, 70, 4475-4483.	5.2	8

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37	Molecular dynamics simulation study on conformational behavior of AÎ²(1â€“40) and AÎ²(1â€“42) in water and methanol. Computational and Theoretical Chemistry, 2009, 907, 51-56.	1.5	7
38	Structural prediction of the interaction of the tumor suppressor p27KIP1 with cyclin A/CDK2 identifies a novel catalytically relevant determinant. BMC Bioinformatics, 2017, 18, 15.	2.6	5
39	Crystal structure of plasma kallikrein reveals the unusual flexibility of the S1 pocket triggered by Glu217. FEBS Letters, 2018, 592, 2658-2667.	2.8	5
40	Crystal structure of the unoccupied murine urokinaseâ€type plasminogen activator receptor (<scp>uPAR</scp>) reveals a tightly packed DIIâ€“DIII unit. FEBS Letters, 2019, 593, 1236-1247.	2.8	4
41	Crystal Structures of Human C4.4A Reveal the Unique Association of Ly6/uPAR/Îµ-neurotoxin Domain. International Journal of Biological Sciences, 2020, 16, 981-993.	6.4	4
42	Molecular and Supramolecular Approach to Highly Photocytotoxic Phthalocyanines with Dual Cell Uptake Pathways and Albumin-Enhanced Tumor Targeting. ACS Applied Materials & Interfaces, 2022, 14, 28581-28590.	8.0	4
43	Solution Structure of SpoIVB Reveals Mechanism of PDZ Domain-Regulated Protease Activity. Frontiers in Microbiology, 2019, 10, 1232.	3.5	3
44	Role of hydrophobic residues for the gaseous formation of helical motifs. Chemical Communications, 2019, 55, 5147-5150.	4.1	3
45	A supramolecular nanocarrier for efficient cancer imaging and therapy by targeting at matriptase. Journal of Controlled Release, 2021, 334, 153-163.	9.9	3
46	Enhanced clot lysis by a single point mutation in a reteplase variant. British Journal of Haematology, 2022, 196, 1076-1085.	2.5	3
47	Identification of Antithrombotic Natural Products Targeting the Major Substrate Binding Pocket of Protein Disulfide Isomerase. Journal of Natural Products, 2022, 85, 1332-1339.	3.0	3
48	Temperature-Independent Ultralong Organic Phosphorescence with a Symmetrical Butterfly-Type Structure. Crystal Growth and Design, 0, , .	3.0	0