Jinyu Li

List of Publications by Year in Descending Order

42 papers	561 citations	13 h-index	22 g-index
50 ext. papers	754 ext. citations	6.2 avg, IF	3.85 L-index

#	Paper	IF	Citations
42	Discovery of a novel Aurora B inhibitor GSK650394 with potent anticancer and anti- dual efficacies .. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2022**, 37, 109-117	5.6	1
41	Enhanced Sampling Approach to the Induced-Fit Docking Problem in Protein-Ligand Binding: The Case of Mono-ADP-Ribosylation Hydrolase Inhibitors. *Journal of Chemical Theory and Computation*, **2021**,	6.4	1
40	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	6.8	2
39	The search for inhibitors of macrodomains for targeting the readers and erasers of mono-ADP-ribosylation. *Drug Discovery Today*, **2021**, 26, 2547-2558	8.8	4
38	A supramolecular nanocarrier for efficient cancer imaging and therapy by targeting at matriptase. *Journal of Controlled Release*, **2021**, 334, 153-163	11.7	1
37	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	6	3
36	Crystal Structures of Human C4.4A Reveal the Unique Association of Ly6/uPAR/□eurotoxin Domain. *International Journal of Biological Sciences*, **2020**, 16, 981-993	11.2	3
35	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,	6.6	7
34	Noncovalent Indocyanine Green Conjugate of C-Phycocyanin: Preparation and Tumor-Associated Macrophages-Targeted Photothermal Therapeutics. *Bioconjugate Chemistry*, **2020**, 31, 1438-1448	6.3	3
33	Specifically targeting cancer proliferation and metastasis processes: the development of matriptase inhibitors. *Cancer and Metastasis Reviews*, **2019**, 38, 507-524	9.6	11
32	Suppression of Tumor Growth and Metastases by Targeted Intervention in Urokinase Activity with Cyclic Peptides. *Journal of Medicinal Chemistry*, **2019**, 62, 2172-2183	8.3	8
31	A novel tumor and mitochondria dual-targeted photosensitizer showing ultra-efficient photodynamic anticancer activities. *Chemical Communications*, **2019**, 55, 866-869	5.8	25
30	Crystal structure of the unoccupied murine urokinase-type plasminogen activator receptor (uPAR) reveals a tightly packed DII-DIII unit. *FEBS Letters*, **2019**, 593, 1236-1247	3.8	4
29	Role of hydrophobic residues for the gaseous formation of helical motifs. *Chemical Communications* , **2019**, 55, 5147-5150	5.8	2
28	Self-Assembled and Size-Controllable Oligonucleotide Nanospheres for Effective Antisense Gene Delivery through an Endocytosis-Independent Pathway. *Angewandte Chemie - International Edition*, **2019**, 58, 5236-5240	16.4	54
27	Self-Assembled and Size-Controllable Oligonucleotide Nanospheres for Effective Antisense Gene Delivery through an Endocytosis-Independent Pathway. *Angewandte Chemie*, **2019**, 131, 5290-5294	3.6	14
26	Bispecific Aptamer Induced Artificial Protein-Pairing: A Strategy for Selective Inhibition of Receptor Function. *Journal of the American Chemical Society*, **2019**, 141, 12673-12681	16.4	54

25	Solution Structure of SpoIVB Reveals Mechanism of PDZ Domain-Regulated Protease Activity. *Frontiers in Microbiology*, **2019**, 10, 1232	5.7	2
24	Structural basis of sequence-specific Holliday junction cleavage by MOC1. *Nature Chemical Biology*, **2019**, 15, 1241-1248	11.7	10
23	tPA Point Mutation at Autolysis Loop Enhances Resistance to PAI-1 Inhibition and Catalytic Activity. *Thrombosis and Haemostasis*, **2019**, 119, 77-86	7	2
22	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	13.1	7
21	Smart Photosensitizer: Tumor-Triggered Oncotherapy by Self-Assembly Photodynamic Nanodots. *ACS Applied Materials & Interfaces*, **2018**, 10, 15369-15380	9.5	20
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	1.8	9
19	Nucleolar-nucleoplasmic shuttling of TARG1 and its control by DNA damage-induced poly-ADP-ribosylation and by nucleolar transcription. *Scientific Reports*, **2018**, 8, 6748	4.9	25
18	Crystal structure of plasma kallikrein reveals the unusual flexibility of the S1 pocket triggered by Glu217. *FEBS Letters*, **2018**, 592, 2658-2667	3.8	4
17	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	1.4	9
16	Molecular basis of rutin inhibition of protein disulfide isomerase (PDI) by combined and experimental methods.. *RSC Advances*, **2018**, 8, 18480-18491	3.7	6
15	Halogen bonding for the design of inhibitors by targeting the S1 pocket of serine proteases.. *RSC Advances*, **2018**, 8, 28189-28197	3.7	7
14	Water desalination across multilayer graphitic carbon nitride membrane: Insights from non-equilibrium molecular dynamics simulations. *Carbon*, **2018**, 140, 131-138	10.4	37
13	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	4.4	7
12	Proton Dynamics in Protein Mass Spectrometry. *Journal of Physical Chemistry Letters*, **2017**, 8, 1105-1112	6.4	26
11	Structural prediction of the interaction of the tumor suppressor p27 with cyclin A/CDK2 identifies a novel catalytically relevant determinant. *BMC Bioinformatics*, **2017**, 18, 15	3.6	2
10	Intramolecular hydrophobic interactions are critical mediators of STAT5 dimerization. *Scientific Reports*, **2016**, 6, 35454	4.9	9
9	Erlotinib Analogue-substituted Zinc(II) Phthalocyanines for Small Molecular Target-based Photodynamic Cancer Therapy. *Chinese Journal of Chemistry*, **2016**, 34, 983-988	4.9	15
8	Computational studies of the binding mechanisms of fullerenes to human serum albumin. *Journal of Molecular Modeling*, **2015**, 21, 177	2	8

7	Mechanistic investigation of the cis/trans isomerization of 2-butene on Pt(1 1 1): DFT study of the influence of the hydrogen coverage. *Journal of Catalysis*, **2014**, 311, 190-198	7.3	20
6	Exploration of the binding of benzimidazole-biphenyl derivatives to hemoglobin using docking and molecular dynamics simulation. *International Journal of Biological Macromolecules*, **2011**, 48, 20-6	7.9	9
5	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, 1941-51	2	12
4	Exploration of the mechanism for LPFFD inhibiting the formation of beta-sheet conformation of A beta(1-42) in water. *Journal of Molecular Modeling*, **2010**, 16, 813-21	2	42
3	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, 789-98	2	35
2	The effect of solvents on the conformations of Amyloid β-peptide (1–42) studied by molecular dynamics simulation. *Computational and Theoretical Chemistry*, **2009**, 895, 1-8		34
1	Molecular dynamics simulation study on conformational behavior of Aβ(1–40) and Aβ(1–42) in water and methanol. *Computational and Theoretical Chemistry*, **2009**, 907, 51-56		5