

Jinyu Li

List of Publications by Year in descending order

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48
papers

929
citations

516215

16
h-index

500791

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. <i>Journal of the American Chemical Society</i> , 2019, 141, 12673-12681.	6.6	102
2	Self-Assembled and Size-Controllable Oligonucleotide Nanospheres for Effective Antisense Gene Delivery through an Endocytosis-Independent Pathway. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 5236-5240.	7.2	97
3	Water desalination across multilayer graphitic carbon nitride membrane: Insights from non-equilibrium molecular dynamics simulations. <i>Carbon</i> , 2018, 140, 131-138.	5.4	75
4	Exploration of the mechanism for LPFFD inhibiting the formation of β -sheet conformation of A β (1-42) in water. <i>Journal of Molecular Modeling</i> , 2010, 16, 813-821.	0.8	48
5	Characterization of the binding of angiotensin II receptor blockers to human serum albumin using docking and molecular dynamics simulation. <i>Journal of Molecular Modeling</i> , 2010, 16, 789-798.	0.8	39
6	A novel tumor and mitochondria dual-targeted photosensitizer showing ultra-efficient photodynamic anticancer activities. <i>Chemical Communications</i> , 2019, 55, 866-869.	2.2	39
7	The effect of solvents on the conformations of Amyloid β -peptide (1-42) studied by molecular dynamics simulation. <i>Computational and Theoretical Chemistry</i> , 2009, 895, 1-8.	1.5	36
8	Proton Dynamics in Protein Mass Spectrometry. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 1105-1112.	2.1	34
9	Smart Photosensitizer: Tumor-Triggered Oncotherapy by Self-Assembly Photodynamic Nanodots. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 15369-15380.	4.0	34
10	Nucleolar-nucleoplasmic shuttling of TARG1 and its control by DNA damage-induced poly-ADP-ribosylation and by nucleolar transcription. <i>Scientific Reports</i> , 2018, 8, 6748.	1.6	32
11	Mechanistic investigation of the cis/trans isomerization of 2-butene on Pt(111): DFT study of the influence of the hydrogen coverage. <i>Journal of Catalysis</i> , 2014, 311, 190-198.	3.1	23
12	Self-Assembled and Size-Controllable Oligonucleotide Nanospheres for Effective Antisense Gene Delivery through an Endocytosis-Independent Pathway. <i>Angewandte Chemie</i> , 2019, 131, 5290-5294.	1.6	23
13	Molecular basis of rutin inhibition of protein disulfide isomerase (PDI) by combined <i>in silico</i> and experimental methods. <i>RSC Advances</i> , 2018, 8, 18480-18491.	1.7	22
14	Structural basis of sequence-specific Holliday junction cleavage by MOC1. <i>Nature Chemical Biology</i> , 2019, 15, 1241-1248.	3.9	21
15	Cryo-electron Microscopy Structure of the Swine Acute Diarrhea Syndrome Coronavirus Spike Glycoprotein Provides Insights into Evolution of Unique Coronavirus Spike Proteins. <i>Journal of Virology</i> , 2020, 94, .	1.5	17
16	Enhanced Sampling Approach to the Induced-Fit Docking Problem in Protein-Ligand Binding: The Case of Mono-ADP-Ribosylation Hydrolase Inhibitors. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 7899-7911.	2.3	17
17	Erlotinib Analogue-Substituted Zinc(II) Phthalocyanines for Small Molecular Target-Based Photodynamic Cancer Therapy. <i>Chinese Journal of Chemistry</i> , 2016, 34, 983-988.	2.6	16
18	Noncovalent Indocyanine Green Conjugate of C-Phycocyanin: Preparation and Tumor-Associated Macrophages-Targeted Photothermal Therapeutics. <i>Bioconjugate Chemistry</i> , 2020, 31, 1438-1448.	1.8	15

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19	Specifically targeting cancer proliferation and metastasis processes: the development of matriptase inhibitors. <i>Cancer and Metastasis Reviews</i> , 2019, 38, 507-524.	2.7	14
20	Probing the interactions of phthalocyanine-based photosensitizers with model phospholipid bilayer by molecular dynamics simulations. <i>Journal of Porphyrins and Phthalocyanines</i> , 2018, 22, 764-770.	0.4	13
21	Assessment of Intracellular Auto-Modification Levels of ARTD10 Using Mono-ADP-Ribose-Specific Macrod domains 2 and 3 of Murine Artd8. <i>Methods in Molecular Biology</i> , 2018, 1813, 41-63.	0.4	13
22	siRNA-Based Carrier-Free System for Synergistic Chemo/Chemodynamic/RNAi Therapy of Drug-Resistant Tumors. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 361-372.	4.0	13
23	Exploration of the binding of proton pump inhibitors to human P450 2C9 based on docking and molecular dynamics simulation. <i>Journal of Molecular Modeling</i> , 2011, 17, 1941-1951.	0.8	12
24	Insights into the binding mechanism of BODIPY-based photosensitizers to human serum albumin: A combined experimental and computational study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2018, 203, 158-165.	2.0	12
25	Halogen bonding for the design of inhibitors by targeting the S1 pocket of serine proteases. <i>RSC Advances</i> , 2018, 8, 28189-28197.	1.7	12
26	Suppression of Tumor Growth and Metastases by Targeted Intervention in Urokinase Activity with Cyclic Peptides. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 2172-2183.	2.9	12
27	The search for inhibitors of macrodomains for targeting the readers and erasers of mono-ADP-ribosylation. <i>Drug Discovery Today</i> , 2021, 26, 2547-2558.	3.2	12
28	Intramolecular hydrophobic interactions are critical mediators of STAT5 dimerization. <i>Scientific Reports</i> , 2016, 6, 35454.	1.6	11
29	Computational studies of the binding mechanisms of fullerenes to human serum albumin. <i>Journal of Molecular Modeling</i> , 2015, 21, 177.	0.8	10
30	Exploration of the binding of benzimidazole-biphenyl derivatives to hemoglobin using docking and molecular dynamics simulation. <i>International Journal of Biological Macromolecules</i> , 2011, 48, 20-26.	3.6	9
31	Using porphyrins as albumin-binding molecules to enhance antitumor efficacies and reduce systemic toxicities of antimicrobial peptides. <i>European Journal of Medicinal Chemistry</i> , 2021, 217, 113382.	2.6	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. <i>Journal of Molecular Liquids</i> , 2021, 333, 115949.	2.3	9
33	Discovery of a novel Aurora B inhibitor GSK650394 with potent anticancer and anti- <i>Aspergillus fumigatus</i> dual efficacies <i>in vitro</i> . <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2022, 37, 109-117.	2.5	9
34	Switch in Relative Stability between <i>cis</i> and <i>trans</i> 2-Butene on Pt(111) as a Function of Experimental Conditions: A Density Functional Theory Study. <i>ACS Catalysis</i> , 2018, 8, 3067-3075.	5.5	8
35	tPA Point Mutation at Autolysis Loop Enhances Resistance to PAI-1 Inhibition and Catalytic Activity. <i>Thrombosis and Haemostasis</i> , 2019, 119, 077-086.	1.8	8
36	Flavonoids as Protein Disulfide Isomerase Inhibitors: Key Molecular and Structural Features for the Interaction. <i>Journal of Agricultural and Food Chemistry</i> , 2022, 70, 4475-4483.	2.4	8

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37	Molecular dynamics simulation study on conformational behavior of $\hat{A}^2(1\hat{\epsilon}40)$ and $\hat{A}^2(1\hat{\epsilon}42)$ in water and methanol. <i>Computational and Theoretical Chemistry</i> , 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. <i>BMC Bioinformatics</i> , 2017, 18, 15.	1.2	5
39	Crystal structure of plasma kallikrein reveals the unusual flexibility of the S1 pocket triggered by Glu217. <i>FEBS Letters</i> , 2018, 592, 2658-2667.	1.3	5
40	Crystal structure of the unoccupied murine urokinase-type plasminogen activator receptor (<sc>uPAR</sc>) reveals a tightly packed DII $\hat{\epsilon}$ DIII unit. <i>FEBS Letters</i> , 2019, 593, 1236-1247.	1.3	4
41	Crystal Structures of Human C4.4A Reveal the Unique Association of Ly6/uPAR/ $\hat{\pm}$ -neurotoxin Domain. <i>International Journal of Biological Sciences</i> , 2020, 16, 981-993.	2.6	4
42	Molecular and Supramolecular Approach to Highly Photocytotoxic Phthalocyanines with Dual Cell Uptake Pathways and Albumin-Enhanced Tumor Targeting. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 28581-28590.	4.0	4
43	Solution Structure of SpoIVB Reveals Mechanism of PDZ Domain-Regulated Protease Activity. <i>Frontiers in Microbiology</i> , 2019, 10, 1232.	1.5	3
44	Role of hydrophobic residues for the gaseous formation of helical motifs. <i>Chemical Communications</i> , 2019, 55, 5147-5150.	2.2	3
45	A supramolecular nanocarrier for efficient cancer imaging and therapy by targeting at matriptase. <i>Journal of Controlled Release</i> , 2021, 334, 153-163.	4.8	3
46	Enhanced clot lysis by a single point mutation in a reteplase variant. <i>British Journal of Haematology</i> , 2022, 196, 1076-1085.	1.2	3
47	Identification of Antithrombotic Natural Products Targeting the Major Substrate Binding Pocket of Protein Disulfide Isomerase. <i>Journal of Natural Products</i> , 2022, 85, 1332-1339.	1.5	3
48	Temperature-Independent Ultralong Organic Phosphorescence with a Symmetrical Butterfly-Type Structure. <i>Crystal Growth and Design</i> , 0, , .	1.4	0