Shiliang Li

List of Publications by Year
in descending order

40 papers	1,454 citations	623734 14 h-index	345221 36 g-index
44 all docs	44 docs citations	44 times ranked	2258 citing authors

#	Article	IF	Citations
1	PharmMapper 2017 update: a web server for potential drug target identification with a comprehensive target pharmacophore database. Nucleic Acids Research, 2017, 45, W356-W360.	14.5	802
2	Novel and potent inhibitors targeting DHODH are broad-spectrum antivirals against RNA viruses including newly-emerged coronavirus SARS-CoV-2. Protein and Cell, 2020, 11, 723-739.	11.0	129
3	Discovery and Rational Design of Natural-Product-Derived 2-Phenyl-3,4-dihydro-2H-benzo[f]chromen-3-amine Analogs as Novel and Potent Dipeptidyl Peptidase 4 (DPP-4) Inhibitors for the Treatment of Type 2 Diabetes. Journal of Medicinal Chemistry, 2016, 59, 6772-6790.	6.4	49
4	Design, Synthesis, X-ray Crystallographic Analysis, and Biological Evaluation of Thiazole Derivatives as Potent and Selective Inhibitors of Human Dihydroorotate Dehydrogenase. Journal of Medicinal Chemistry, 2015, 58, 1123-1139.	6.4	47
5	Discovery of Potent and Noncovalent Reversible EGFR Kinase Inhibitors of EGFR^{L858R/T790M/C797S}. ACS Medicinal Chemistry Letters, 2019, 10, 869-873.	2.8	39
6	Quercetin inhibits virulence properties of Porphyromas gingivalis in periodontal disease. Scientific Reports, 2020, 10, 18313.	3.3	39
7	iDrug: a web-accessible and interactive drug discovery and design platform. Journal of Cheminformatics, 2014, 6, 28.	6.1	30
8	Systematic Analysis of the Multiple Bioactivities of Green Tea through a Network Pharmacology Approach. Evidence-based Complementary and Alternative Medicine, 2014, 2014, 1-11.	1.2	29
9	Deep Learning Based Drug Metabolites Prediction. Frontiers in Pharmacology, 2019, 10, 1586.	3.5	24
10	Discovery of a Natural-Product-Derived Preclinical Candidate for Once-Weekly Treatment of Type 2 Diabetes. Journal of Medicinal Chemistry, 2019, 62, 2348-2361.	6.4	23
11	Multi-Body Interactions in Molecular Docking Program Devised with Key Water Molecules in Protein Binding Sites. Molecules, 2018, 23, 2321.	3.8	21
12	A Broad Antiviral Strategy: Inhibitors of Human DHODH Pave the Way for Host-Targeting Antivirals against Emerging and Re-Emerging Viruses. Viruses, 2022, 14, 928.	3.3	20
13	Identification of Inhibitors against p90 Ribosomal S6 Kinase 2 (RSK2) through Structure-Based Virtual Screening with the Inhibitor-Constrained Refined Homology Model. Journal of Chemical Information and Modeling, 2011, 51, 2939-2947.	5.4	19
14	Rational Design of Benzylidenehydrazinyl-Substituted Thiazole Derivatives as Potent Inhibitors of Human Dihydroorotate Dehydrogenase with in Vivo Anti-arthritic Activity. Scientific Reports, 2015, 5, 14836.	3.3	19
15	Lipopolysaccharide Preparation Derived From Porphyromonas gingivalis Induces a Weaker Immuno-Inflammatory Response in BV-2 Microglial Cells Than Escherichia coli by Differentially Activating TLR2/4-Mediated NF-ÎºB/STAT3 Signaling Pathways. Frontiers in Cellular and Infection Microbiology, 2021, 11, 606986.	3.9	19
16	Design, synthesis, molecular modeling, and biological evaluation of acrylamide derivatives as potent inhibitors of human dihydroorotate dehydrogenase for the treatment of rheumatoid arthritis. Acta Pharmaceutica Sinica B, 2021, 11, 795-809.	12.0	14
17	Mebhydrolin ameliorates glucose homeostasis in type 2 diabetic mice by functioning as a selective FXR antagonist. Metabolism: Clinical and Experimental, 2021, 119, 154771.	3.4	14
18	Isoindole-1,3-dione derivatives as RSK2 inhibitors: synthesis, molecular docking simulation and SAR analysis. MedChemComm, 2016, 7, 292-296.	3.4	12

#	Article	IF	Citations
19	Structure-based design of potent human dihydroorotate dehydrogenase inhibitors as anticancer agents. MedChemComm, 2016, 7, 1441-1448.	3.4	11
20	Discovery of Natural Products as Novel and Potent FXR Antagonists by Virtual Screening. Frontiers in Chemistry, 2018, 6, 140.	3.6	10
21	A fast protein binding site comparison algorithm for proteomeâ€wide protein function prediction and drug repurposing. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1541-1556.	2.6	9
22	Synthesis, structureâ€“activity relationship and binding mode analysis of 4-thiazolidinone derivatives as novel inhibitors of human dihydroorotate dehydrogenase. MedChemComm, 2017, 8, 1297-1302.	3.4	8
23	Statistical Analysis, Investigation, and Prediction of the Water Positions in the Binding Sites of Proteins. Journal of Chemical Information and Modeling, 2017, 57, 1517-1528.	5.4	8
24	Drug Design of â€œUndruggableâ€•Targets. Chinese Journal of Chemistry, 2019, 37, 501-512.	4.9	8
25	Synthesis and biological evaluation of a novel Î²-D-2â€²-deoxy-2â€²-Î±-fluoro-2â€²-Î²-C-(fluoromethyl)uridine phosphoramidate prodrug for the treatment of hepatitis C virus infection. European Journal of Medicinal Chemistry, 2018, 143, 107-113.	5.5	7
26	Structural and genetic analysis of <scp>START</scp> superfamily protein <scp>MSMEG</scp>_0129 from MycobacteriumÂsmegmatis. FEBS Letters, 2018, 592, 1445-1457.	2.8	6
27	RD-Metabolizer: an integrated and reaction types extensive approach to predict metabolic sites and metabolites of drug-like molecules. Chemistry Central Journal, 2017, 11, 65.	2.6	5
28	Discovery of a natural fluorescent probe targeting the Plasmodium falciparum cysteine protease falcipain-2. Science China Life Sciences, 2020, 63, 1016-1025.	4.9	4
29	Discovery, Optimization, and Structureâ€“Activity Relationship Study of Novel and Potent RSK4 Inhibitors as Promising Agents for the Treatment of Esophageal Squamous Cell Carcinoma. Journal of Medicinal Chemistry, 2021, 64, 13572-13587.	6.4	4
30	Triazole and Benzotriazole Derivatives as Novel Inhibitors for p90 Ribosomal S6 Protein Kinase 2: Synthesis, Molecular Docking and SAR Analysis. Chinese Journal of Chemistry, 2013, 31, 1192-1198.	4.9	3
31	Design, Synthesis, and Evaluation of Ribose-Modified Anilinopyrimidine Derivatives as EGFR Tyrosine Kinase Inhibitors. Frontiers in Chemistry, 2017, 5, 101.	3.6	3
32	Design and Synthesis of a Series of Novel Macrocycle Janus Kinase 2 Inhibitors. Chinese Journal of Chemistry, 2019, 37, 1259-1263.	4.9	3
33	Design, Synthesis and <scp>SAR</scp> Studies of Novel and Potent Dipeptidyl Peptidase 4 Inhibitors. Chinese Journal of Chemistry, 2021, 39, 115-120.	4.9	3
34	Biological evaluation of quinoline derivatives as inhibitors of human dihydroorotate dehydrogenase. MedChemComm, 2016, 7, 853-858.	3.4	2
35	Structural Optimization and Structureâ€“Activity Relationship of 4-Thiazolidinone Derivatives as Novel Inhibitors of Human Dihydroorotate Dehydrogenase. Molecules, 2019, 24, 2780.	3.8	2
36	Design, Synthesis, and Structureâ€“Activity Relationship Study of Potent MAPK11 Inhibitors. Molecules, 2022, 27, 203.	3.8	2

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37	Systematic evaluation and optimization of highâ€performance liquid chromatography separation of polyoxins. Journal of Separation Science, 2020, 43, 3006-3016.	2.5	1
38	Molecular Docking for Ligand-Receptor Binding Process Based on Heterogeneous Computing. Scientific Programming, 2022, 2022, 1-13.	0.7	1
39	ePharmer : An integrated and graphical software for pharmacophoreâ€based virtual screening. Journal of Computational Chemistry, 2021, 42, 2181-2195.	3.3	0
40	Cover Image, Volume 89, Issue 11. Proteins: Structure, Function and Bioinformatics, 2021, 89, .	2.6	0