

# Shiliang Li

## List of Publications by Year in descending order

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40  
papers

1,454  
citations

623734

14  
h-index

345221

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all docs

44  
docs citations

44  
times ranked

2258  
citing authors

#	ARTICLE	IF	CITATIONS
1	Molecular Docking for Ligand-Receptor Binding Process Based on Heterogeneous Computing. <i>Scientific Programming</i> , 2022, 2022, 1-13.	0.7	1
2	Design, Synthesis, and Structure-Activity Relationship Study of Potent MAPK11 Inhibitors. <i>Molecules</i> , 2022, 27, 203.	3.8	2
3	A Broad Antiviral Strategy: Inhibitors of Human DHODH Pave the Way for Host-Targeting Antivirals against Emerging and Re-Emerging Viruses. <i>Viruses</i> , 2022, 14, 928.	3.3	20
4	Design, synthesis, molecular modeling, and biological evaluation of acrylamide derivatives as potent inhibitors of human dihydroorotate dehydrogenase for the treatment of rheumatoid arthritis. <i>Acta Pharmaceutica Sinica B</i> , 2021, 11, 795-809.	12.0	14
5	Design, Synthesis and SAR Studies of Novel and Potent Dipeptidyl Peptidase 4 Inhibitors. <i>Chinese Journal of Chemistry</i> , 2021, 39, 115-120.	4.9	3
6	Lipopolysaccharide Preparation Derived From <i>Porphyromonas gingivalis</i> Induces a Weaker Immuno-Inflammatory Response in BV-2 Microglial Cells Than <i>Escherichia coli</i> by Differentially Activating TLR2/4-Mediated NF- $\kappa$ B/STAT3 Signaling Pathways. <i>Frontiers in Cellular and Infection Microbiology</i> , 2021, 11, 606986.	3.9	19
7	Mebhydrolin ameliorates glucose homeostasis in type 2 diabetic mice by functioning as a selective FXR antagonist. <i>Metabolism: Clinical and Experimental</i> , 2021, 119, 154771.	3.4	14
8	A fast protein binding site comparison algorithm for proteome-wide protein function prediction and drug repurposing. <i>Proteins: Structure, Function and Bioinformatics</i> , 2021, 89, 1541-1556.	2.6	9
9	ePharmer : An integrated and graphical software for pharmacophore-based virtual screening. <i>Journal of Computational Chemistry</i> , 2021, 42, 2181-2195.	3.3	0
10	Discovery, Optimization, and Structure-Activity Relationship Study of Novel and Potent RSK4 Inhibitors as Promising Agents for the Treatment of Esophageal Squamous Cell Carcinoma. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 13572-13587.	6.4	4
11	Cover Image, Volume 89, Issue 11. <i>Proteins: Structure, Function and Bioinformatics</i> , 2021, 89, .	2.6	0
12	Novel and potent inhibitors targeting DHODH are broad-spectrum antivirals against RNA viruses including newly-emerged coronavirus SARS-CoV-2. <i>Protein and Cell</i> , 2020, 11, 723-739.	11.0	129
13	Quercetin inhibits virulence properties of <i>Porphyromonas gingivalis</i> in periodontal disease. <i>Scientific Reports</i> , 2020, 10, 18313.	3.3	39
14	Systematic evaluation and optimization of high-performance liquid chromatography separation of polyoxins. <i>Journal of Separation Science</i> , 2020, 43, 3006-3016.	2.5	1
15	Discovery of a natural fluorescent probe targeting the <i>Plasmodium falciparum</i> cysteine protease falcipain-2. <i>Science China Life Sciences</i> , 2020, 63, 1016-1025.	4.9	4
16	Structural Optimization and Structure-Activity Relationship of 4-Thiazolidinone Derivatives as Novel Inhibitors of Human Dihydroorotate Dehydrogenase. <i>Molecules</i> , 2019, 24, 2780.	3.8	2
17	Design and Synthesis of a Series of Novel Macrocyclic Janus Kinase 2 Inhibitors. <i>Chinese Journal of Chemistry</i> , 2019, 37, 1259-1263.	4.9	3
18	Discovery of a Natural-Product-Derived Preclinical Candidate for Once-Weekly Treatment of Type 2 Diabetes. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 2348-2361.	6.4	23

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19	Discovery of Potent and Noncovalent Reversible EGFR Kinase Inhibitors of EGFR <sup>L858R/T790M/C797S</sup> . ACS Medicinal Chemistry Letters, 2019, 10, 869-873.	2.8	39
20	Drug Design of "Undruggable" Targets. Chinese Journal of Chemistry, 2019, 37, 501-512.	4.9	8
21	Deep Learning Based Drug Metabolites Prediction. Frontiers in Pharmacology, 2019, 10, 1586.	3.5	24
22	Structural and genetic analysis of START superfamily protein MSMEG <sub>0129</sub> from <i>Mycobacterium smegmatis</i> . FEBS Letters, 2018, 592, 1445-1457.	2.8	6
23	Synthesis and biological evaluation of a novel 2'-deoxy-2-fluoro-2'-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
24	Multi-Body Interactions in Molecular Docking Program Devised with Key Water Molecules in Protein Binding Sites. Molecules, 2018, 23, 2321.	3.8	21
25	Discovery of Natural Products as Novel and Potent FXR Antagonists by Virtual Screening. Frontiers in Chemistry, 2018, 6, 140.	3.6	10
26	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
27	Synthesis, structure-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
28	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
29	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
30	Design, Synthesis, and Evaluation of Ribose-Modified Anilinopyrimidine Derivatives as EGFR Tyrosine Kinase Inhibitors. Frontiers in Chemistry, 2017, 5, 101.	3.6	3
31	Discovery and Rational Design of Natural-Product-Derived 2-Phenyl-3,4-dihydro-2H-benzo[ <i>f</i> ]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
32	Structure-based design of potent human dihydroorotate dehydrogenase inhibitors as anticancer agents. MedChemComm, 2016, 7, 1441-1448.	3.4	11
33	Biological evaluation of quinoline derivatives as inhibitors of human dihydroorotate dehydrogenase. MedChemComm, 2016, 7, 853-858.	3.4	2
34	Isoindole-1,3-dione derivatives as RSK2 inhibitors: synthesis, molecular docking simulation and SAR analysis. MedChemComm, 2016, 7, 292-296.	3.4	12
35	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
36	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

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37	Systematic Analysis of the Multiple Bioactivities of Green Tea through a Network Pharmacology Approach. <i>Evidence-based Complementary and Alternative Medicine</i> , 2014, 2014, 1-11.	1.2	29
38	iDrug: a web-accessible and interactive drug discovery and design platform. <i>Journal of Cheminformatics</i> , 2014, 6, 28.	6.1	30
39	Triazole and Benzotriazole Derivatives as Novel Inhibitors for p90 Ribosomal S6 Protein Kinase 2: Synthesis, Molecular Docking and SAR Analysis. <i>Chinese Journal of Chemistry</i> , 2013, 31, 1192-1198.	4.9	3
40	Identification of Inhibitors against p90 Ribosomal S6 Kinase 2 (RSK2) through Structure-Based Virtual Screening with the Inhibitor-Constrained Refined Homology Model. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 2939-2947.	5.4	19