Zhe Li

List of Publications by Year
in descending order

32	1,173	394286 19	434063 31
papers	citations	h-index	g-index

35	35	35	1914
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Free energy perturbation (FEP)-guided scaffold hopping. Acta Pharmaceutica Sinica B, 2022, 12, 1351-1362.	5.7	12
2	Structure-based discovery of orally efficient inhibitors via unique interactions with H-pocket of PDE8 for the treatment of vascular dementia. Acta Pharmaceutica Sinica B, 2022, 12, 3103-3112.	5.7	4
3	Structural Modifications of Nimodipine Lead to Novel PDE1 Inhibitors with Anti-pulmonary Fibrosis Effects. Journal of Medicinal Chemistry, 2022, 65, 8444-8455.	2.9	6
4	Therapeutic targets and potential agents for the treatment of COVIDâ€19. Medicinal Research Reviews, 2021, 41, 1775-1797.	5.0	21
5	Reply to Ma and Wang: Reliability of various in vitro activity assays on SARS-CoV-2 main protease inhibitors. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	15
6	Design, Synthesis, and Evaluation of Dihydropyranopyrazole Derivatives as Novel PDE2 Inhibitors for the Treatment of Alzheimerâ€™s Disease. Molecules, 2021, 26, 3034.	1.7	8
7	Perspective of drug design with high-performance computing. National Science Review, 2021, 8, nwab105.	4.6	1
8	Reply to Behnam and Klein: Potential role of the His-tag in C-terminal His-tagged SARS-CoV-2 main protease. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	1
9	Catalytic Roles of Coenzyme Pyridoxal-5â€²-phosphate (PLP) in PLP-Dependent Enzymes: Reaction Pathway for Methionine-Î³-Lyase-Catalyzed <scp>l</scp>-Methionine Depletion. ACS Catalysis, 2020, 10, 2198-2210.	5.5	14
10	Identify potent SARS-CoV-2 main protease inhibitors via accelerated free energy perturbation-based virtual screening of existing drugs. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 27381-27387.	3.3	174
11	Rational Design of 2-Chloroadenine Derivatives as Highly Selective Phosphodiesterase 8A Inhibitors. Journal of Medicinal Chemistry, 2020, 63, 15852-15863.	2.9	9
12	Discovery and Optimization of Chromone Derivatives as Novel Selective Phosphodiesterase 10 Inhibitors. ACS Chemical Neuroscience, 2020, 11, 1058-1071.	1.7	7
13	Discovery and Optimization of Î±-Mangostin Derivatives as Novel PDE4 Inhibitors for the Treatment of Vascular Dementia. Journal of Medicinal Chemistry, 2020, 63, 3370-3380.	2.9	20
14	Potential therapeutic effects of dipyridamole in the severely ill patients with COVID-19. Acta Pharmaceutica Sinica B, 2020, 10, 1205-1215.	5.7	193
15	SIRT6 protects vascular endothelial cells from angiotensin II-induced apoptosis and oxidative stress by promoting the activation of Nrf2/ARE signaling. European Journal of Pharmacology, 2019, 859, 172516.	1.7	46
16	Absolute Binding Free Energy Calculation and Design of a Subnanomolar Inhibitor of Phosphodiesterase-10. Journal of Medicinal Chemistry, 2019, 62, 2099-2111.	2.9	47
17	Discovery of Potent, Selective, and Orally Bioavailable Inhibitors against Phosphodiesterase-9, a Novel Target for the Treatment of Vascular Dementia. Journal of Medicinal Chemistry, 2019, 62, 4218-4224.	2.9	15
18	Novel Phosphodiesterase Inhibitors for Cognitive Improvement in Alzheimerâ€™s Disease. Journal of Medicinal Chemistry, 2018, 61, 5467-5483.	2.9	83

#	Article	IF	Citations
19	Optimization of Chromeno[2,3-c]pyrrol-9(2H)-ones as Highly Potent, Selective, and Orally Bioavailable PDE5 Inhibitors: Structureâ€“Activity Relationship, X-ray Crystal Structure, and Pharmacodynamic Effect on Pulmonary Arterial Hypertension. Journal of Medicinal Chemistry, 2018, 61, 8468-8473.	2.9	21
20	Discovery of Novel Phosphodiesterase-2A Inhibitors by Structure-Based Virtual Screening, Structural Optimization, and Bioassay. Journal of Chemical Information and Modeling, 2017, 57, 355-364.	2.5	40
21	Discovery and modelling studies of natural ingredients from Gaultheria yunnanensi s (FRANCH.) against phosphodiesterase-4. European Journal of Medicinal Chemistry, 2016, 114, 134-140.	2.6	19
22	Structural Asymmetry of Phosphodiesterase-9A and a Unique Pocket for Selective Binding of a Potent Enantiomeric Inhibitor. Molecular Pharmacology, 2015, 88, 836-845.	1.0	23
23	Molecular dynamics-based discovery of novel phosphodiesterase-9A inhibitors with non-pyrazolopyrimidinone scaffolds. Molecular BioSystems, 2015, 11, 115-125.	2.9	21
24	Ab Initio QM/MM Study Shows a Highly Dissociated S_N2 Hydrolysis Mechanism for the cGMP-Specific Phosphodiesterase-5. Journal of Chemical Theory and Computation, 2014, 10, 5448-5457.	2.3	9
25	Discovery of a Phosphodiesterase 9A Inhibitor as a Potential Hypoglycemic Agent. Journal of Medicinal Chemistry, 2014, 57, 10304-10313.	2.9	53
26	Discovery of 3-(4-hydroxybenzyl)-1-(thiophen-2-yl)chromeno[2,3-c]pyrrol-9(2H)-one as a phosphodiesterase-5 inhibitor and its complex crystal structure. Biochemical Pharmacology, 2014, 89, 86-98.	2.0	25
27	AG-690/11026014, a novel PARP-1 inhibitor, protects cardiomyocytes from AngII-induced hypertrophy. Molecular and Cellular Endocrinology, 2014, 392, 14-22.	1.6	29
28	The molecular basis for the inhibition of phosphodiesterase-4D by three natural resveratrol analogs. Isolation, molecular docking, molecular dynamics simulations, binding free energy, and bioassay. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2013, 1834, 2089-2096.	1.1	23
29	The Molecular Basis for the Selectivity of Tadalafil toward Phosphodiesterase 5 and 6: A Modeling Study. Journal of Chemical Information and Modeling, 2013, 53, 3044-3053.	2.5	32
30	Identification of Novel Phosphodiesterase-4D Inhibitors Prescreened by Molecular Dynamics-Augmented Modeling and Validated by Bioassay. Journal of Chemical Information and Modeling, 2013, 53, 972-981.	2.5	37
31	Structure-Based Discovery of Highly Selective Phosphodiesterase-9A Inhibitors and Implications for Inhibitor Design. Journal of Medicinal Chemistry, 2012, 55, 8549-8558.	2.9	58
32	Moracin M from Morus alba L. is a natural phosphodiesterase-4 inhibitor. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 3261-3264.	1.0	55