

Zhe Li

List of Publications by Year in descending order

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Version: 2024-02-01

32
papers

1,173
citations

394286

19
h-index

434063

31
g-index

35
all docs

35
docs citations

35
times ranked

1914
citing authors

#	ARTICLE	IF	CITATIONS
1	Potential therapeutic effects of dipyrindamole in the severely ill patients with COVID-19. <i>Acta Pharmaceutica Sinica B</i> , 2020, 10, 1205-1215.	5.7	193
2	Identify potent SARS-CoV-2 main protease inhibitors via accelerated free energy perturbation-based virtual screening of existing drugs. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 27381-27387.	3.3	174
3	Novel Phosphodiesterase Inhibitors for Cognitive Improvement in Alzheimer's Disease. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 5467-5483.	2.9	83
4	Structure-Based Discovery of Highly Selective Phosphodiesterase-9A Inhibitors and Implications for Inhibitor Design. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 8549-8558.	2.9	58
5	Moracin M from <i>Morus alba</i> L. is a natural phosphodiesterase-4 inhibitor. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2012, 22, 3261-3264.	1.0	55
6	Discovery of a Phosphodiesterase 9A Inhibitor as a Potential Hypoglycemic Agent. <i>Journal of Medicinal Chemistry</i> , 2014, 57, 10304-10313.	2.9	53
7	Absolute Binding Free Energy Calculation and Design of a Subnanomolar Inhibitor of Phosphodiesterase-10. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 2099-2111.	2.9	47
8	SIRT6 protects vascular endothelial cells from angiotensin II-induced apoptosis and oxidative stress by promoting the activation of Nrf2/ARE signaling. <i>European Journal of Pharmacology</i> , 2019, 859, 172516.	1.7	46
9	Discovery of Novel Phosphodiesterase-2A Inhibitors by Structure-Based Virtual Screening, Structural Optimization, and Bioassay. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 355-364.	2.5	40
10	Identification of Novel Phosphodiesterase-4D Inhibitors Prescreened by Molecular Dynamics-Augmented Modeling and Validated by Bioassay. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 972-981.	2.5	37
11	The Molecular Basis for the Selectivity of Tadalafil toward Phosphodiesterase 5 and 6: A Modeling Study. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 3044-3053.	2.5	32
12	AG-690/11026014, a novel PARP-1 inhibitor, protects cardiomyocytes from AngII-induced hypertrophy. <i>Molecular and Cellular Endocrinology</i> , 2014, 392, 14-22.	1.6	29
13	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. <i>Biochemical Pharmacology</i> , 2014, 89, 86-98.	2.0	25
14	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. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2013, 1834, 2089-2096.	1.1	23
15	Structural Asymmetry of Phosphodiesterase-9A and a Unique Pocket for Selective Binding of a Potent Enantiomeric Inhibitor. <i>Molecular Pharmacology</i> , 2015, 88, 836-845.	1.0	23
16	Molecular dynamics-based discovery of novel phosphodiesterase-9A inhibitors with non-pyrazolopyrimidinone scaffolds. <i>Molecular BioSystems</i> , 2015, 11, 115-125.	2.9	21
17	Optimization of Chromeno[2,3-c]pyrrol-9(2H)-ones as Highly Potent, Selective, and Orally Bioavailable PDE5 Inhibitors: Structure-Activity Relationship, X-ray Crystal Structure, and Pharmacodynamic Effect on Pulmonary Arterial Hypertension. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 8468-8473.	2.9	21
18	Therapeutic targets and potential agents for the treatment of COVID-19. <i>Medicinal Research Reviews</i> , 2021, 41, 1775-1797.	5.0	21

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19	Discovery and Optimization of Î±-Mangostin Derivatives as Novel PDE4 Inhibitors for the Treatment of Vascular Dementia. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 3370-3380.	2.9	20
20	Discovery and modelling studies of natural ingredients from <i>Gaultheria yunnanensis</i> (FRANCH.) against phosphodiesterase-4. <i>European Journal of Medicinal Chemistry</i> , 2016, 114, 134-140.	2.6	19
21	Discovery of Potent, Selective, and Orally Bioavailable Inhibitors against Phosphodiesterase-9, a Novel Target for the Treatment of Vascular Dementia. <i>Journal of Medicinal Chemistry</i> , 2019, 62, 4218-4224.	2.9	15
22	Reply to Ma and Wang: Reliability of various in vitro activity assays on SARS-CoV-2 main protease inhibitors. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	15
23	Catalytic Roles of Coenzyme Pyridoxal-5-phosphate (PLP) in PLP-Dependent Enzymes: Reaction Pathway for Methionine-Î³-Lyase-Catalyzed <sc>l</sc>-Methionine Depletion. <i>ACS Catalysis</i> , 2020, 10, 2198-2210.	5.5	14
24	Free energy perturbation (FEP)-guided scaffold hopping. <i>Acta Pharmaceutica Sinica B</i> , 2022, 12, 1351-1362.	5.7	12
25	Ab Initio QM/MM Study Shows a Highly Dissociated S_N2 Hydrolysis Mechanism for the cGMP-Specific Phosphodiesterase-5. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 5448-5457.	2.3	9
26	Rational Design of 2-Chloroadenine Derivatives as Highly Selective Phosphodiesterase 8A Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 15852-15863.	2.9	9
27	Design, Synthesis, and Evaluation of Dihydropyranopyrazole Derivatives as Novel PDE2 Inhibitors for the Treatment of Alzheimer's Disease. <i>Molecules</i> , 2021, 26, 3034.	1.7	8
28	Discovery and Optimization of Chromone Derivatives as Novel Selective Phosphodiesterase 10 Inhibitors. <i>ACS Chemical Neuroscience</i> , 2020, 11, 1058-1071.	1.7	7
29	Structural Modifications of Nimodipine Lead to Novel PDE1 Inhibitors with Anti-pulmonary Fibrosis Effects. <i>Journal of Medicinal Chemistry</i> , 2022, 65, 8444-8455.	2.9	6
30	Structure-based discovery of orally efficient inhibitors via unique interactions with H-pocket of PDE8 for the treatment of vascular dementia. <i>Acta Pharmaceutica Sinica B</i> , 2022, 12, 3103-3112.	5.7	4
31	Perspective of drug design with high-performance computing. <i>National Science Review</i> , 2021, 8, nwab105.	4.6	1
32	Reply to Behnam and Klein: Potential role of the His-tag in C-terminal His-tagged SARS-CoV-2 main protease. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	3.3	1