Liangren Zhang

List of Publications by Year
in descending order

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86 papers	1,839 citations	236833 25 h-index	315616 38 g-index
87 all docs	87 docs citations	87 times ranked	2176 citing authors

#	Article	IF	Citations
1	Discovery of novel ataxia telangiectasia mutated (ATM) kinase modulators: Computational simulation, biological evaluation and cancer combinational chemotherapy study. European Journal of Medicinal Chemistry, 2022, 233, 114196.	2.6	4
2	Optimization of 4-arylthiophene-3-carboxylic acid derivatives as inhibitors of ANO1: Lead optimization studies toward their analgesic efficacy for inflammatory pain. European Journal of Medicinal Chemistry, 2022, 237, 114413.	2.6	5
3	CMNPD: a comprehensive marine natural products database towards facilitating drug discovery from the ocean. Nucleic Acids Research, 2021, 49, D509-D515.	6.5	105
4	Discovery of 4-arylthiophene-3-carboxylic acid as inhibitor of ANO1 and its effect as analgesic agent. Acta Pharmaceutica Sinica B, 2021, 11, 1947-1964.	5.7	13
5	Vacuolin-1 inhibits endosomal trafficking and metastasis via CapZÎ². Oncogene, 2021, 40, 1775-1791.	2.6	14
6	The Discovery of Novel ACA Derivatives as Specific TRPM2 Inhibitors that Reduce Ischemic Injury Both In Vitro and In Vivo. Journal of Medicinal Chemistry, 2021, 64, 3976-3996.	2.9	16
7	Target Prediction Model for Natural Products Using Transfer Learning. International Journal of Molecular Sciences, 2021, 22, 4632.	1.8	9
8	Discovery of Novel and Potent N-Methyl-<scp>d</scp>-aspartate Receptor Positive Allosteric Modulators with Antidepressant-like Activity in Rodent Models. Journal of Medicinal Chemistry, 2021, 64, 5551-5576.	2.9	12
9	Chemical Space, Scaffolds, and Halogenated Compounds of CMNPD: A Comprehensive Chemoinformatic Analysis. Journal of Chemical Information and Modeling, 2021, 61, 3323-3336.	2.5	4
10	Synthesis and Biological Evaluation of Novel Triazine Derivatives as Positive Allosteric Modulators of Î±7 Nicotinic Acetylcholine Receptors. Journal of Medicinal Chemistry, 2021, 64, 12379-12396.	2.9	6
11	Functional Characterization and Crystal Structure of the Bifunctional Thioesterase Catalyzing Epimerization and Cyclization in Skyllamycin Biosynthesis. ACS Catalysis, 2021, 11, 11733-11741.	5.5	8
12	Design, synthesis and biological activities of benzo[d]imidazo[1,2-a]imidazole derivatives as TRPM2-specfic inhibitors. European Journal of Medicinal Chemistry, 2021, 225, 113750.	2.6	3
13	A unique ligandâ€steered strategy for CC chemokine receptor 2 homology modeling to facilitate structureâ€based virtual screening. Chemical Biology and Drug Design, 2021, 97, 944-961.	1.5	3
14	Challenging Reverse Screening: A Benchmark Study for Comprehensive Evaluation. Molecular Informatics, 2021, , 2100063.	1.4	1
15	DeepScaffold: A Comprehensive Tool for Scaffold-Based De Novo Drug Discovery Using Deep Learning. Journal of Chemical Information and Modeling, 2020, 60, 77-91.	2.5	84
16	Design, synthesis and biological activities of piperidine-spirooxadiazole derivatives as Î±7 nicotinic receptor antagonists. European Journal of Medicinal Chemistry, 2020, 207, 112774.	2.6	8
17	Discovery of 2-(2-aminobenzo[d]thiazol-6-yl) benzo[d]oxazol-5-amine derivatives that regulated HPV relevant cellular pathway and prevented cervical cancer from abnormal proliferation. European Journal of Medicinal Chemistry, 2020, 204, 112556.	2.6	2
18	Medicinal chemistry perspective of TRPM2 channel inhibitors: where we are and where we might be heading?. Drug Discovery Today, 2020, 25, 2326-2334.	3.2	10

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19	TF3P: Three-Dimensional Force Fields Fingerprint Learned by Deep Capsular Network. Journal of Chemical Information and Modeling, 2020, 60, 2754-2765.	2.5	9
20	Privileged Scaffold Analysis of Natural Products with Deep Learningâ€based Indication Prediction Model. Molecular Informatics, 2020, 39, e2000057.	1.4	10
21	Rational modification, synthesis and biological evaluation of 3,4-dihydroquinoxalin-2(1H)-one derivatives as potent and selective c-Jun N-terminal kinase 3 (JNK3) inhibitors. European Journal of Medicinal Chemistry, 2020, 201, 112445.	2.6	17
22	Pose Filter-Based Ensemble Learning Enables Discovery of Orally Active, Nonsteroidal Farnesoid X Receptor Agonists. Journal of Chemical Information and Modeling, 2020, 60, 1202-1214.	2.5	7
23	Discovery and antibacterial study of potential PPK1 inhibitors against uropathogenic E. coli. Journal of Enzyme Inhibition and Medicinal Chemistry, 2020, 35, 1224-1232.	2.5	12
24	Discovery of fused heterocyclic carboxamide derivatives as novel Î±7-nAChR agonists: Synthesis, preliminary SAR and biological evaluation. European Journal of Medicinal Chemistry, 2019, 182, 111618.	2.6	7
25	Multistage Screening Reveals 3-Substituted Indolin-2-one Derivatives as Novel and Isoform-Selective c-Jun N-terminal Kinase 3 (JNK3) Inhibitors: Implications to Drug Discovery for Potential Treatment of Neurodegenerative Diseases. Journal of Medicinal Chemistry, 2019, 62, 6645-6664.	2.9	38
26	Identification and characterization of benzo[d]oxazol-2(3H)-one derivatives as the first potent and selective small-molecule inhibitors of chromodomain protein CDYL. European Journal of Medicinal Chemistry, 2019, 182, 111656.	2.6	11
27	Direct Gating of the TRPM2 Channel by cADPR via Specific Interactions with the ADPR Binding Pocket. Cell Reports, 2019, 27, 3684-3695.e4.	2.9	45
28	Rational Design and Identification of Smallâ€Molecule Allosteric Inhibitors of CD38. ChemBioChem, 2019, 20, 2485-2493.	1.3	6
29	Discovery of novel glycogen synthase kinase-3Î± inhibitors: Structure-based virtual screening, preliminary SAR and biological evaluation for treatment of acute myeloid leukemia. European Journal of Medicinal Chemistry, 2019, 171, 221-234.	2.6	19
30	Graph-based generative models for de Novo drug design. Drug Discovery Today: Technologies, 2019, 32-33, 45-53.	4.0	15
31	Design, synthesis and biological activities of 2,3-dihydroquinazolin-4(1H)-one derivatives as TRPM2 inhibitors. European Journal of Medicinal Chemistry, 2018, 152, 235-252.	2.6	29
32	Calciumâ€Mobilizing Behaviors of Neutral Cyclic ADPâ€Ribose Mimics that Integrate Modifications to the Nucleobase, Northern Ribose and Pyrophosphate. ChemBioChem, 2018, 19, 1444-1451.	1.3	3
33	Maximal Unbiased Benchmarking Data Sets for Human Chemokine Receptors and Comparative Analysis. Journal of Chemical Information and Modeling, 2018, 58, 1104-1120.	2.5	4
34	Selective inhibition of <scp>TRPM</scp>2 channel by two novel synthesized <scp>ADPR</scp> analogues. Chemical Biology and Drug Design, 2018, 91, 552-566.	1.5	27
35	Discovery of new GSK-3Î² inhibitors through structure-based virtual screening. Bioorganic and Medicinal Chemistry Letters, 2018, 28, 160-166.	1.0	19
36	<scp>d</scp>-/<scp>l</scp>-Isothymidine incorporation in the core sequence of aptamer BC15 enhanced its binding affinity to the hnRNP A1 protein. Organic and Biomolecular Chemistry, 2018, 16, 7488-7497.	1.5	5

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37	Synthesis and Biological Evaluation of Fused Tricyclic Heterocycle Piperazine (Piperidine) Derivatives As Potential Multireceptor Atypical Antipsychotics. Journal of Medicinal Chemistry, 2018, 61, 10017-10039.	2.9	39
38	Multi-objective de novo drug design with conditional graph generative model. Journal of Cheminformatics, 2018, 10, 33.	2.8	193
39	Discovery of N-(Naphtho[1,2-b]Furan-5-Yl) Benzenesulfonamides as Novel Selective Inhibitors of Triple-Negative Breast Cancer (TNBC). Molecules, 2018, 23, 678.	1.7	4
40	Scale-Up Synthesis and Identification of GLYX-13, a NMDAR Glycine-Site Partial Agonist for the Treatment of Major Depressive Disorder. Molecules, 2018, 23, 996.	1.7	3
41	Identification of the ADPR binding pocket in the NUDT9 homology domain of TRPM2. Journal of General Physiology, 2017, 149, 219-235.	0.9	49
42	Design, synthesis, and biological evaluation of imidazo[1,2- b]pyridazine derivatives as mTOR inhibitors. European Journal of Medicinal Chemistry, 2017, 129, 135-150.	2.6	24
43	Identifying Glyceraldehyde 3-Phosphate Dehydrogenase as a Cyclic Adenosine Diphosphoribose Binding Protein by Photoaffinity Proteinâ€“Ligand Labeling Approach. Journal of the American Chemical Society, 2017, 139, 156-170.	6.6	30
44	Identification of Novel Vacuolin-1 Analogues as Autophagy Inhibitors by Virtual Drug Screening and Chemical Synthesis. Molecules, 2017, 22, 891.	1.7	17
45	The scoring bias in reverse docking and the score normalization strategy to improve success rate of target fishing. PLoS ONE, 2017, 12, e0171433.	1.1	19
46	Synthesis and biological activities of indolizine derivatives as alpha-7 nAChR agonists. European Journal of Medicinal Chemistry, 2016, 115, 94-108.	2.6	35
47	Cyclic Adenosine 5â€²-Diphosphoribose (cADPR) Mimics Used as Molecular Probes in Cell Signaling. Chemical Record, 2015, 15, 511-523.	2.9	4
48	Comparative Analysis of Pharmacophore Features and Quantitative Structureâ€“Activity Relationships for <scp>CD</scp>38 Covalent and Nonâ€covalent Inhibitors. Chemical Biology and Drug Design, 2015, 86, 1411-1424.	1.5	17
49	Enrichment Assessment of Multiple Virtual Screening Strategies for Tollâ€Like Receptor 8 Agonists Based on a Maximal Unbiased Benchmarking Data Set. Chemical Biology and Drug Design, 2015, 86, 1226-1241.	1.5	11
50	Integrating Pharmacophore into Membrane Molecular Dynamics Simulations to Improve Homology Modeling of <scp>G</scp> Proteinâ€coupled Receptors with Ligand Selectivity: A_{2A} Adenosine Receptor as an Example. Chemical Biology and Drug Design, 2015, 86, 1438-1450.	1.5	7
51	Benchmarking methods and data sets for ligand enrichment assessment in virtual screening. Methods, 2015, 71, 146-157.	1.9	40
52	An Unbiased Method To Build Benchmarking Sets for Ligand-Based Virtual Screening and its Application To GPCRs. Journal of Chemical Information and Modeling, 2014, 54, 1433-1450.	2.5	46
53	Stability and bioactivity of thrombin binding aptamers modified with<scp>d</scp>-/<scp>l</scp>-isothymidine in the loop regions. Organic and Biomolecular Chemistry, 2014, 12, 8866-8876.	1.5	38
54	Unfolding and Conformational Variations of Thrombinâ€Binding DNA Aptamers: Synthesis, Circular Dichroism and Molecular Dynamics Simulations. ChemMedChem, 2014, 9, 993-1001.	1.6	15

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55	Design, Synthesis and SAR Studies of NAD Analogues as Potent Inhibitors towards CD38 NADase. Molecules, 2014, 19, 15754-15767.	1.7	26
56	Design, synthesis and biological evaluation of indolizine derivatives as HIV-1 VIFâ€“ElonginC interaction inhibitors. Molecular Diversity, 2013, 17, 221-243.	2.1	41
57	Computational Identification of a New Binding Site in Influenza Virus Hemagglutinin for Membrane Fusion Inhibitors. Chemical Biology and Drug Design, 2013, 82, 267-274.	1.5	1
58	Indolizine Derivatives as <scp>HIV</scp>â€‘1 <scp>VIF</scp>â€“Elongin<scp>C</scp> Interaction Inhibitors. Chemical Biology and Drug Design, 2013, 81, 730-741.	1.5	46
59	Computational investigation of interactions between Cdc37 and celastrol. Molecular Simulation, 2013, 39, 270-278.	0.9	4
60	Toll-Like Receptor 7 Agonists: Chemical Feature Based Pharmacophore Identification and Molecular Docking Studies. PLoS ONE, 2013, 8, e56514.	1.1	14
61	Small-Molecule Inhibition of Human Immunodeficiency Virus Type 1 Replication by Targeting the Interaction between Vif and ElonginC. Journal of Virology, 2012, 86, 5497-5507.	1.5	63
62	A Novel Fluorescent Cell Membrane-permeable Caged Cyclic ADP-ribose Analogue. Journal of Biological Chemistry, 2012, 287, 24774-24783.	1.6	27
63	Synthesis and Calcium Mobilization Activity of cADPR Analogues Which Integrate Nucleobase, Northern and Southern Ribose Modifications. Molecules, 2012, 17, 4343-4356.	1.7	7
64	Catalysis-Based Inhibitors of the Calcium Signaling Function of CD38. Biochemistry, 2012, 51, 555-564.	1.2	31
65	A Cell Permeable NPE Caged ADP-Ribose for Studying TRPM2. PLoS ONE, 2012, 7, e51028.	1.1	23
66	Design, Synthesis and Biological Evaluation of Noncovalent Inhibitors of Human CD38 NADase. ChemMedChem, 2012, 7, 223-228.	1.6	21
67	Design and synthesis of cADPR analogues with simplified ribose and nucleobase. Journal of Chinese Pharmaceutical Sciences, 2012, 21, .	0.4	2
68	Novel nucleobase-simplified cyclic ADP-ribose analogue: A concise synthesis and Ca2+-mobilizing activity in T-lymphocytes. Organic and Biomolecular Chemistry, 2010, 8, 1843.	1.5	16
69	Concise Syntheses of Trifluoromethylated Cyclic and Acyclic Analogues of cADPR. Molecules, 2010, 15, 8689-8701.	1.7	11
70	Structural basis for the specific interaction of chicken haemoglobin with bromophenol blue: a computational analysis. Molecular Physics, 2010, 108, 215-220.	0.8	1
71	Covalent complexes of proteasome model with peptide aldehyde inhibitors MG132 and MG101: docking and molecular dynamics study. Journal of Molecular Modeling, 2009, 15, 1481-1490.	0.8	30
72	An efficient synthesis of (R)- and (S)-baclofen via desymmetrization. Tetrahedron Letters, 2009, 50, 6166-6168.	0.7	24

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73	Three-dimensional structure of HIV-1 VIF constructed by comparative modeling and the function characterization analyzed by molecular dynamics simulation. Organic and Biomolecular Chemistry, 2007, 5, 617.	1.5	30
74	Synthesis and recognition of novel isonucleoside triphosphates by DNA polymerases. Bioorganic and Medicinal Chemistry, 2007, 15, 3019-3025.	1.4	23
75	Synthesis and Agonist Activity of Cyclic ADP-Ribose Analogues with Substitution of the Northern Ribose by Ether or Alkane Chains. Journal of Medicinal Chemistry, 2006, 49, 5501-5512.	2.9	35
76	Structural insights into the effect of isonucleosides on B-DNA duplexes using molecular-dynamics simulations. Journal of Molecular Modeling, 2006, 12, 781-791.	0.8	6
77	Analysis of the interactions of ribonuclease inhibitor with kanamycin. Journal of Molecular Modeling, 2005, 11, 80-86.	0.8	3
78	A Minimal Structural Analogue of Cyclic ADP-ribose. Journal of Biological Chemistry, 2005, 280, 15952-15959.	1.6	40
79	Amplification and propagation of pacemaker Ca2+ signals by cyclic ADP-ribose and the type 3 ryanodine receptor in T cells. Journal of Cell Science, 2004, 117, 2141-2149.	1.2	41
80	Synthesis and Biological Evaluation of Novel Membrane-Permeant Cyclic ADP-Ribose Mimics:ÂN1-[(5â€˜Ââ€˜-O-Phosphorylethoxy)methyl]-5â€˜-O-phosphorylinosine 5â€˜,5â€˜Ââ€˜-Cyclicpyrophosphate (cIDPRE) and 8-Substituted Derivatives. Journal of Medicinal Chemistry, 2004, 47, 5674-5682.	2.0	51
81	Solid-Phase Synthesis of Dipeptide-Conjugated Nucleosides and Their Interaction with RNA. Helvetica Chimica Acta, 2003, 86, 3516-3524.	1.0	8
82	Synthesis of 2-amino-2-deoxy-Î²-glycosyl-(1â†’5)-nucleosides and the interaction with RNA. Bioorganic and Medicinal Chemistry, 2003, 11, 3273-3278.	1.4	10
83	Synthesis Of Spin Labeled Conjugate Of Peptide and Peptide Nucleic Acid. Synthetic Communications, 1999, 29, 1519-1525.	1.1	3
84	Synthesis and Duplex Stabilization of Oligonucleotides Consisting of Isonucleosides. Helvetica Chimica Acta, 1999, 82, 2037-2043.	1.0	19
85	8-chloroadenosine induces apoptosis in human MOLT-4 cell line. Science Bulletin, 1997, 42, 592-597.	1.7	0
86	Assignments of Nonexchangeable Proton Resonances and the Solution Structures of dâ€“TGGGT. Spectroscopy Letters, 1993, 26, 1537-1546.	0.5	1