

Liangren Zhang

List of Publications by Year in descending order

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236925
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87
all docs

87
docs citations

87
times ranked

2176
citing authors

#	ARTICLE	IF	CITATIONS
1	Multi-objective de novo drug design with conditional graph generative model. Journal of Cheminformatics, 2018, 10, 33.	6.1	193
2	CMNPD: a comprehensive marine natural products database towards facilitating drug discovery from the ocean. Nucleic Acids Research, 2021, 49, D509-D515.	14.5	105
3	DeepScaffold: A Comprehensive Tool for Scaffold-Based De Novo Drug Discovery Using Deep Learning. Journal of Chemical Information and Modeling, 2020, 60, 77-91.	5.4	84
4	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.	3.4	63
5	Synthesis and Biological Evaluation of Novel Membrane-Permeant Cyclic ADP-Ribose Mimics: AN1-[(5'-O-Phosphorylethoxy)methyl]-5'-O-phosphorylinosine 5',5'-Cyclicpyrophosphate (cADPRE) and 8-Substituted Derivatives. Journal of Medicinal Chemistry, 2004, 47, 5674-5682.	6.4	51
6	Identification of the ADPR binding pocket in the NUDT9 homology domain of TRPM2. Journal of General Physiology, 2017, 149, 219-235.	1.9	49
7	Indolizine Derivatives as HIV-1 VIF-ElonginC Interaction Inhibitors. Chemical Biology and Drug Design, 2013, 81, 730-741.	3.2	46
8	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.	5.4	46
9	Direct Gating of the TRPM2 Channel by cADPR via Specific Interactions with the ADPR Binding Pocket. Cell Reports, 2019, 27, 3684-3695.e4.	6.4	45
10	Amplification and propagation of pacemaker Ca ²⁺ signals by cyclic ADP-ribose and the type 3 ryanodine receptor in T cells. Journal of Cell Science, 2004, 117, 2141-2149.	2.0	41
11	Design, synthesis and biological evaluation of indolizine derivatives as HIV-1 VIF-ElonginC interaction inhibitors. Molecular Diversity, 2013, 17, 221-243.	3.9	41
12	A Minimal Structural Analogue of Cyclic ADP-ribose. Journal of Biological Chemistry, 2005, 280, 15952-15959.	3.4	40
13	Benchmarking methods and data sets for ligand enrichment assessment in virtual screening. Methods, 2015, 71, 146-157.	3.8	40
14	Synthesis and Biological Evaluation of Fused Tricyclic Heterocycle Piperazine (Piperidine) Derivatives As Potential Multireceptor Atypical Antipsychotics. Journal of Medicinal Chemistry, 2018, 61, 10017-10039.	6.4	39
15	Stability and bioactivity of thrombin binding aptamers modified with dC-dI-isothymidine in the loop regions. Organic and Biomolecular Chemistry, 2014, 12, 8866-8876.	2.8	38
16	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.	6.4	38
17	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.	6.4	35
18	Synthesis and biological activities of indolizine derivatives as alpha-7 nAChR agonists. European Journal of Medicinal Chemistry, 2016, 115, 94-108.	5.5	35

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19	Catalysis-Based Inhibitors of the Calcium Signaling Function of CD38. <i>Biochemistry</i> , 2012, 51, 555-564.	2.5	31
20	Three-dimensional structure of HIV-1 VIF constructed by comparative modeling and the function characterization analyzed by molecular dynamics simulation. <i>Organic and Biomolecular Chemistry</i> , 2007, 5, 617.	2.8	30
21	Covalent complexes of proteasome model with peptide aldehyde inhibitors MG132 and MG101: docking and molecular dynamics study. <i>Journal of Molecular Modeling</i> , 2009, 15, 1481-1490.	1.8	30
22	Identifying Glyceraldehyde 3-Phosphate Dehydrogenase as a Cyclic Adenosine Diphosphoribose Binding Protein by Photoaffinity Proteinâ€“Ligand Labeling Approach. <i>Journal of the American Chemical Society</i> , 2017, 139, 156-170.	13.7	30
23	Design, synthesis and biological activities of 2,3-dihydroquinazolin-4(1H)-one derivatives as TRPM2 inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2018, 152, 235-252.	5.5	29
24	A Novel Fluorescent Cell Membrane-permeable Caged Cyclic ADP-ribose Analogue. <i>Journal of Biological Chemistry</i> , 2012, 287, 24774-24783.	3.4	27
25	Selective inhibition of <scp>TRPM</scp>2 channel by two novel synthesized <scp>ADPR</scp> analogues. <i>Chemical Biology and Drug Design</i> , 2018, 91, 552-566.	3.2	27
26	Design, Synthesis and SAR Studies of NAD Analogues as Potent Inhibitors towards CD38 NADase. <i>Molecules</i> , 2014, 19, 15754-15767.	3.8	26
27	An efficient synthesis of (R)- and (S)-baclofen via desymmetrization. <i>Tetrahedron Letters</i> , 2009, 50, 6166-6168.	1.4	24
28	Design, synthesis, and biological evaluation of imidazo[1,2- b]pyridazine derivatives as mTOR inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2017, 129, 135-150.	5.5	24
29	Synthesis and recognition of novel isonucleoside triphosphates by DNA polymerases. <i>Bioorganic and Medicinal Chemistry</i> , 2007, 15, 3019-3025.	3.0	23
30	A Cell Permeable NPE Caged ADP-Ribose for Studying TRPM2. <i>PLoS ONE</i> , 2012, 7, e51028.	2.5	23
31	Design, Synthesis and Biological Evaluation of Noncovalent Inhibitors of Human CD38 NADase. <i>ChemMedChem</i> , 2012, 7, 223-228.	3.2	21
32	Synthesis and Duplex Stabilization of Oligonucleotides Consisting of Isonucleosides. <i>Helvetica Chimica Acta</i> , 1999, 82, 2037-2043.	1.6	19
33	Discovery of new GSK-3Î² inhibitors through structure-based virtual screening. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2018, 28, 160-166.	2.2	19
34	Discovery of novel glycogen synthase kinase-3Î± inhibitors: Structure-based virtual screening, preliminary SAR and biological evaluation for treatment of acute myeloid leukemia. <i>European Journal of Medicinal Chemistry</i> , 2019, 171, 221-234.	5.5	19
35	The scoring bias in reverse docking and the score normalization strategy to improve success rate of target fishing. <i>PLoS ONE</i> , 2017, 12, e0171433.	2.5	19
36	Comparative Analysis of Pharmacophore Features and Quantitative Structureâ€“Activity Relationships for <scp>CD</scp>38 Covalent and Nonâ€“covalent Inhibitors. <i>Chemical Biology and Drug Design</i> , 2015, 86, 1411-1424.	3.2	17

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37	Identification of Novel Vacuolin-1 Analogues as Autophagy Inhibitors by Virtual Drug Screening and Chemical Synthesis. <i>Molecules</i> , 2017, 22, 891.	3.8	17
38	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. <i>European Journal of Medicinal Chemistry</i> , 2020, 201, 112445.	5.5	17
39	Novel nucleobase-simplified cyclic ADP-ribose analogue: A concise synthesis and Ca ²⁺ -mobilizing activity in T-lymphocytes. <i>Organic and Biomolecular Chemistry</i> , 2010, 8, 1843.	2.8	16
40	The Discovery of Novel ACA Derivatives as Specific TRPM2 Inhibitors that Reduce Ischemic Injury Both In Vitro and In Vivo. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 3976-3996.	6.4	16
41	Unfolding and Conformational Variations of Thrombin- α -Binding DNA Aptamers: Synthesis, Circular Dichroism and Molecular Dynamics Simulations. <i>ChemMedChem</i> , 2014, 9, 993-1001.	3.2	15
42	Graph-based generative models for de Novo drug design. <i>Drug Discovery Today: Technologies</i> , 2019, 32-33, 45-53.	4.0	15
43	Vacuolin-1 inhibits endosomal trafficking and metastasis via CapZ ¹² . <i>Oncogene</i> , 2021, 40, 1775-1791.	5.9	14
44	Toll-Like Receptor 7 Agonists: Chemical Feature Based Pharmacophore Identification and Molecular Docking Studies. <i>PLoS ONE</i> , 2013, 8, e56514.	2.5	14
45	Discovery of 4-arylthiophene-3-carboxylic acid as inhibitor of ANO1 and its effect as analgesic agent. <i>Acta Pharmaceutica Sinica B</i> , 2021, 11, 1947-1964.	12.0	13
46	Discovery of Novel and Potent N-Methyl-D-aspartate Receptor Positive Allosteric Modulators with Antidepressant-like Activity in Rodent Models. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 5551-5576.	6.4	12
47	Discovery and antibacterial study of potential PPK1 inhibitors against uropathogenic E. coli. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2020, 35, 1224-1232.	5.2	12
48	Concise Syntheses of Trifluoromethylated Cyclic and Acyclic Analogues of cADPR. <i>Molecules</i> , 2010, 15, 8689-8701.	3.8	11
49	Enrichment Assessment of Multiple Virtual Screening Strategies for Toll-Like Receptor 8 Agonists Based on a Maximal Unbiased Benchmarking Data Set. <i>Chemical Biology and Drug Design</i> , 2015, 86, 1226-1241.	3.2	11
50	Identification and characterization of benzo[d]oxazol-2(3H)-one derivatives as the first potent and selective small-molecule inhibitors of chromodomain protein CDYL. <i>European Journal of Medicinal Chemistry</i> , 2019, 182, 111656.	5.5	11
51	Synthesis of 2-amino-2-deoxy- β -glycosyl-(1 α '5)-nucleosides and the interaction with RNA. <i>Bioorganic and Medicinal Chemistry</i> , 2003, 11, 3273-3278.	3.0	10
52	Medicinal chemistry perspective of TRPM2 channel inhibitors: where we are and where we might be heading?. <i>Drug Discovery Today</i> , 2020, 25, 2326-2334.	6.4	10
53	Privileged Scaffold Analysis of Natural Products with Deep Learning-based Indication Prediction Model. <i>Molecular Informatics</i> , 2020, 39, e2000057.	2.5	10
54	TF3P: Three-Dimensional Force Fields Fingerprint Learned by Deep Capsular Network. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 2754-2765.	5.4	9

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55	Target Prediction Model for Natural Products Using Transfer Learning. <i>International Journal of Molecular Sciences</i> , 2021, 22, 4632.	4.1	9
56	Solid-Phase Synthesis of Dipeptide-Conjugated Nucleosides and Their Interaction with RNA. <i>Helvetica Chimica Acta</i> , 2003, 86, 3516-3524.	1.6	8
57	Design, synthesis and biological activities of piperidine-spirooxadiazole derivatives as $\alpha 7$ nicotinic receptor antagonists. <i>European Journal of Medicinal Chemistry</i> , 2020, 207, 112774.	5.5	8
58	Functional Characterization and Crystal Structure of the Bifunctional Thioesterase Catalyzing Epimerization and Cyclization in Skylamycin Biosynthesis. <i>ACS Catalysis</i> , 2021, 11, 11733-11741.	11.2	8
59	Synthesis and Calcium Mobilization Activity of cADPR Analogues Which Integrate Nucleobase, Northern and Southern Ribose Modifications. <i>Molecules</i> , 2012, 17, 4343-4356.	3.8	7
60	Integrating Pharmacophore into Membrane Molecular Dynamics Simulations to Improve Homology Modeling of G Protein-coupled Receptors with Ligand Selectivity: A_{2A} Adenosine Receptor as an Example. <i>Chemical Biology and Drug Design</i> , 2015, 86, 1438-1450.	3.2	7
61	Discovery of fused heterocyclic carboxamide derivatives as novel $\alpha 7$ -nAChR agonists: Synthesis, preliminary SAR and biological evaluation. <i>European Journal of Medicinal Chemistry</i> , 2019, 182, 111618.	5.5	7
62	Pose Filter-Based Ensemble Learning Enables Discovery of Orally Active, Nonsteroidal Farnesoid X Receptor Agonists. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 1202-1214.	5.4	7
63	Structural insights into the effect of isonucleosides on B-DNA duplexes using molecular-dynamics simulations. <i>Journal of Molecular Modeling</i> , 2006, 12, 781-791.	1.8	6
64	Rational Design and Identification of Small-Molecule Allosteric Inhibitors of CD38. <i>ChemBioChem</i> , 2019, 20, 2485-2493.	2.6	6
65	Synthesis and Biological Evaluation of Novel Triazine Derivatives as Positive Allosteric Modulators of $\alpha 7$ Nicotinic Acetylcholine Receptors. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 12379-12396.	6.4	6
66	dC -Isothymidine incorporation in the core sequence of aptamer BC15 enhanced its binding affinity to the hnRNP A1 protein. <i>Organic and Biomolecular Chemistry</i> , 2018, 16, 7488-7497.	2.8	5
67	Optimization of 4-arylthiophene-3-carboxylic acid derivatives as inhibitors of ANO1: Lead optimization studies toward their analgesic efficacy for inflammatory pain. <i>European Journal of Medicinal Chemistry</i> , 2022, 237, 114413.	5.5	5
68	Computational investigation of interactions between Cdc37 and celastrol. <i>Molecular Simulation</i> , 2013, 39, 270-278.	2.0	4
69	Cyclic Adenosine 5'-Diphosphoribose (cADPR) Mimics Used as Molecular Probes in Cell Signaling. <i>Chemical Record</i> , 2015, 15, 511-523.	5.8	4
70	Maximal Unbiased Benchmarking Data Sets for Human Chemokine Receptors and Comparative Analysis. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 1104-1120.	5.4	4
71	Discovery of N-(Naphtho[1,2-b]Furan-5-Yl) Benzenesulfonamides as Novel Selective Inhibitors of Triple-Negative Breast Cancer (TNBC). <i>Molecules</i> , 2018, 23, 678.	3.8	4
72	Chemical Space, Scaffolds, and Halogenated Compounds of CMNPD: A Comprehensive Chemoinformatic Analysis. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 3323-3336.	5.4	4

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73	Discovery of novel ataxia telangiectasia mutated (ATM) kinase modulators: Computational simulation, biological evaluation and cancer combinational chemotherapy study. <i>European Journal of Medicinal Chemistry</i> , 2022, 233, 114196.	5.5	4
74	Synthesis Of Spin Labeled Conjugate Of Peptide and Peptide Nucleic Acid. <i>Synthetic Communications</i> , 1999, 29, 1519-1525.	2.1	3
75	Analysis of the interactions of ribonuclease inhibitor with kanamycin. <i>Journal of Molecular Modeling</i> , 2005, 11, 80-86.	1.8	3
76	Calcium-Mobilizing Behaviors of Neutral Cyclic ADP-Ribose Mimics that Integrate Modifications to the Nucleobase, Northern Ribose and Pyrophosphate. <i>ChemBioChem</i> , 2018, 19, 1444-1451.	2.6	3
77	Scale-Up Synthesis and Identification of GLYX-13, a NMDAR Glycine-Site Partial Agonist for the Treatment of Major Depressive Disorder. <i>Molecules</i> , 2018, 23, 996.	3.8	3
78	Design, synthesis and biological activities of benzo[d]imidazo[1,2-a]imidazole derivatives as TRPM2-specific inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2021, 225, 113750.	5.5	3
79	A unique ligand-steered strategy for CC chemokine receptor 2 homology modeling to facilitate structure-based virtual screening. <i>Chemical Biology and Drug Design</i> , 2021, 97, 944-961.	3.2	3
80	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. <i>European Journal of Medicinal Chemistry</i> , 2020, 204, 112556.	5.5	2
81	Design and synthesis of cADPR analogues with simplified ribose and nucleobase. <i>Journal of Chinese Pharmaceutical Sciences</i> , 2012, 21, .	0.1	2
82	Assignments of Nonexchangeable Proton Resonances and the Solution Structures of dTGGGT. <i>Spectroscopy Letters</i> , 1993, 26, 1537-1546.	1.0	1
83	Structural basis for the specific interaction of chicken haemoglobin with bromophenol blue: a computational analysis. <i>Molecular Physics</i> , 2010, 108, 215-220.	1.7	1
84	Computational Identification of a New Binding Site in Influenza Virus Hemagglutinin for Membrane Fusion Inhibitors. <i>Chemical Biology and Drug Design</i> , 2013, 82, 267-274.	3.2	1
85	Challenging Reverse Screening: A Benchmark Study for Comprehensive Evaluation. <i>Molecular Informatics</i> , 2021, , 2100063.	2.5	1
86	8-chloroadenosine induces apoptosis in human MOLT-4 cell line. <i>Science Bulletin</i> , 1997, 42, 592-597.	1.7	0