Jiang Hualiang

List of Publications by Year
in descending order

82 papers	8,849 citations	159585 30 h-index	60623 81 g-index
89 all docs	89 docs citations	89 times ranked	13190 citing authors

#	Article	IF	Citations
1	Design, Synthesis, and Biological Evaluation of Peptidomimetic Aldehydes as Broad-Spectrum Inhibitors against Enterovirus and SARS-CoV-2. Journal of Medicinal Chemistry, 2022, 65, 2794-2808.	6.4	52
2	Facing small and biased data dilemma in drug discovery with enhanced federated learning approaches. Science China Life Sciences, 2022, 65, 529-539.	4.9	17
3	Drug target inference by mining transcriptional data using a novel graph convolutional network framework. Protein and Cell, 2022, 13, 281-301.	11.0	18
4	Computational characterization of transducer recognition of Î²2 adrenergic receptor. Biochemical and Biophysical Research Communications, 2022, 592, 67-73.	2.1	6
5	Structures of the Omicron spike trimer with ACE2 and an anti-Omicron antibody. Science, 2022, 375, 1048-1053.	12.6	216
6	Molecular basis for allosteric agonism and G protein subtype selectivity of galanin receptors. Nature Communications, 2022, 13, 1364.	12.8	23
7	Structural basis of leukotriene B4 receptor 1 activation. Nature Communications, 2022, 13, 1156.	12.8	19
8	Structural insights into ligand binding and activation of the human thyrotropin-releasing hormone receptor. Cell Research, 2022, 32, 855-857.	12.0	4
9	Dual-acting antitumor agents targeting the A2A adenosine receptor and histone deacetylases: Design and synthesis of 4-(furan-2-yl)-1H-pyrazolo[3,4-d]pyrimidin-6-amine derivatives. European Journal of Medicinal Chemistry, 2022, 236, 114326.	5.5	5
10	Oral remdesivir derivative VV116 is a potent inhibitor of respiratory syncytial virus with efficacy in mouse model. Signal Transduction and Targeted Therapy, 2022, 7, 123.	17.1	14
11	Why is the SARS-CoV-2 Omicron variant milder?. Innovation(China), 2022, 3, 100251.	9.1	12
12	Beneficial effects exerted by hydroxychloroquine in treating COVID-19 patients via protecting multiple organs. Science China Life Sciences, 2021, 64, 330-333.	4.9	12
13	Cryo-EM structure determination captures new chemical modification of protein. Science China Life Sciences, 2021, 64, 1781-1783.	4.9	1
14	Structural insights into the human D1 and D2 dopamine receptor signaling complexes. Cell, 2021, 184, 931-942.e18.	28.9	140
15	Mechanism of dopamine binding and allosteric modulation of the human D1 dopamine receptor. Cell Research, 2021, 31, 593-596.	12.0	48
16	Structural basis for inhibition of the SARS-CoV-2 RNA polymerase by suramin. Nature Structural and Molecular Biology, 2021, 28, 319-325.	8.2	104
17	Structures of the human dopamine D3 receptor-Gi complexes. Molecular Cell, 2021, 81, 1147-1159.e4.	9.7	51
18	Structural insights into the lipid and ligand regulation of serotonin receptors. Nature, 2021, 592, 469-473.	27.8	138

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19	Drug discovery and development targeting the life cycle of SARS-CoV-2. Fundamental Research, 2021, 1, 151-165.	3.3	9
20	Effects of Shuanghuanglian oral liquids on patients with COVID-19: a randomized, open-label, parallel-controlled, multicenter clinical trial. Frontiers of Medicine, 2021, 15, 704-717.	3.4	33
21	Graph neural networks for automated de novo drug design. Drug Discovery Today, 2021, 26, 1382-1393.	6.4	71
22	Identification of pyrogallol as a warhead in design of covalent inhibitors for the SARS-CoV-2 3CL protease. Nature Communications, 2021, 12, 3623.	12.8	111
23	SARS-CoV-2 envelope protein causes acute respiratory distress syndrome (ARDS)-like pathological damages and constitutes an antiviral target. Cell Research, 2021, 31, 847-860.	12.0	102
24	Targeting sorting nexin 10 improves mouse colitis via inhibiting PIKfyve-mediated TBK1/c-Rel signaling activation. Pharmacological Research, 2021, 169, 105679.	7.1	3
25	Structures of full-length glycoprotein hormone receptor signalling complexes. Nature, 2021, 598, 688-692.	27.8	52
26	Design and development of an oral remdesivir derivative VV116 against SARS-CoV-2. Cell Research, 2021, 31, 1212-1214.	12.0	71
27	Constitutive signal bias mediated by the human GHRHR splice variant 1. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	13
28	Structure-Based Design of Dual-Acting Compounds Targeting Adenosine A_{2A} Receptor and Histone Deacetylase as Novel Tumor Immunotherapeutic Agents. Journal of Medicinal Chemistry, 2021, 64, 16573-16597.	6.4	16
29	Structural basis for activation of the growth hormone-releasing hormone receptor. Nature Communications, 2020, 11, 5205.	12.8	57
30	Automated design and optimization of multitarget schizophrenia drug candidates by deep learning. European Journal of Medicinal Chemistry, 2020, 204, 112572.	5.5	25
31	Potential treatment of COVID-19 by inhibitors of human dihydroorotateÂdehydrogenase. Protein and Cell, 2020, 11, 699-702.	11.0	18
32	Structure of Mpro from SARS-CoV-2 and discovery of its inhibitors. Nature, 2020, 582, 289-293.	27.8	3,133
33	Revisiting Aldehyde Oxidase Mediated Metabolism in Drug-like Molecules: An Improved Computational Model. Journal of Medicinal Chemistry, 2020, 63, 6523-6537.	6.4	10
34	Structural basis for inhibition of the RNA-dependent RNA polymerase from SARS-CoV-2 by remdesivir. Science, 2020, 368, 1499-1504.	12.6	950
35	Structure-based design of antiviral drug candidates targeting the SARS-CoV-2 main protease. Science, 2020, 368, 1331-1335.	12.6	1,135
36	Nature brings new avenues to the therapy of central nervous system diseasesâ€"An overview of possible treatments derived from natural products. Science China Life Sciences, 2019, 62, 1332-1367.	4.9	20

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37	High-resolution mapping of brain vasculature and its impairment in the hippocampus of Alzheimer's disease mice. National Science Review, 2019, 6, 1223-1238.	9.5	65
38	Dynamic modifications of biomacromolecules: mechanism and chemical interventions. Science China Life Sciences, 2019, 62, 1459-1471.	4.9	14
39	Pharmacokinetics-Driven Optimization of 4(3H)-Pyrimidinones as Phosphodiesterase Type 5 Inhibitors Leading to TPN171, a Clinical Candidate for the Treatment of Pulmonary Arterial Hypertension. Journal of Medicinal Chemistry, 2019, 62, 4979-4990.	6.4	25
40	China's reform of the regulatory system for medical products and its impact. National Science Review, 2019, 6, 1-1.	9.5	13
41	Allostery in Drug Development. Advances in Experimental Medicine and Biology, 2019, 1163, 1-23.	1.6	15
42	The Mechanism by Which Luteolin Disrupts the Cytoplasmic Membrane of Methicillin-Resistant Staphylococcus aureus. Journal of Physical Chemistry B, 2018, 122, 1427-1438.	2.6	18
43	Computational chemical biology and drug design: Facilitating protein structure, function, and modulation studies. Medicinal Research Reviews, 2018, 38, 914-950.	10.5	38
44	Structure of the glucagon receptor in complex with a glucagon analogue. Nature, 2018, 553, 106-110.	27.8	109
45	Characterizing the interactions of two lipid modifications with lipid rafts: farnesyl anchors vs. palmitoyl anchors. European Biophysics Journal, 2018, 47, 19-30.	2.2	5
46	Artificial intelligence in drug design. Science China Life Sciences, 2018, 61, 1191-1204.	4.9	145
47	Discovery of new antimalarial agents: Second-generation dual inhibitors against FP-2 and PfDHFR via fragments assembely. Bioorganic and Medicinal Chemistry, 2017, 25, 6467-6478.	3.0	12
48	Discovery of potent 2,4-difluoro-linker poly(ADP-ribose) polymerase 1 inhibitors with enhanced water solubility and in vivo anticancer efficacy. Acta Pharmacologica Sinica, 2017, 38, 1521-1532.	6.1	8
49	Computational Studies on Acetylcholinesterases. Molecules, 2017, 22, 1324.	3.8	33
50	Probing the structure and dynamics of caveolin-1 in a caveolae-mimicking asymmetric lipid bilayer model. European Biophysics Journal, 2016, 45, 511-521.	2.2	18
51	Small-Molecule Targeting of E3 Ligase Adaptor SPOP in Kidney Cancer. Cancer Cell, 2016, 30, 474-484.	16.8	74
52	Effects of ion interactions with a cholesterol-rich bilayer. Biochemical and Biophysical Research Communications, 2015, 468, 125-129.	2.1	8
53	Discovery of Benzylidene Derivatives as Potent Syk Inhibitors: Synthesis, SAR Analysis, and Biological Evaluation. Archiv Der Pharmazie, 2015, 348, 463-474.	4.1	4
54	Design, Synthesis, and Biological Evaluation of Novel Nonsteroidal Farnesoidâ€…X Receptor (FXR) Antagonists: Molecular Basis of FXR Antagonism. ChemMedChem, 2015, 10, 1184-1199.	3.2	16

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55	Combinatorial Pharmacophore-Based 3D-QSAR Analysis and Virtual Screening of FGFR1 Inhibitors. International Journal of Molecular Sciences, 2015, 16, 13407-13426.	4.1	26
56	Discovery of Novel Small Molecule Anti-HCV Agents via the CypA Inhibitory Mechanism Using O-Acylation-Directed Lead Optimization. Molecules, 2015, 20, 10342-10359.	3.8	16
57	A Genetic Algorithm Based Support Vector Machine Model for Blood-Brain Barrier Penetration Prediction. BioMed Research International, 2015, 2015, 1-13.	1.9	23
58	TarPred: a web application for predicting therapeutic and side effect targets of chemical compounds. Bioinformatics, 2015, 31, 2049-2051.	4.1	52
59	Identification, synthesis and pharmacological evaluation of novel anti-EV71 agents via cyclophilin A inhibition. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 5682-5686.	2.2	11
60	Estimation of acute oral toxicity in rat using local lazy learning. Journal of Cheminformatics, 2014, 6, 26.	6.1	30
61	iDrug: a web-accessible and interactive drug discovery and design platform. Journal of Cheminformatics, 2014, 6, 28.	6.1	30
62	Protein tyrosine phosphatase receptor U (PTPRU) is required for glioma growth and motility. Carcinogenesis, 2014, 35, 1901-1910.	2.8	30
63	Structural Basis for Molecular Recognition at Serotonin Receptors. Science, 2013, 340, 610-614.	12.6	454
64	Free energy landscape for the binding process of Huperzine A to acetylcholinesterase. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 4273-4278.	7.1	79
65	Accelerating All-Atom Normal Mode Analysis with Graphics Processing Unit. Journal of Chemical Theory and Computation, 2011, 7, 1595-1603.	5.3	5
66	SHAFTS: A Hybrid Approach for 3D Molecular Similarity Calculation. 1. Method and Assessment of Virtual Screening. Journal of Chemical Information and Modeling, 2011, 51, 2372-2385.	5.4	145
67	First Reaction of a Chiral Glyâ€Ni(II) Complex in Water. Chinese Journal of Chemistry, 2010, 28, 422-428.	4.9	3
68	Facile Creation of 3â€Indolylâ€3â€hydroxyâ€2â€oxindoles by an Organocatalytic Enantioselective Friedelâ€“Crafts Reaction of Indoles with Isatins. Advanced Synthesis and Catalysis, 2010, 352, 833-838.	4.3	92
69	A Direct Amineâ€Palladium Acetate Cocatalyzed Saegusa Oxidation Reaction of Unmodified Aldehydes to Î±,Î²â€Unsaturated Aldehydes. Advanced Synthesis and Catalysis, 2009, 351, 1229-1232.	4.3	88
70	Silverâ€Catalyzed Intramolecular Cyclization of oâ€(1â€Alkynyl)benzamides: Efficient Synthesis of (1H)â€Isochromenâ€1â€imines. Advanced Synthesis and Catalysis, 2009, 351, 2605-2610.	4.3	57
71	Goldâ€and Silverâ€Catalyzed Intramolecular Hydroamination of Terminal Alkynes: Waterâ€Triggered Chemoâ€ and Regioselective Synthesis of Fused Tricyclic Xanthines. Advanced Synthesis and Catalysis, 2009, 351, 2770-2778.	4.3	55
72	Refinement and 3Dâ€QSAR Studies of Inhibitors of Cyclophilin A Containing Amide Linker. QSAR and Combinatorial Science, 2009, 28, 183-193.	1.4	4

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73	Reduced Catalytic Activity of P450 2A6 Mutants with Coumarin: A Computational Investigation. Journal of Chemical Theory and Computation, 2009, 5, 1411-1420.	5.3	22
74	Research progress in cation-Ï€ interactions. Science in China Series B: Chemistry, 2008, 51, 709-717.	0.8	24
75	The open-close mechanism of M2 channel protein in influenza A virus: A computational study on the hydrogen bonds and cation-Ï€ interactions among His37 and Trp41. Science in China Series B: Chemistry, 2008, 51, 768-775.	0.8	6
76	Ionicâ€Liquidâ€Supported Total Synthesis of Sansalvamide A Peptide. Synthetic Communications, 2008, 38, 239-248.	2.1	20
77	Microwaveâ€Assisted Dehalogenation of Î±â€Haloketones by Zinc and Ammonium Chloride in Alcohol. Synthetic Communications, 2008, 38, 567-575.	2.1	12
78	Transformation of Aryl Acyloin Oâ€Alkyl and Oâ€Phenyl Derivatives to Ketones. Synthetic Communications, 2007, 37, 149-156.	2.1	18
79	Cation sitting in aromatic cages:ab initio computational studies on tetramethylammoniumâ€“(benzene)n (n=3â€“4) complexes. Journal of Physical Organic Chemistry, 2007, 20, 448-453.	1.9	10
80	Techniques used for the discovery of therapeutic compounds: The case of SARS. Drug Discovery Today: Technologies, 2006, 3, 277-283.	4.0	8
81	Cinanserin Is an Inhibitor of the 3C-Like Proteinase of Severe Acute Respiratory Syndrome Coronavirus and Strongly Reduces Virus Replication In Vitro. Journal of Virology, 2005, 79, 7095-7103.	3.4	185
82	Focused Library Design Based on Hit and Target Structures: Method and Application in Drug Discovery. , 0, , 108-124.		0