Fang Bai

List of Publications by Year
in descending order

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36 papers	6,492 citations	279701 23 h-index	360920 35 g-index
38 all docs	38 docs citations	38 times ranked	10476 citing authors

#	Article	IF	Citations
1	Structure of Mpro from SARS-CoV-2 and discovery of its inhibitors. Nature, 2020, 582, 289-293.	13.7	3,133
2	Structure-based design of antiviral drug candidates targeting the SARS-CoV-2 main protease. Science, 2020, 368, 1331-1335.	6.0	1,135
3	Structural Basis for Molecular Recognition at Serotonin Receptors. Science, 2013, 340, 610-614.	6.0	454
4	Anti-SARS-CoV-2 activities in vitro of Shuanghuanglian preparations and bioactive ingredients. Acta Pharmacologica Sinica, 2020, 41, 1167-1177.	2.8	314
5	Targeting CPT1A-mediated fatty acid oxidation sensitizes nasopharyngeal carcinoma to radiation therapy. Theranostics, 2018, 8, 2329-2347.	4.6	155
6	NEET Proteins: A New Link Between Iron Metabolism, Reactive Oxygen Species, and Cancer. Antioxidants and Redox Signaling, 2019, 30, 1083-1095.	2.5	129
7	Enhancing intracellular accumulation and target engagement of PROTACs with reversible covalent chemistry. Nature Communications, 2020, 11, 4268.	5.8	112
8	Redox-dependent gating of VDAC by mitoNEET. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 19924-19929.	3.3	85
9	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.	3.3	79
10	Elucidating the druggable interface of proteinâ^'protein interactions using fragment docking and coevolutionary analysis. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E8051-E8058.	3.3	65
11	The Fe-S cluster-containing NEET proteins mitoNEET and NAF-1 as chemotherapeutic targets in breast cancer. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 3698-3703.	3.3	64
12	Breast cancer tumorigenicity is dependent on high expression levels of NAF-1 and the lability of its Fe-S clusters. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 10890-10895.	3.3	64
13	Identification of matrine as a promising novel drug for hepatic steatosis and glucose intolerance with <scp>HSP</scp>72 as an upstream target. British Journal of Pharmacology, 2015, 172, 4303-4318.	2.7	60
14	Discovery of Pteridin-7(8H)-one-Based Irreversible Inhibitors Targeting the Epidermal Growth Factor Receptor (EGFR) Kinase T790M/L858R Mutant. Journal of Medicinal Chemistry, 2013, 56, 7821-7837.	2.9	58
15	Gambogic acid identifies an isoform-specific druggable pocket in the middle domain of Hsp90Î². Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E4801-9.	3.3	52
16	A multi-targeting drug design strategy for identifying potent anti-SARS-CoV-2 inhibitors. Acta Pharmacologica Sinica, 2022, 43, 483-493.	2.8	43
17	Cyndi: a multi-objective evolution algorithm based method for bioactive molecular conformational generation. BMC Bioinformatics, 2009, 10, 101.	1.2	42
18	Interactions between mitoNEET and NAF-1 in cells. PLoS ONE, 2017, 12, e0175796.	1.1	42

#	Article	IF	Citations
19	Discovery of potential small molecular SARS-CoV-2 entry blockers targeting the spike protein. Acta Pharmacologica Sinica, 2022, 43, 788-796.	2.8	40
20	Kinetics-Driven Drug Design Strategy for Next-Generation Acetylcholinesterase Inhibitors to Clinical Candidate. Journal of Medicinal Chemistry, 2021, 64, 1844-1855.	2.9	32
21	Fast and effective identification of the bioactive compounds and their targets from medicinal plants via computational chemical biology approach. MedChemComm, 2011, 2, 471.	3.5	29
22	Bioactive conformational generation of small molecules: A comparative analysis between force-field and multiple empirical criteria based methods. BMC Bioinformatics, 2010, 11, 545.	1.2	26
23	Discovery of novel selective inhibitors for EGFR-T790M/L858R. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 1365-1370.	1.0	24
24	Recent advances in predicting proteinâ€“protein interactions with the aid of artificial intelligence algorithms. Current Opinion in Structural Biology, 2022, 73, 102344.	2.6	24
25	A VDAC1-mediated NEET protein chain transfers [2Fe-2S] clusters between the mitochondria and the cytosol and impacts mitochondrial dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	3.3	20
26	A Generic Force Field for Protein Coarse-Grained Molecular Dynamics Simulation. International Journal of Molecular Sciences, 2012, 13, 14451-14469.	1.8	18
27	Veratramine modulates AP-1-dependent gene transcription by directly binding to programmable DNA. Nucleic Acids Research, 2018, 46, 546-557.	6.5	17
28	An Accurate Metalloprotein-Specific Scoring Function and Molecular Docking Program Devised by a Dynamic Sampling and Iteration Optimization Strategy. Journal of Chemical Information and Modeling, 2015, 55, 833-847.	2.5	15
29	Probing the Allosteric Inhibition Mechanism of a Spike Protein Using Molecular Dynamics Simulations and Active Compound Identifications. Journal of Medicinal Chemistry, 2022, 65, 2827-2835.	2.9	15
30	BAP1 forms a trimer with HMGB1 and HDAC1 that modulates gene Ã— environment interaction with asbestos. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	14
31	Target-Based Virtual Screening and LC/MS-Guided Isolation Procedure for Identifying Phloroglucinol-Terpenoid Inhibitors of SARS-CoV-2. Journal of Natural Products, 2022, 85, 327-336.	1.5	13
32	The nature of proton-coupled electron transfer in a blue light using flavin domain. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	3.3	12
33	The anti-apoptotic proteins NAF-1 and iASPP interact to drive apoptosis in cancer cells. Chemical Science, 2019, 10, 665-673.	3.7	11
34	In Silico Elucidation of the Plausible Inhibitory Potential of Withaferin A of Withania Somnifera Medicinal Herb Against Breast Cancer Targeting Estrogen Receptor. Current Pharmaceutical Biotechnology, 2020, 21, 842-851.	0.9	3
35	A Statistical Thermodynamic Model for Ligands Interacting With Ion Channels: Theoretical Model and Experimental Validation of the KCNQ2 Channel. Frontiers in Pharmacology, 2018, 9, 150.	1.6	2
36	The binding proximity of methyl Î²-lilacinobioside isolated from Caralluma retrospiciens with topoisomerase II attributes apoptosis in breast cancer cell line. Saudi Journal of Biological Sciences, 2018, 25, 1826-1833.	1.8	1