Fang Bai

List of Publications by Year
in descending order

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36 papers	6,492 citations	279487 23 h-index	360668 35 g-index
38 all docs	38 docs citations	38 times ranked	10476 citing authors

#	Article	IF	Citations
1	A multi-targeting drug design strategy for identifying potent anti-SARS-CoV-2 inhibitors. Acta Pharmacologica Sinica, 2022, 43, 483-493.	2.8	43
2	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
3	Discovery of potential small molecular SARS-CoV-2 entry blockers targeting the spike protein. Acta Pharmacologica Sinica, 2022, 43, 788-796.	2.8	40
4	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
5	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
6	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
7	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
8	Kinetics-Driven Drug Design Strategy for Next-Generation Acetylcholinesterase Inhibitors to Clinical Candidate. Journal of Medicinal Chemistry, 2021, 64, 1844-1855.	2.9	32
9	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
10	Anti-SARS-CoV-2 activities in vitro of Shuanghuanglian preparations and bioactive ingredients. Acta Pharmacologica Sinica, 2020, 41, 1167-1177.	2.8	314
11	Enhancing intracellular accumulation and target engagement of PROTACs with reversible covalent chemistry. Nature Communications, 2020, 11, 4268.	5.8	112
12	Structure of Mpro from SARS-CoV-2 and discovery of its inhibitors. Nature, 2020, 582, 289-293.	13.7	3,133
13	Structure-based design of antiviral drug candidates targeting the SARS-CoV-2 main protease. Science, 2020, 368, 1331-1335.	6.0	1,135
14	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
15	The anti-apoptotic proteins NAF-1 and iASPP interact to drive apoptosis in cancer cells. Chemical Science, 2019, 10, 665-673.	3.7	11
16	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
17	NEET Proteins: A New Link Between Iron Metabolism, Reactive Oxygen Species, and Cancer. Antioxidants and Redox Signaling, 2019, 30, 1083-1095.	2.5	129
18	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

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19	Veratramine modulates AP-1-dependent gene transcription by directly binding to programmable DNA. Nucleic Acids Research, 2018, 46, 546-557.	6.5	17
20	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
21	Targeting CPT1A-mediated fatty acid oxidation sensitizes nasopharyngeal carcinoma to radiation therapy. Theranostics, 2018, 8, 2329-2347.	4.6	155
22	Interactions between mitoNEET and NAF-1 in cells. PLoS ONE, 2017, 12, e0175796.	1.1	42
23	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
24	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
25	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
26	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
27	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
28	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
29	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
30	Structural Basis for Molecular Recognition at Serotonin Receptors. Science, 2013, 340, 610-614.	6.0	454
31	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
32	A Generic Force Field for Protein Coarse-Grained Molecular Dynamics Simulation. International Journal of Molecular Sciences, 2012, 13, 14451-14469.	1.8	18
33	Discovery of novel selective inhibitors for EGFR-T790M/L858R. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 1365-1370.	1.0	24
34	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
35	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
36	Cyndi: a multi-objective evolution algorithm based method for bioactive molecular conformational generation. BMC Bioinformatics, 2009, 10, 101.	1.2	42