Jie Xia

List of Publications by Year in descending order

30 papers	599 citations	687363 13 h-index	642732 23 g-index
30 all docs	30 docs citations	30 times ranked	959 citing authors

#	Article	IF	Citations
1	Advances in GPCR Modeling Evaluated by the GPCR Dock 2013 Assessment: Meeting New Challenges. Structure, 2014, 22, 1120-1139.	3.3	149
2	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
3	Benchmarking methods and data sets for ligand enrichment assessment in virtual screening. Methods, 2015, 71, 146-157.	3.8	40
4	N-thiadiazole-4-hydroxy-2-quinolone-3-carboxamides bearing heteroaromatic rings as novel antibacterial agents: Design, synthesis, biological evaluation and target identification. European Journal of Medicinal Chemistry, 2020, 188, 112022.	5.5	36
5	Discovery of novel isoflavone derivatives as AChE/BuChE dual-targeted inhibitors: synthesis, biological evaluation and molecular modelling. Journal of Enzyme Inhibition and Medicinal Chemistry, 2017, 32, 968-977.	5.2	32
6	Mechanism-based design, synthesis and biological studies of N5-substituted tetrahydrofolate analogs as inhibitors of cobalamin-dependent methionine synthase and potential anticancer agents. European Journal of Medicinal Chemistry, 2012, 58, 228-236.	5.5	27
7	Comparative Modeling and Benchmarking Data Sets for Human Histone Deacetylases and Sirtuin Families. Journal of Chemical Information and Modeling, 2015, 55, 374-388.	5.4	25
8	Synthesis and biological activity evaluation of 20-epi-salinomycin and its 20-O-acyl derivatives. RSC Advances, 2016, 6, 41885-41890.	3.6	23
9	Design, Synthesis and Biological Evaluation of Noncovalent Inhibitors of Human CD38 NADase. ChemMedChem, 2012, 7, 223-228.	3.2	21
10	Study on pharmacokinetics and tissue distribution of single dose oral tryptanthrin in Kunming mice by validated reversed-phase high-performance liquid chromatography with ultraviolet detection. Integrative Medicine Research, 2017, 6, 269-279.	1.8	16
11	Screening of cytochrome P450 3A4 inhibitors via in silico and in vitro approaches. RSC Advances, 2018, 8, 34783-34792.	3.6	16
12	HDAC3iâ€Finder: A Machine Learningâ€based Computational Tool to Screen for HDAC3 Inhibitors. Molecular Informatics, 2021, 40, e2000105.	2.5	16
13	The discovery of novel HDAC3 inhibitors via virtual screening and in vitro bioassay. Journal of Enzyme Inhibition and Medicinal Chemistry, 2018, 33, 525-535.	5.2	15
14	Design and synthesis of conformationally constrained salinomycin derivatives. European Journal of Medicinal Chemistry, 2017, 138, 353-356.	5.5	14
15	Discovery of potent PTP1B inhibitors via structure-based drug design, synthesis and in vitro bioassay of Norathyriol derivatives. Bioorganic Chemistry, 2019, 86, 224-234.	4.1	13
16	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.	3.2	11
17	Virtual Screening against Phosphoglycerate Kinase 1 in Quest of Novel Apoptosis Inhibitors. Molecules, 2017, 22, 1029.	3.8	11
18	The Development of Target-Specific Pose Filter Ensembles To Boost Ligand Enrichment for Structure-Based Virtual Screening. Journal of Chemical Information and Modeling, 2017, 57, 1414-1425.	5.4	10

#	Article	IF	Citations
19	MUBDâ€DecoyMaker 2.0: A Python GUI Application to Generate Maximal Unbiased Benchmarking Data Sets for Virtual Drug Screening. Molecular Informatics, 2020, 39, e1900151.	2.5	10
20	Computational representations of proteinâ€“ligand interfaces for structure-based virtual screening. Expert Opinion on Drug Discovery, 2021, 16, 1175-1192.	5.0	10
21	Bacterial Lipoprotein Biosynthetic Pathway as a Potential Target for Structure-based Design of Antibacterial Agents. Current Medicinal Chemistry, 2020, 27, 1132-1150.	2.4	10
22	A Thoroughly Validated Virtual Screening Strategy for Discovery of Novel HDAC3 Inhibitors. International Journal of Molecular Sciences, 2017, 18, 137.	4.1	8
23	Activation of FXR and inhibition of EZH2 synergistically inhibit colorectal cancer through cooperatively accelerating FXR nuclear location and upregulating CDX2 expression. Cell Death and Disease, 2022, 13, 388.	6.3	8
24	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.	5.4	7
25	Discovery ofN-quinazolinone-4-hydroxy-2-quinolone-3-carboxamides as DNA gyrase B-targeted antibacterial agents. Journal of Enzyme Inhibition and Medicinal Chemistry, 2022, 37, 1620-1631.	5.2	6
26	Histone deacetylase 3-selective inhibitor RGFP966 ameliorates impaired glucose tolerance through Î²-cell protection. Toxicology and Applied Pharmacology, 2020, 406, 115189.	2.8	5
27	Maximal Unbiased Benchmarking Data Sets for Human Chemokine Receptors and Comparative Analysis. Journal of Chemical Information and Modeling, 2018, 58, 1104-1120.	5.4	4
28	Anti-MRSA drug discovery by ligand-based virtual screening and biological evaluation. Bioorganic Chemistry, 2021, 114, 105042.	4.1	4
29	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.	3.2	3
30	Serum Pharmacochemistry Combining Network Pharmacology to Discover the Active Constituents and Effect of Xijiao Dihuang Tang Prescription for Treatment of Blood-Heat and Blood-Stasis Syndrome-Related Disease. Oxidative Medicine and Cellular Longevity, 2022, 2022, 1-25.	4.0	3