Dan-feng Shi

List of Publications by Year
in descending order

35	849	471371 17	501076 28
papers	citations	h-index	g-index

35	35	35	1302
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Molecular dynamics simulations and novel drug discovery. Expert Opinion on Drug Discovery, 2018, 13, 23-37.	2.5	292
2	Investigate the mechanisms of Chinese medicine Fuzhengkangai towards EGFR mutation-positive lung adenocarcinomas by network pharmacology. BMC Complementary and Alternative Medicine, 2018, 18, 293.	3.7	37
3	Ligand induced change of Î²₂adrenergic receptor from active to inactive conformation and its implication for the closed/open state of the water channel: insight from molecular dynamics simulation, free energy calculation and Markov state model analysis. Physical Chemistry Chemical Physics, 2014, 16, 15874.	1.3	35
4	Molecular dynamics simulation, binding free energy calculation and unbinding pathway analysis on selectivity difference between FKBP51 and FKBP52: Insight into the molecular mechanism of isoform selectivity. Proteins: Structure, Function and Bioinformatics, 2018, 86, 43-56.	1.5	35
5	Xanthatin Promotes Apoptosis via Inhibiting Thioredoxin Reductase and Eliciting Oxidative Stress. Molecular Pharmaceutics, 2018, 15, 3285-3296.	2.3	34
6	Computational Insight Into the Small Molecule Intervening PD-L1 Dimerization and the Potential Structure-Activity Relationship. Frontiers in Chemistry, 2019, 7, 764.	1.8	33
7	Desmodeleganine, a new alkaloid from the leaves of Desmodium elegans as a potential monoamine oxidase inhibitor. FÃ¬toterapÃ¬Ã¢, 2014, 98, 160-165.	1.1	28
8	Fluorophore-Dependent Cleavage of Disulfide Bond Leading to a Highly Selective Fluorescent Probe of Thioredoxin. Analytical Chemistry, 2019, 91, 8524-8531.	3.2	26
9	Revealing inhibition difference between PFI-2 enantiomers against SETD7 by molecular dynamics simulations, binding free energy calculations and unbinding pathway analysis. Scientific Reports, 2017, 7, 46547.	1.6	25
10	Influence of EGCG on Î±â€synuclein (Î±S) aggregation and identification of their possible binding mode: A computational study using molecular dynamics simulation. Chemical Biology and Drug Design, 2018, 91, 162-171.	1.5	24
11	Synthesis of naphthazarin derivatives and identification of novel thioredoxin reductase inhibitor as potential anticancer agent. European Journal of Medicinal Chemistry, 2017, 140, 435-447.	2.6	23
12	Synthesis and quantitative structureâ€“activity relationship (QSAR) study of C7-oxime ester derivatives of obacunone as insecticidal agents. RSC Advances, 2015, 5, 31700-31707.	1.7	21
13	Protective V127 prion variant prevents prion disease by interrupting the formation of dimer and fibril from molecular dynamics simulations. Scientific Reports, 2016, 6, 21804.	1.6	21
14	Understanding the structural and energetic basis of PD-1 and monoclonal antibodies bound to PD-L1: A molecular modeling perspective. Biochimica Et Biophysica Acta - General Subjects, 2018, 1862, 576-588.	1.1	21
15	Influence of Chirality of Crizotinib on Its MTH1 Protein Inhibitory Activity: Insight from Molecular Dynamics Simulations and Binding Free Energy Calculations. PLoS ONE, 2015, 10, e0145219.	1.1	20
16	4-Hydroxy Pyridones from Heterologous Expression and Cultivation of the Native Host. Journal of Natural Products, 2020, 83, 3338-3346.	1.5	19
17	Identification of a new pyruvate kinase M2 isoform (PKM2) activator for the treatment of non-small-cell lung cancer (NSCLC). Chemical Biology and Drug Design, 2018, 92, 1851-1858.	1.5	17
18	Computational study on the selective inhibition mechanism of MS402 to the first and second bromodomains of BRD4. Proteins: Structure, Function and Bioinformatics, 2019, 87, 3-11.	1.5	16

#	Article	IF	Citations
19	Structural Modification of Aminophenylarsenoxides Generates Candidates for Leukemia Treatment via Thioredoxin Reductase Inhibition. Journal of Medicinal Chemistry, 2021, 64, 16132-16146.	2.9	16
20	Virtual screening-guided discovery of thioredoxin reductase inhibitors. Toxicology and Applied Pharmacology, 2019, 370, 106-116.	1.3	15
21	pH-Induced Misfolding Mechanism of Prion Protein: Insights from Microsecond-Accelerated Molecular Dynamics Simulations. ACS Chemical Neuroscience, 2019, 10, 2718-2729.	1.7	13
22	Targeting Thioredoxin Reductase by Ibrutinib Promotes Apoptosis of SMMC-7721 Cells. Journal of Pharmacology and Experimental Therapeutics, 2019, 369, 212-222.	1.3	10
23	How Does Agonist and Antagonist Binding Lead to Different Conformational Ensemble Equilibria of the Î¼-Opioid Receptor: Insight from Long-Time Gaussian Accelerated Molecular Dynamics Simulation. ACS Chemical Neuroscience, 2019, 10, 1575-1584.	1.7	9
24	Two new iridoid glycosides from the fruit of Gardenia jasminoides. Natural Product Research, 2022, 36, 186-192.	1.0	9
25	Phenolic acids and their glycosides from the rhizomes of Cimicifuga dahurica. FÃ¬toterapÃ¬Ã¢, 2019, 134, 485-492.	1.1	8
26	Identifying the molecular basis of Jinhong tablets against chronic superficial gastritis via chemical profile identification and symptom-guided network pharmacology analysis. Journal of Pharmaceutical Analysis, 2022, 12, 65-76.	2.4	8
27	Three new cycloart-7-ene triterpenoid glycosides from Cimicifuga dahurica and their anti-inflammatory effects. Natural Product Research, 2021, 35, 3634-3643.	1.0	7
28	Inhibition of Monoamine Oxidase by Stilbenes from Rheum palmatum. Iranian Journal of Pharmaceutical Research, 2016, 15, 885-892.	0.3	6
29	Computational studies on horseshoe shape pocket of human orexin receptor type 2 and boat conformation of suvorexant by molecular dynamics simulations. Chemical Biology and Drug Design, 2018, 92, 1221-1231.	1.5	4
30	Systematically identifying the antiâ€inflammatory constituents of Cimicifuga dahurica by UPLCâ€“Q/TOFâ€“MS combined with network pharmacology analysis. Biomedical Chromatography, 2021, 35, e5177.	0.8	4
31	Arteannoides Uâ€“Z: Six undescribed sesquiterpenoids with anti-inflammatory activities from the aerial parts of Artemisia annua (Qinghao). FÃ¬toterapÃ¬Ã¢, 2021, 154, 105002.	1.1	4
32	A new nitrogen-containing iridoid glycoside from lonicera macranthoides. Natural Product Research, 2021, 35, 3432-3438.	1.0	3
33	Deciphering the Allosteric Effect of Antagonist Vismodegib on Smoothened Receptor Deactivation Using Metadynamics Simulation. Frontiers in Chemistry, 2019, 7, 406.	1.8	2
34	Metabolic profiles of Jinâ€hong tablets in rats by ultraâ€performance liquid chromatography coupled with quadrupole timeâ€ofâ€flight tandem mass spectrometry. Biomedical Chromatography, 2021, 35, e5072.	0.8	2
35	Discovery of novel IDO1 inhibitors via structure-based virtual screening and biological assays. Journal of Computer-Aided Molecular Design, 2021, 35, 679-694.	1.3	2