Dan-feng Shi

List of Publications by Year
in descending order

35	849	471509 17	501196 28
papers	citations	h-index	g-index

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

#	Article	IF	Citations
1	Two new iridoid glycosides from the fruit of Gardenia jasminoides. Natural Product Research, 2022, 36, 186-192.	1.8	9
2	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.	5.3	8
3	Three new cycloart-7-ene triterpenoid glycosides from Cimicifuga dahurica and their anti-inflammatory effects. Natural Product Research, 2021, 35, 3634-3643.	1.8	7
4	A new nitrogen-containing iridoid glycoside from lonicera macranthoides. Natural Product Research, 2021, 35, 3432-3438.	1.8	3
5	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.	1.7	2
6	Discovery of novel IDO1 inhibitors via structure-based virtual screening and biological assays. Journal of Computer-Aided Molecular Design, 2021, 35, 679-694.	2.9	2
7	Systematically identifying the antiâ€inflammatory constituents of Cimicifuga dahurica by UPLCâ€Q/TOFâ€MS combined with network pharmacology analysis. Biomedical Chromatography, 2021, 35, e5177.	1.7	4
8	Arteannoides Uâ€Z: Six undescribed sesquiterpenoids with anti-inflammatory activities from the aerial parts of Artemisia annua (Qinghao). FÃ¬toterapÃ¬Ã¢, 2021, 154, 105002.	2.2	4
9	Structural Modification of Aminophenylarsenoxides Generates Candidates for Leukemia Treatment via Thioredoxin Reductase Inhibition. Journal of Medicinal Chemistry, 2021, 64, 16132-16146.	6.4	16
10	4-Hydroxy Pyridones from Heterologous Expression and Cultivation of the Native Host. Journal of Natural Products, 2020, 83, 3338-3346.	3.0	19
11	Computational Insight Into the Small Molecule Intervening PD-L1 Dimerization and the Potential Structure-Activity Relationship. Frontiers in Chemistry, 2019, 7, 764.	3.6	33
12	Fluorophore-Dependent Cleavage of Disulfide Bond Leading to a Highly Selective Fluorescent Probe of Thioredoxin. Analytical Chemistry, 2019, 91, 8524-8531.	6.5	26
13	Deciphering the Allosteric Effect of Antagonist Vismodegib on Smoothened Receptor Deactivation Using Metadynamics Simulation. Frontiers in Chemistry, 2019, 7, 406.	3.6	2
14	pH-Induced Misfolding Mechanism of Prion Protein: Insights from Microsecond-Accelerated Molecular Dynamics Simulations. ACS Chemical Neuroscience, 2019, 10, 2718-2729.	3.5	13
15	Virtual screening-guided discovery of thioredoxin reductase inhibitors. Toxicology and Applied Pharmacology, 2019, 370, 106-116.	2.8	15
16	Phenolic acids and their glycosides from the rhizomes of Cimicifuga dahurica. FÃ¬toterapÃ¬Ã¢, 2019, 134, 485-492.	2.2	8
17	Targeting Thioredoxin Reductase by Ibrutinib Promotes Apoptosis of SMMC-7721 Cells. Journal of Pharmacology and Experimental Therapeutics, 2019, 369, 212-222.	2.5	10
18	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.	3.5	9

#	Article	IF	Citations
19	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.	2.6	16
20	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.	3.2	4
21	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.	2.4	21
22	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.	3.2	24
23	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.	2.6	35
24	Molecular dynamics simulations and novel drug discovery. Expert Opinion on Drug Discovery, 2018, 13, 23-37.	5.0	292
25	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
26	Xanthatin Promotes Apoptosis via Inhibiting Thioredoxin Reductase and Eliciting Oxidative Stress. Molecular Pharmaceutics, 2018, 15, 3285-3296.	4.6	34
27	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.	3.2	17
28	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.	3.3	25
29	Synthesis of naphthazarin derivatives and identification of novel thioredoxin reductase inhibitor as potential anticancer agent. European Journal of Medicinal Chemistry, 2017, 140, 435-447.	5.5	23
30	Protective V127 prion variant prevents prion disease by interrupting the formation of dimer and fibril from molecular dynamics simulations. Scientific Reports, 2016, 6, 21804.	3.3	21
31	Inhibition of Monoamine Oxidase by Stilbenes from Rheum palmatum. Iranian Journal of Pharmaceutical Research, 2016, 15, 885-892.	0.5	6
32	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.	2.5	20
33	Synthesis and quantitative structureâ€“activity relationship (QSAR) study of C7-oxime ester derivatives of obacunone as insecticidal agents. RSC Advances, 2015, 5, 31700-31707.	3.6	21
34	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.	2.8	35
35	Desmodeleganine, a new alkaloid from the leaves of Desmodium elegans as a potential monoamine oxidase inhibitor. FÃ¬toterapÃ¬Ã¢, 2014, 98, 160-165.	2.2	28