Xiao-Jun Yao

List of Publications by Year in descending order

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335	9,426	53660	76769
papers	citations	45 h-index	74 g-index

336	336	336	11571
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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
2	Ginseng polysaccharides alter the gut microbiota and kynurenine/tryptophan ratio, potentiating the antitumour effect of antiprogrammed cell death 1/programmed cell death ligand 1 (anti-PD-1/PD-L1) immunotherapy. Gut, 2022, 71, 734-745.	6.1	177
3	Pyronaridine induces apoptosis in nonâ€small cell lung cancer cells by upregulating death receptor 5 expression and inhibiting epidermal growth factor receptor. Chemical Biology and Drug Design, 2022, 99, 83-91.	1.5	8
4	Recent Advances in Computer-aided Antiviral Drug Design Targeting HIV-1 Integrase and Reverse Transcriptase Associated Ribonuclease H. Current Medicinal Chemistry, 2022, 29, 1664-1676.	1.2	3
5	Molecular dynamics simulations reveal the disruption mechanism of a 2,4â€thiazolidinedione derivative <scp>C30</scp> against tau hexapeptide (<scp>PHF6</scp>) oligomer. Proteins: Structure, Function and Bioinformatics, 2022, 90, 142-154.	1.5	3
6	Synthesis and biological activity of 1H-imidazo[4,5-f][1,10]phenanthroline as a potential antitumor agent with PI3K/AKT/mTOR signaling. European Journal of Pharmacology, 2022, 915, 174514.	1.7	2
7	Emodin induces apoptosis and suppresses non-small-cell lung cancer growth via downregulation of sPLA2-IIa. Phytomedicine, 2022, 95, 153786.	2.3	21
8	Application advances of deep learning methods for de novo drug design and molecular dynamics simulation. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, e1581.	6.2	49
9	The prediction of proteinâ€“ligand unbinding for modern drug discovery. Expert Opinion on Drug Discovery, 2022, 17, 191-205.	2.5	7
10	Structural Engineering of Covalent Organic Frameworks Comprising Two Electron Acceptors Improves Photocatalytic Performance. ChemSusChem, 2022, 15, .	3.6	11
11	Simple hybrid dithiafulvenes-triphenylamine systems as dopant-free hole-transporting materials for efficient perovskite solar cells. Journal of Energy Chemistry, 2022, 68, 293-299.	7.1	6
12	Discovery of N-(4-(Benzyloxy)-phenyl)-sulfonamide Derivatives as Novel Antagonists of the Human Androgen Receptor Targeting the Activation Function 2. Journal of Medicinal Chemistry, 2022, 65, 2507-2521.	2.9	8
13	Resistance looms for KRAS G12C inhibitors and rational tackling strategies. , 2022, 229, 108050.		34
14	Molecular Modeling Study on the Interaction Mechanism between the LRRK2 G2019S Mutant and Type I Inhibitors by Integrating Molecular Dynamics Simulation, Binding Free Energy Calculations, and Pharmacophore Modeling. ACS Chemical Neuroscience, 2022, 13, 599-612.	1.7	11
15	Discovery of Novel HPK1 Inhibitors Through Structure-Based Virtual Screening. Frontiers in Pharmacology, 2022, 13, 850855.	1.6	5
16	Andrographolide suppresses non-small-cell lung cancer progression through induction of autophagy and antitumor immune response. Pharmacological Research, 2022, 179, 106198.	3.1	21
17	Absolute Configuration Determination of Two Diastereomeric Neovasifuranones A and B from Fusarium oxysporum R1 by a Combination of Mosherâ€™s Method and Chiroptical Approach. Journal of Fungi (Basel, Switzerland), 2022, 8, 40.	1.5	5
18	Covalent Protein Modification: An Unignorable Factor for Bisphenol A-Induced Hepatotoxicity. Environmental Science & Technology, 2022, 56, 9536-9545.	4.6	9

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19	An adaptive graph learning method for automated molecular interactions and properties predictions. Nature Machine Intelligence, 2022, 4, 645-651.	8.3	15
20	Synthesis and anticancer evaluations of novel 1H-imidazole [4,5-f][1,10] phenanthroline derivative for the treatment of colorectal cancer. European Journal of Pharmacology, 2022, 928, 175120.	1.7	5
21	RELATION: A Deep Generative Model for Structure-Based De Novo Drug Design. Journal of Medicinal Chemistry, 2022, 65, 9478-9492.	2.9	36
22	Subtype-selective mechanisms of negative allosteric modulators binding to group I metabotropic glutamate receptors. Acta Pharmacologica Sinica, 2021, 42, 1354-1367.	2.8	25
23	TrimNet: learning molecular representation from triplet messages for biomedicine. Briefings in Bioinformatics, 2021, 22, .	3.2	28
24	MolAICal: a soft tool for 3D drug design of protein targets by artificial intelligence and classical algorithm. Briefings in Bioinformatics, 2021, 22, .	3.2	163
25	Early lung cancer diagnostic biomarker discovery by machine learning methods. Translational Oncology, 2021, 14, 100907.	1.7	99
26	Roles of Ion Fluxes, Metabolism, and Redox Balance in Cancer Therapy. Antioxidants and Redox Signaling, 2021, 34, 1108-1127.	2.5	4
27	A new two-dimensional all-sp³ carbon allotrope with an indirect band gap and superior carrier mobility. Physical Chemistry Chemical Physics, 2021, 23, 2906-2913.	1.3	7
28	Accuracy or novelty: what can we gain from target-specific machine-learning-based scoring functions in virtual screening?. Briefings in Bioinformatics, 2021, 22, .	3.2	26
29	Diarylheptanoid analogues from the rhizomes of Zingiber officinale and their anti-tumour activity. RSC Advances, 2021, 11, 29376-29384.	1.7	4
30	Discovery of pentapeptide-inhibitor hits targeting FKBP51 by combining computational modeling and X-ray crystallography. Computational and Structural Biotechnology Journal, 2021, 19, 4079-4091.	1.9	1
31	Insights into the molecular mechanism of positive cooperativity between partial agonist MK-8666 and full allosteric agonist AP8 of hGPR40 by Gaussian accelerated molecular dynamics (GaMD) simulations. Computational and Structural Biotechnology Journal, 2021, 19, 3978-3989.	1.9	17
32	Exploring the thermodynamic, kinetic and inhibitory mechanisms of 5-iTU targeting mitotic kinase haspin by integrated molecular dynamics. Physical Chemistry Chemical Physics, 2021, 23, 18404-18413.	1.3	3
33	Discovery of a new inhibitor targeting PD-L1 for cancer immunotherapy. Neoplasia, 2021, 23, 281-293.	2.3	18
34	Uncovering the Effect of pS202/pT205/pS208 Triple Phosphorylations on the Conformational Features of the Key Fragment G192â€“T212 of Tau Protein. ACS Chemical Neuroscience, 2021, 12, 1039-1048.	1.7	4
35	An online target and rapid screening method for Î±â€glucosidase inhibitors based on capillary electrophoresis. Electrophoresis, 2021, 42, 1221-1228.	1.3	2
36	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

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37	Inhomogeneous charge distribution of simple substances. International Journal of Modern Physics B, 2021, 35, 2150147.	1.0	1
38	Identification and characterization of a novel mutant isocitrate dehydrogenase 1 inhibitor for glioma treatment. Biochemical and Biophysical Research Communications, 2021, 551, 38-45.	1.0	4
39	An efficient and hydrophobic molecular doping in perovskite solar cells. Nano Energy, 2021, 82, 105751.	8.2	35
40	Potential prognostic factors in progression-free survival for patients with cervical cancer. BMC Cancer, 2021, 21, 531.	1.1	10
41	Quantitative analysis of the relationship of derivatization reagents and detection sensitivity of electrospray ionization-triple quadrupole tandem mass spectrometry: Hydrazines as prototypes. Analytica Chimica Acta, 2021, 1158, 338402.	2.6	3
42	Understanding the Polypharmacological Profiles of Triple Reuptake Inhibitors by Molecular Simulation. ACS Chemical Neuroscience, 2021, 12, 2013-2026.	1.7	18
43	Introducing block design in graph neural networks for molecular properties prediction. Chemical Engineering Journal, 2021, 414, 128817.	6.6	17
44	Deep Scoring Neural Network Replacing the Scoring Function Components to Improve the Performance of Structure-Based Molecular Docking. ACS Chemical Neuroscience, 2021, 12, 2133-2142.	1.7	11
45	Computational Insights Into the Inhibition Mechanism of Proanthocyanidin B2 on Tau Hexapeptide (PHF6) Oligomer. Frontiers in Chemistry, 2021, 9, 666043.	1.8	6
46	Plumbagin suppresses non-small cell lung cancer progression through downregulating ARF1 and by elevating CD8+ T cells. Pharmacological Research, 2021, 169, 105656.	3.1	9
47	Virtual Screening and Biological Activity Evaluation of New Potent Inhibitors Targeting LRRK2 Kinase Domain. ACS Chemical Neuroscience, 2021, 12, 3214-3224.	1.7	10
48	Preclinical Evaluation of [⁶⁴Cu]NOTA-CP01 as a PET Imaging Agent for Metastatic Esophageal Squamous Cell Carcinoma. Molecular Pharmaceutics, 2021, 18, 3638-3648.	2.3	6
49	Luteolin and its derivative apigenin suppress the inducible PD-L1 expression to improve anti-tumor immunity in KRAS-mutant lung cancer. Cancer Letters, 2021, 515, 36-48.	3.2	91
50	A norbisabolane and an arabitol benzoate from Talaromyces marneffei, an endophytic fungus of Epilobium angustifolium. FÃ¬toterapÃ¬Ã¢, 2021, 153, 104948.	1.1	3
51	In silico study of intrinsic dynamics of full-length apo-ACE2 and RBD-ACE2 complex. Computational and Structural Biotechnology Journal, 2021, 19, 5455-5465.	1.9	11
52	Anticoagulant Dodecapeptide Suppresses Thrombosis In Vivo by Inhibiting the Thrombin Exosite-I Binding Site. Journal of Agricultural and Food Chemistry, 2021, 69, 10920-10931.	2.4	4
53	RetroPrime: A Diverse, plausible and Transformer-based method for Single-Step retrosynthesis predictions. Chemical Engineering Journal, 2021, 420, 129845.	6.6	44
54	Selectively targeting individual bromodomain: Drug discovery and molecular mechanisms. Pharmacological Research, 2021, 172, 105804.	3.1	16

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55	(Â±)-Caryopterisines A and B, dimeric monoterpene alkaloids with unprecedented 6/5/5/5/6 pentacyclic rings scaffold from Caryopteris glutinosa. Bioorganic Chemistry, 2021, 116, 105364.	2.0	2
56	WADDAICA: A webserver for aiding protein drug design by artificial intelligence and classical algorithm. Computational and Structural Biotechnology Journal, 2021, 19, 3573-3579.	1.9	17
57	A new strategy for constructing a dispiro-based dopant-free hole-transporting material: spatial configuration of spiro-bifluorene changes from a perpendicular to parallel arrangement. Chemical Science, 2021, 12, 8548-8555.	3.7	14
58	A new two-dimensional semiconducting carbon allotrope with direct band gap: a first-principles prediction. Journal of Physics Condensed Matter, 2021, 33, 045502.	0.7	6
59	SMART v1.0: A Database for Small Molecules with Functional Implications in Plants. Interdisciplinary Sciences, Computational Life Sciences, 2021, , 1.	2.2	3
60	Structural Basis of a Human Neutralizing Antibody Specific to the SARS-CoV-2 Spike Protein Receptor-Binding Domain. Microbiology Spectrum, 2021, 9, e0135221.	1.2	13
61	Structural Modification of Aminophenylarsenoxides Generates Candidates for Leukemia Treatment via Thioredoxin Reductase Inhibition. Journal of Medicinal Chemistry, 2021, 64, 16132-16146.	2.9	16
62	A method establishment and comparison of in vivo lung cancer model development platforms for evaluation of tumour metabolism and pharmaceutical efficacy. Phytomedicine, 2021, 96, 153831.	2.3	1
63	3D-QSAR, Molecular Docking, and MD Simulations of Anthraquinone Derivatives as PGAM1 Inhibitors. Frontiers in Pharmacology, 2021, 12, 764351.	1.6	6
64	Compound C620-0696, a new potent inhibitor targeting BPTF, the chromatin-remodeling factor in non-small-cell lung cancer. Frontiers of Medicine, 2020, 14, 60-67.	1.5	19
65	Two new compounds, Talaromycin A and B, isolated from an endophytic fungus, Talaromyces aurantiacus. Natural Product Research, 2020, 34, 2802-2808.	1.0	8
66	Elucidating the tight-binding mechanism of two oral anticoagulants to factor Xa by using induced-fit docking and molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2020, 38, 625-633.	2.0	35
67	Investigation on the fungicide resistance mechanism against Botrytis cinerea Î²-tubulin inhibitor zoxamide by computational study. Journal of Biomolecular Structure and Dynamics, 2020, 38, 4304-4312.	2.0	4
68	Discovery of potential Toxoplasma gondii CDPK1 inhibitors with new scaffolds based on the combination of QSAR and scaffoldâ€hopping method with in vitro validation. Chemical Biology and Drug Design, 2020, 95, 476-484.	1.5	2
69	The specific binding of a new 1,2,3-triazole to three blood proteins and it's appended rhodamine complex for selective detection of Hg2+. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 228, 117728.	2.0	9
70	Structurally diverse sesquiterpenoids from the aerial parts of Artemisia annua (Qinghao) and their striking systemically anti-inflammatory activities. Bioorganic Chemistry, 2020, 103, 104221.	2.0	15
71	Discovery of Icotinib-1,2,3-Triazole Derivatives as IDO1 Inhibitors. Frontiers in Pharmacology, 2020, 11, 579024.	1.6	13
72	Long-term aspirin use for primary cancer prevention: An updated systematic review and subgroup meta-analysis of 29 randomized clinical trials. Journal of Cancer, 2020, 11, 6460-6473.	1.2	12

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73	IPM712, a vanillin derivative as potential antitumor agents, displays better antitumor activity in colorectal cancers cell lines. European Journal of Pharmaceutical Sciences, 2020, 152, 105464.	1.9	18
74	Revealing the Positive Binding Cooperativity Mechanism between the Orthosteric and the Allosteric Antagonists of CCR2 by Metadynamics and Gaussian Accelerated Molecular Dynamics Simulations. ACS Chemical Neuroscience, 2020, 11, 628-637.	1.7	12
75	Evodiamine suppresses non-small cell lung cancer by elevating CD8+ T cells and downregulating the MUC1-C/PD-L1 axis. Journal of Experimental and Clinical Cancer Research, 2020, 39, 249.	3.5	56
76	Discovery of Novel IDH1 Inhibitor Through Comparative Structure-Based Virtual Screening. Frontiers in Pharmacology, 2020, 11, 579768.	1.6	15
77	The study on the interactions of two 1,2,3-triazoles with several biological macromolecules by multiple spectroscopic methodologies and molecular docking. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 243, 118795.	2.0	5
78	Dolutegravir derivative inhibits proliferation and induces apoptosis of non-small cell lung cancer cells via calcium signaling pathway. Pharmacological Research, 2020, 161, 105129.	3.1	23
79	Nrf2: a dark horse in Alzheimer's disease treatment. Ageing Research Reviews, 2020, 64, 101206.	5.0	131
80	Clinical significance of LSECtin and its association with PVR in non-small-cell lung cancer patients. Annals of Translational Medicine, 2020, 8, 1393-1393.	0.7	1
81	Vertical Phase Separated Cesium Fluoride Doping Organic Electron Transport Layer: A Facile and Efficient â€œBridgeâ€•Linked Heterojunction for Perovskite Solar Cells. Advanced Functional Materials, 2020, 30, 2001418.	7.8	44
82	The misfolding mechanism of the key fragment R3 of tau protein: a combined molecular dynamics simulation and Markov state model study. Physical Chemistry Chemical Physics, 2020, 22, 10968-10980.	1.3	18
83	Chelidonine selectively inhibits the growth of gefitinib-resistant non-small cell lung cancer cells through the EGFR-AMPK pathway. Pharmacological Research, 2020, 159, 104934.	3.1	21
84	Network pharmacological approach for elucidating the mechanisms of traditional Chinese medicine in treating COVID-19 patients. Pharmacological Research, 2020, 159, 105043.	3.1	26
85	Modulation of gut microbiota to overcome resistance to immune checkpoint blockade in cancer immunotherapy. Current Opinion in Pharmacology, 2020, 54, 1-10.	1.7	35
86	Unraveling the Molecular Mechanism of Prion H2 C-Terminus Misfolding by Metadynamics Simulations. ACS Chemical Neuroscience, 2020, 11, 772-782.	1.7	3
87	Binding affinity and dissociation pathway predictions for a series of USP7 inhibitors with pyrimidinone scaffold by multiple computational methods. Physical Chemistry Chemical Physics, 2020, 22, 5487-5499.	1.3	9
88	The binding mode of vilazodone in the human serotonin transporter elucidated by ligand docking and molecular dynamics simulations. Physical Chemistry Chemical Physics, 2020, 22, 5132-5144.	1.3	33
89	Novel approach toward hole-transporting layer doped by hydrophobic Lewis acid through infiltrated diffusion doping for perovskite solar cells. Nano Energy, 2020, 70, 104509.	8.2	67
90	Prognostic significance of tumor poliovirus receptor and CTLA4 expression in patients with surgically resected non-small-cell lung cancer. Journal of Cancer Research and Clinical Oncology, 2020, 146, 1441-1450.	1.2	11

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91	Selective Inhibition of HDAC1 by Macrocyclic Polypeptide for the Treatment of Glioblastoma: A Binding Mechanistic Analysis Based on Molecular Dynamics. Frontiers in Molecular Biosciences, 2020, 7, 41.	1.6	9
92	Comprehensive Evaluation of Fourteen Docking Programs on Proteinâ€“Peptide Complexes. Journal of Chemical Theory and Computation, 2020, 16, 3959-3969.	2.3	90
93	Editorial: Computational Approaches in Drug Discovery and Precision Medicine. Frontiers in Chemistry, 2020, 8, 639449.	1.8	3
94	Pretreatment neutrophil-to-lymphocyte ratio is a predictive biomarker for EGFR TKI-treated patients with advanced EGFR- mutant Non-small cell lung cancer. Translational Cancer Research, 2020, 9, 2875-2883.	0.4	5
95	miRâ€20b promotes growth of nonâ€small cell lung cancer through a positive feedback loop of the Wnt/Î²â€catenin signaling pathway. International Journal of Oncology, 2020, 56, 470-479.	1.4	5
96	Macrolide sesquiterpene pyridine alkaloids from the stems of Tripterygium regelii. Journal of Natural Medicines, 2019, 73, 23-33.	1.1	10
97	p53 sensitizes chemoresistant non-small cell lung cancer via elevation of reactive oxygen species and suppression of EGFR/PI3K/AKT signaling. Cancer Cell International, 2019, 19, 188.	1.8	45
98	Aggreganoids Aâ€“F, Carbon-Bridged Sesquiterpenoid Dimers and Trimers from Lindera aggregata. Organic Letters, 2019, 21, 5753-5756.	2.4	29
99	Discovery of a novel protein kinase C activator from Croton tiglium for inhibition of non-small cell lung cancer. Phytomedicine, 2019, 65, 153100.	2.3	10
100	Disclosing the Mechanism of Spontaneous Aggregation and Template-Induced Misfolding of the Key Hexapeptide (PHF6) of Tau Protein Based on Molecular Dynamics Simulation. ACS Chemical Neuroscience, 2019, 10, 4810-4823.	1.7	27
101	Wortmannine H, a phenylpentenol isolated from an endophytic fungus, Talaromyces wortmannii LGT-4. Natural Product Research, 2019, 35, 1-6.	1.0	3
102	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
103	MicroRNA-421 confers paclitaxel resistance by binding to the KEAP1 3â€²UTR and predicts poor survival in non-small cell lung cancer. Cell Death and Disease, 2019, 10, 821.	2.7	56
104	Non-volatile pungent compounds isolated from Zingiber officinale and their mechanisms of action. Food and Function, 2019, 10, 1203-1211.	2.1	14
105	Disclosing the Template-Induced Misfolding Mechanism of Tau Protein by Studying the Dissociation of the Boundary Chain from the Formed Tau Fibril Based on a Steered Molecular Dynamics Simulation. ACS Chemical Neuroscience, 2019, 10, 1854-1865.	1.7	14
106	A vanillin derivative suppresses the growth of HT29 cells through the Wnt/Î²-catenin signaling pathway. European Journal of Pharmacology, 2019, 849, 43-49.	1.7	23
107	Prediction of the Antioxidant Response Elements' Response of Compound by Deep Learning. Frontiers in Chemistry, 2019, 7, 385.	1.8	24
108	Identification of metabolic vulnerabilities of receptor tyrosine kinases-driven cancer. Nature Communications, 2019, 10, 2701.	5.8	82

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109	Fluorophore-Dependent Cleavage of Disulfide Bond Leading to a Highly Selective Fluorescent Probe of Thioredoxin. Analytical Chemistry, 2019, 91, 8524-8531.	3.2	26
110	Linderalides Aâ€“D, Disesquiterpenoidâ€“Geranylbenzofuranone Conjugates from Lindera aggregata. Journal of Organic Chemistry, 2019, 84, 8242-8247.	1.7	21
111	Deciphering the Allosteric Effect of Antagonist Vismodegib on Smoothened Receptor Deactivation Using Metadynamics Simulation. Frontiers in Chemistry, 2019, 7, 406.	1.8	2
112	pH-Induced Misfolding Mechanism of Prion Protein: Insights from Microsecond-Accelerated Molecular Dynamics Simulations. ACS Chemical Neuroscience, 2019, 10, 2718-2729.	1.7	13
113	Importance of protein flexibility in ranking ERK2 Type I1/2inhibitor affinities: a computational study. RSC Advances, 2019, 9, 12441-12454.	1.7	5
114	Importance of Incorporating Protein Flexibility in Molecule Modeling: A Theoretical Study on Type I1/2 NIK Inhibitors. Frontiers in Pharmacology, 2019, 10, 345.	1.6	11
115	Virtual screening-guided discovery of thioredoxin reductase inhibitors. Toxicology and Applied Pharmacology, 2019, 370, 106-116.	1.3	15
116	Target discovery of chlorogenic acid derivatives from the flower buds of Lonicera macranthoides and their MAO B inhibitory mechanism. FÃ¬toterapÃ¬Ã¢, 2019, 134, 297-304.	1.1	19
117	Raman Spectroscopic Differences between Ephedrine and Pseudoephedrine. Journal of Forensic Sciences, 2019, 64, 1482-1485.	0.9	3
118	A surgical case of ciliated muconodular papillary tumor. Thoracic Cancer, 2019, 10, 1019-1022.	0.8	5
119	Structure based virtual screening of novel noncompetitive antagonistâ€‰ofâ€‰Î±-amino-3-hydroxy-5-methyl-4-isoxazolepropionic acid (AMPA) receptor. Journal of Biotechnology, 2019, 295, 9-18.	1.9	3
120	Investigation of ECD conformational transition mechanism of GLP-1R by molecular dynamics simulations and Markov state model. Physical Chemistry Chemical Physics, 2019, 21, 8470-8481.	1.3	19
121	Cordycepin Inhibits Drug-resistance Non-small Cell Lung Cancer Progression by Activating AMPK Signaling Pathway. Pharmacological Research, 2019, 144, 79-89.	3.1	66
122	Phenolic acids and their glycosides from the rhizomes of Cimicifuga dahurica. FÃ¬toterapÃ¬Ã¢, 2019, 134, 485-492.	1.1	8
123	Targeting Thioredoxin Reductase by Ibrutinib Promotes Apoptosis of SMMC-7721 Cells. Journal of Pharmacology and Experimental Therapeutics, 2019, 369, 212-222.	1.3	10
124	Identification of a new inhibitor of KRASâ€PDEÎ´ interaction targeting KRAS mutant nonsmall cell lung cancer. International Journal of Cancer, 2019, 145, 1334-1345.	2.3	29
125	How Does Chirality Determine the Selective Inhibition of Histone Deacetylase 6? A Lesson from Trichostatin A Enantiomers Based on Molecular Dynamics. ACS Chemical Neuroscience, 2019, 10, 2467-2480.	1.7	86
126	DeepDock: Enhancing Ligand-protein Interaction Prediction by a Combination of Ligand and Structure Information. , 2019, , .		15

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127	Neferine induces autophagy-dependent cell death in apoptosis-resistant cancers via ryanodine receptor and Ca2+-dependent mechanism. Scientific Reports, 2019, 9, 20034.	1.6	44
128	Importance of a crystalline water network in docking-based virtual screening: a case study of BRD4. Physical Chemistry Chemical Physics, 2019, 21, 25276-25289.	1.3	19
129	Conformation Transition of Intracellular Part of Glucagon Receptor in Complex With Agonist Glucagon by Conventional and Accelerated Molecular Dynamics Simulations. Frontiers in Chemistry, 2019, 7, 851.	1.8	5
130	Resistance mechanism of the oncogenic Î²3â€Î±C deletion mutation in <scp>BRAF</scp> kinase to dabrafenib and vemurafenib revealed by molecular dynamics simulations and binding free energy calculations. Chemical Biology and Drug Design, 2019, 93, 177-187.	1.5	6
131	Carbon Nanoparticles Inhibit the Aggregation of Prion Protein as Revealed by Experiments and Atomistic Simulations. Journal of Chemical Information and Modeling, 2019, 59, 1909-1918.	2.5	16
132	How graphene affects the misfolding of human prion protein: A combined experimental and molecular dynamics simulation study. Environmental Research, 2019, 171, 1-10.	3.7	7
133	Potent Antagonists of RORÎ³t, Cardenolides from Calotropis gigantea, Exhibit Discrepant Effects on the Differentiation of T Lymphocyte Subsets. Molecular Pharmaceutics, 2019, 16, 798-807.	2.3	10
134	The molecular mechanism of pHâ€regulating C3dâ€CR2 interactions: Insights from molecular dynamics simulation. Chemical Biology and Drug Design, 2019, 93, 628-637.	1.5	0
135	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
136	Are the Apo Proteins Suitable for the Rational Discovery of Allosteric Drugs?. Journal of Chemical Information and Modeling, 2019, 59, 597-604.	2.5	18
137	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
138	Computational study of the binding mechanism between farnesoid X receptor Î± and antagonist N-benzyl-N-(3-(tertbutyl)-4-hydroxyphenyl)-2,6-dichloro-4-(dimethylamino) benzamide. Journal of Biomolecular Structure and Dynamics, 2019, 37, 1628-1640.	2.0	9
139	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
140	Computer-Aided Formulation Design for a Highly Soluble Luteinâ€“Cyclodextrin Multiple-Component Delivery System. Molecular Pharmaceutics, 2018, 15, 1664-1673.	2.3	46
141	Definition and classification system of glacial lake for inventory and hazards study. Journal of Chinese Geography, 2018, 28, 193-205.	1.5	66
142	The molecular mechanism of two coreceptor binding site antibodies X5 and 17b neutralizing <scp>HIV</scp>â€1: Insights from molecular dynamics simulation. Chemical Biology and Drug Design, 2018, 92, 1357-1365.	1.5	2
143	Astragalus polysaccharide enhanced antitumor effects of Apatinib in gastric cancer AGS cells by inhibiting AKT signalling pathway. Biomedicine and Pharmacotherapy, 2018, 100, 176-183.	2.5	44
144	Inhibition of KRAS-dependent lung cancer cell growth by deltarasin: blockage of autophagy increases its cytotoxicity. Cell Death and Disease, 2018, 9, 216.	2.7	41

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145	Computational identification of the binding mechanism of a triple reuptake inhibitor amitifadine for the treatment of major depressive disorder. Physical Chemistry Chemical Physics, 2018, 20, 6606-6616.	1.3	125
146	(Â±)-Sativamides A and B, Two Pairs of Racemic Nor-Lignanamide Enantiomers from the Fruits of Cannabis sativa. Journal of Organic Chemistry, 2018, 83, 2376-2381.	1.7	18
147	Benchmark Study Based on 2P2I_{DB} to Gain Insights into the Discovery of Small-Molecule PPI Inhibitors. Journal of Physical Chemistry B, 2018, 122, 2544-2555.	1.2	12
148	Dimeric Cadinane Sesquiterpenoid Derivatives from Artemisia annua. Organic Letters, 2018, 20, 453-456.	2.4	39
149	What Contributes to Serotoninâ€“Norepinephrine Reuptake Inhibitorsâ€™ Dual-Targeting Mechanism? The Key Role of Transmembrane Domain 6 in Human Serotonin and Norepinephrine Transporters Revealed by Molecular Dynamics Simulation. ACS Chemical Neuroscience, 2018, 9, 1128-1140.	1.7	225
150	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
151	Glacier changes in the Qilian Mountains in the past half-century: Based on the revised First and Second Chinese Glacier Inventory. Journal of Chinese Geography, 2018, 28, 206-220.	1.5	70
152	Exploring the Binding Mechanism of Metabotropic Glutamate Receptor 5 Negative Allosteric Modulators in Clinical Trials by Molecular Dynamics Simulations. ACS Chemical Neuroscience, 2018, 9, 1492-1502.	1.7	108
153	QSPRs for estimating nematic transition temperatures of pyridine-containing liquid crystalline compounds. Liquid Crystals, 2018, 45, 238-249.	0.9	8
154	Suppression of Lipogenesis via Reactive Oxygen Speciesâ€“AMPK Signaling for Treating Malignant and Proliferative Diseases. Antioxidants and Redox Signaling, 2018, 28, 339-357.	2.5	39
155	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
156	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
157	Molecular dynamics simulations and novel drug discovery. Expert Opinion on Drug Discovery, 2018, 13, 23-37.	2.5	292
158	Computational characterization of the selective inhibition of human norepinephrine and serotonin transporters by an escitalopram scaffold. Physical Chemistry Chemical Physics, 2018, 20, 29513-29527.	1.3	37
159	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
160	Phytotoxic ent-Isopimarane-Type Diterpenoids from Euphorbia hylonoma. Journal of Natural Products, 2018, 81, 2381-2391.	1.5	18
161	Steroids-specific target library for steroids target prediction. Steroids, 2018, 140, 83-91.	0.8	4
162	Comprehensive assessment of nine docking programs on type II kinase inhibitors: prediction accuracy of sampling power, scoring power and screening power. Briefings in Bioinformatics, 2018, , .	3.2	16

#	Article	IF	Citations
163	Krukovine Suppresses KRAS-Mutated Lung Cancer Cell Growth and Proliferation by Inhibiting the RAF-ERK Pathway and Inactivating AKT Pathway. Frontiers in Pharmacology, 2018, 9, 958.	1.6	19
164	Binding Performance of Human Intravenous Immunoglobulin and 20(S)-7-Ethylcamptothecin. Molecules, 2018, 23, 2389.	1.7	0
165	Investigation of the inhibition effect of arachidonic acid on the core structure of the HIV-1 gp41. Journal of Pharmaceutical and Biomedical Analysis, 2018, 161, 377-382.	1.4	0
166	Descriptor Selection via Log-Sum Regularization for the Biological Activities of Chemical Structure. International Journal of Molecular Sciences, 2018, 19, 30.	1.8	15
167	Xanthatin Promotes Apoptosis via Inhibiting Thioredoxin Reductase and Eliciting Oxidative Stress. Molecular Pharmaceutics, 2018, 15, 3285-3296.	2.3	34
168	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
169	Identification of a Novel Protein Arginine Methyltransferase 5 Inhibitor in Non-small Cell Lung Cancer by Structure-Based Virtual Screening. Frontiers in Pharmacology, 2018, 9, 173.	1.6	23
170	Honokiol Inhibits Proliferation, Invasion and Induces Apoptosis Through Targeting Lyn Kinase in Human Lung Adenocarcinoma Cells. Frontiers in Pharmacology, 2018, 9, 558.	1.6	14
171	A Method for Rapid Screening of Anilide-Containing AMPK Modulators Based on Computational Docking and Biological Validation. Frontiers in Pharmacology, 2018, 9, 710.	1.6	9
172	Gossypol Inhibits Non-small Cell Lung Cancer Cells Proliferation by Targeting EGFRL858R/T790M. Frontiers in Pharmacology, 2018, 9, 728.	1.6	20
173	The Binding Mechanism Between Inositol Phosphate (InsP) and the Jasmonate Receptor Complex: A Computational Study. Frontiers in Plant Science, 2018, 9, 963.	1.7	9
174	Classical molecular dynamics and metadynamics simulations decipher the mechanism of CBP30 selectively inhibiting CBP/p300 bromodomains. Organic and Biomolecular Chemistry, 2018, 16, 6521-6530.	1.5	17
175	Proscillaridin A induces apoptosis and suppresses non-small-cell lung cancer tumor growth via calcium-induced DR4 upregulation. Cell Death and Disease, 2018, 9, 696.	2.7	44
176	Prediction of the binding mode and resistance profile for a dual-target pyrrolyl diketo acid scaffold against HIV-1 integrase and reverse-transcriptase-associated ribonuclease H. Physical Chemistry Chemical Physics, 2018, 20, 23873-23884.	1.3	31
177	Phenolic Constituents Isolated from the Twigs of Cinnamomum cassia and Their Potential Neuroprotective Effects. Journal of Natural Products, 2018, 81, 1333-1342.	1.5	40
178	Inhibition of invasion by N -trans -feruloyloctopamine via AKT, p38MAPK and EMT related signals in hepatocellular carcinoma cells. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 989-993.	1.0	30
179	The in silico identification of human bile salt export pump (ABCB11) inhibitors associated with cholestatic drug-induced liver injury. Molecular BioSystems, 2017, 13, 417-424.	2.9	8
180	Identification of mitoxantrone as a new inhibitor of ROS1 fusion protein in non-small cell lung cancer cells. MedChemComm, 2017, 8, 621-624.	3.5	6

#	Article	IF	Citations
181	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
182	Comparison of computational model and X-ray crystal structure of human serotonin transporter: potential application for the pharmacology of human monoamine transporters. Molecular Simulation, 2017, 43, 1089-1098.	0.9	21
183	Differentiating Physicochemical Properties between Addictive and Nonaddictive ADHD Drugs Revealed by Molecular Dynamics Simulation Studies. ACS Chemical Neuroscience, 2017, 8, 1416-1428.	1.7	61
184	The folding mechanism and key metastable state identification of the PrP127â€“147 monomer studied by molecular dynamics simulations and Markov state model analysis. Physical Chemistry Chemical Physics, 2017, 19, 11249-11259.	1.3	16
185	Molecular basis of P450 OleTJE: an investigation of substrate binding mechanism and major pathways. Journal of Computer-Aided Molecular Design, 2017, 31, 483-495.	1.3	16
186	Molecular dynamics simulation on the inhibition mechanism of peptideâ€based inhibitor of islet amyloid polypeptide (<scp>IAPP</scp>) to islet amyloid polypeptide (<scp>IAPP</scp>_{22â€“28}) oligomers. Chemical Biology and Drug Design, 2017, 90, 31-39.	1.5	10
187	A highly selective Schiff base fluorescent chemosensor for Lu³⁺. Analytical Methods, 2017, 9, 6254-6260.	1.3	7
188	Revealing vilazodone's binding mechanism underlying its partial agonism to the 5-HT_{1A} receptor in the treatment of major depressive disorder. Physical Chemistry Chemical Physics, 2017, 19, 28885-28896.	1.3	41
189	Identification of a potent kinase inhibitor targeting EML4-ALK fusion protein in non-small cell lung cancer. MedChemComm, 2017, 8, 1914-1918.	3.5	0
190	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
191	Selective inhibition mechanism of RVX-208 to the second bromodomain of bromo and extraterminal proteins: insight from microsecond molecular dynamics simulations. Scientific Reports, 2017, 7, 8857.	1.6	26
192	Suppressing mPGES-1 expression by sinomenine ameliorates inflammation and arthritis. Biochemical Pharmacology, 2017, 142, 133-144.	2.0	60
193	Differentiating physicochemical properties between NDRIs and sNRIs clinically important for the treatment of ADHD. Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 2766-2777.	1.1	56
194	Computational study of the binding mechanism of medium chain acyl-CoA synthetase with substrate in Methanosarcina acetivorans. Journal of Biotechnology, 2017, 259, 160-167.	1.9	8
195	Linear Ïƒ-holeâ‹¯C Oâ‹¯Ïƒ-hole intermolecular interactions between carbon monoxide and dihalogen molecules XY (X, Y = Cl, Br). Journal of Molecular Graphics and Modelling, 2017, 76, 419-428.	1.3	6
196	Norsampsone E, an unprecedented decarbonyl polycyclic polyprenylated acylphloroglucinol with a homoadamantyl core from Hypericum sampsonii. RSC Advances, 2017, 7, 33113-33119.	1.7	7
197	Aphapolins A and B: Two Nemoralisin Diterpenoids Isolated from Aphanamixis polystachya (Wall.) R. Parker. European Journal of Organic Chemistry, 2017, 2017, 4429-4433.	1.2	16
198	Prediction of nematic transition temperatures of quinoline-containing liquid crystalline compounds from molecular structure. Liquid Crystals, 2017, 44, 2337-2347.	0.9	1

#	Article	IF	Citations
199	Experimental and Theoretical Insights into the Inhibition Mechanism of Prion Fibrillation by Resveratrol and its Derivatives. ACS Chemical Neuroscience, 2017, 8, 2698-2707.	1.7	16
200	Molecular Dynamics Simulation Study on the Binding and Stabilization Mechanism of Antiprion Compounds to the â€œHot Spotâ€•Region of PrP^C. ACS Chemical Neuroscience, 2017, 8, 2446-2456.	1.7	10
201	Discovery of small molecules binding to the normal conformation of prion by combining virtual screening and multiple biological activity evaluation methods. Journal of Computer-Aided Molecular Design, 2017, 31, 1053-1062.	1.3	5
202	The glycanâ€mediated mechanism on the interactions of gp120 with <scp>CD</scp>4 and antibody: Insights from molecular dynamics simulation. Chemical Biology and Drug Design, 2017, 90, 1237-1246.	1.5	6
203	A Strategy To Boost the Efficiency of Rhodanine Electron Acceptor for Organic Dye: From Nonconjugation to Conjugation. ACS Applied Materials & Interfaces, 2017, 9, 25225-25231.	4.0	32
204	Shikonin inhibits gefitinib-resistant non-small cell lung cancer by inhibiting TrxR and activating the EGFR proteasomal degradation pathway. Pharmacological Research, 2017, 115, 45-55.	3.1	74
205	Chiral separation and absolute configurations of two pairs of racemic polyprenylated benzophenones from Hypericum sampsonii. FÃ¬toterapÃ¬Ã¢, 2017, 116, 39-44.	1.1	11
206	Interaction of intravenous immunoglobulin and three 20(S)-camptothecin analogs: maintaining higher circulatory levels of the biologically active species. Medicinal Chemistry Research, 2017, 26, 3286-3295.	1.1	1
207	Identification of potential genetic causal variants for rheumatoid arthritis by whole-exome sequencing. Oncotarget, 2017, 8, 111119-111129.	0.8	20
208	Identification of a New Potent Inhibitor Targeting KRAS in Non-small Cell Lung Cancer Cells. Frontiers in Pharmacology, 2017, 8, 823.	1.6	34
209	New Abietane and Kaurane Type Diterpenoids from the Stems of Tripterygium regelii. International Journal of Molecular Sciences, 2017, 18, 147.	1.8	13
210	Association between Charlson comorbidity index score and outcome in patients with stage IIIB-IV non-small cell lung cancer. BMC Pulmonary Medicine, 2017, 17, 112.	0.8	45
211	Isoliquiritigenin suppresses human T Lymphocyte activation via covalently binding cysteine 46 of IÏºB kinase. Oncotarget, 2017, 8, 34223-34235.	0.8	10
212	Thalidezine, a novel AMPK activator, eliminates apoptosis-resistant cancer cells through energy-mediated autophagic cell death. Oncotarget, 2017, 8, 30077-30091.	0.8	34
213	Novel direct AMPK activator suppresses non-small cell lung cancer through inhibition of lipid metabolism. Oncotarget, 2017, 8, 96089-96102.	0.8	21
214	Clinical statistics analysis on the characteristics of pneumoconiosis of Chinese miner population. Journal of Thoracic Disease, 2016, 8, 2203-2211.	0.6	11
215	Compound Library Screening Identified Cardiac Glycoside Digitoxin as an Effective Growth Inhibitor of Gefitinib-Resistant Non-Small Cell Lung Cancer via Downregulation of Î±-Tubulin and Inhibition of Microtubule Formation. Molecules, 2016, 21, 374.	1.7	24
216	Hernandezine, a novel AMPK activator induces autophagic cell death in drug-resistant cancers. Oncotarget, 2016, 7, 8090-8104.	0.8	74

#	Article	IF	Citations
217	Organohalogeniteâ€Catalyzed Spiroketalization: Enantioselective Synthesis of Bisbenzannulated Spiroketal Cores. Advanced Synthesis and Catalysis, 2016, 358, 370-374.	2.1	16
218	Hypersampsones Sâ€“W, new polycyclic polyprenylated acylphloroglucinols from Hypericum sampsonii. RSC Advances, 2016, 6, 50887-50894.	1.7	19
219	Comprehensive evaluation of ten docking programs on a diverse set of proteinâ€“ligand complexes: the prediction accuracy of sampling power and scoring power. Physical Chemistry Chemical Physics, 2016, 18, 12964-12975.	1.3	669
220	Indolo-quinoline boron difluoride dyes: synthesis and spectroscopic properties. Organic and Biomolecular Chemistry, 2016, 14, 4185-4188.	1.5	10
221	Tangeretin, a citrus pentamethoxyflavone, antagonizes ABCB1-mediated multidrug resistance by inhibiting its transport function. Pharmacological Research, 2016, 110, 193-204.	3.1	31
222	The solvent at antigen-binding site regulated C3dâ€“CR2 interactions through the C-terminal tail of C3d at different ion strengths: insights from molecular dynamics simulation. Biochimica Et Biophysica Acta - General Subjects, 2016, 1860, 2220-2231.	1.1	5
223	The characterization of 1-(4-bromophenyl)-5-phenyl-1H-1,2,3-triazole on acute toxicity, antimicrobial activities, photophysical property, and binding to two globular proteins. Journal of Photochemistry and Photobiology B: Biology, 2016, 164, 191-203.	1.7	2
224	Combined use of PI3K and MEK inhibitors synergistically inhibits lung cancer with EGFR and KRAS mutations. Oncology Reports, 2016, 36, 365-375.	1.2	15
225	Colletotrilactam Aâ€“D, novel lactams from Colletotrichum gloeosporioides GT-7, a fungal endophyte of Uncaria rhynchophylla. FÃ¬toterapÃ¬Ã¢, 2016, 113, 158-163.	1.1	21
226	Revealing the molecular mechanism of different residence times of ERK2 inhibitors via binding free energy calculation and unbinding pathway analysis. Chemometrics and Intelligent Laboratory Systems, 2016, 158, 91-101.	1.8	16
227	Advanced research technology for discovery of new effective compounds from Chinese herbal medicine and their molecular targets. Pharmacological Research, 2016, 111, 546-555.	3.1	25
228	Exploring the Inhibitory Mechanism of Approved Selective Norepinephrine Reuptake Inhibitors and Reboxetine Enantiomers by Molecular Dynamics Study. Scientific Reports, 2016, 6, 26883.	1.6	46
229	Investigation of allosteric modulation mechanism of metabotropic glutamate receptor 1 by molecular dynamics simulations, free energy and weak interaction analysis. Scientific Reports, 2016, 6, 21763.	1.6	23
230	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
231	Efficacy and safety of angiogenesis inhibitors in advanced gastric cancer: a systematic review and meta-analysis. Journal of Hematology and Oncology, 2016, 9, 111.	6.9	45
232	Computational study on the unbinding pathways of B-RAF inhibitors and its implication for the difference of residence time: insight from random acceleration and steered molecular dynamics simulations. Physical Chemistry Chemical Physics, 2016, 18, 5622-5629.	1.3	38
233	Identification of the inhibitory mechanism of FDA approved selective serotonin reuptake inhibitors: an insight from molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2016, 18, 3260-3271.	1.3	66
234	Targeting Tyrosine Kinase Inhibitor-Resistant Non-Small Cell Lung Cancer by Inducing Epidermal Growth Factor Receptor DegradationviaMethionine 790 Oxidation. Antioxidants and Redox Signaling, 2016, 24, 263-279.	2.5	70

#	Article	IF	Citations
235	Computational study on the drug resistance mechanism of hepatitis C virus NS5B RNA-dependent RNA polymerase mutants to BMS-791325 by molecular dynamics simulation and binding free energy calculations. Chemometrics and Intelligent Laboratory Systems, 2016, 154, 185-193.	1.8	18
236	Insights into conformational regulation of PfMATE transporter from Pyrococcus furiosus induced by alternating protonation state of Asp41 residue: A molecular dynamics simulation study. Biochimica Et Biophysica Acta - General Subjects, 2016, 1860, 1173-1180.	1.1	5
237	Sesquiterpenoids and tirucallane triterpenoids from the roots of Scorzonera divaricata. Phytochemistry, 2016, 124, 86-98.	1.4	38
238	A new furanosteroid from Talaromyces sp. lgt-4, a fungal endophyte isolated from Tripterygium wilfordii. Natural Product Research, 2016, 30, 2137-2141.	1.0	21
239	Two new compounds, deacetylisowortmins A and B, isolated from an endophytic Fungus, Talaromyces wortmannii LGT-4. Natural Product Research, 2016, 30, 1623-1627.	1.0	18
240	Electric-field and strain-tunable electronic properties of MoS₂/h-BN/graphene vertical heterostructures. Physical Chemistry Chemical Physics, 2016, 18, 3159-3164.	1.3	42
241	HydPred: a novel method for the identification of protein hydroxylation sites that reveals new insights into human inherited disease. Molecular BioSystems, 2016, 12, 490-498.	2.9	10
242	Computational Study of the Binding Mechanism of Actin-Depolymerizing Factor 1 with Actin in Arabidopsis thaliana. PLoS ONE, 2016, 11, e0159053.	1.1	4
243	SCD1 is associated with tumor promotion, late stage and poor survival in lung adenocarcinoma. Oncotarget, 2016, 7, 39970-39979.	0.8	69
244	Inhibition of Monoamine Oxidase by Stilbenes from Rheum palmatum. Iranian Journal of Pharmaceutical Research, 2016, 15, 885-892.	0.3	6
245	(Z)3,4,5,4â€²-trans-tetramethoxystilbene, a new analogue of resveratrol, inhibits gefitinb-resistant non-small cell lung cancer via selectively elevating intracellular calcium level. Scientific Reports, 2015, 5, 16348.	1.6	38
246	Nobiletin enhances the efficacy of chemotherapeutic agents in ABCB1 overexpression cancer cells. Scientific Reports, 2015, 5, 18789.	1.6	70
247	Rapid identification of new minor chemical constituents from Smilacis Glabrae Rhizoma by combined use of UHPLCâ€Qâ€TOFâ€MS, preparative HPLC and UHPLCâ€SPEâ€NMRâ€MS techniques. Phytochemical Analysis, 2015, 26, 428-435.	1.2	17
248	The Molecular Mechanism of Bisphenol A (BPA) as an Endocrine Disruptor by Interacting with Nuclear Receptors: Insights from Molecular Dynamics (MD) Simulations. PLoS ONE, 2015, 10, e0120330.	1.1	73
249	A Highly Efficient Gene Expression Programming (GEP) Model for Auxiliary Diagnosis of Small Cell Lung Cancer. PLoS ONE, 2015, 10, e0125517.	1.1	20
250	Effects of the Pathogenic Mutation A117V and the Protective Mutation H111S on the Folding and Aggregation of PrP106-126: Insights from Replica Exchange Molecular Dynamics Simulations. PLoS ONE, 2015, 10, e0125899.	1.1	7
251	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
252	Binding of Citreoviridin to Human Serum Albumin: Multispectroscopic and Molecular Docking. BioMed Research International, 2015, 2015, 1-8.	0.9	11

#	Article	IF	Citations
253	Mutation of cysteine 46 in IKK-beta increases inflammatory responses. Oncotarget, 2015, 6, 31805-31819.	0.8	26
254	Dithiafulvenylâ€“triphenylamine organic dyes with alkyl chains for efficient coadsorbent-free dye-sensitized solar cells. RSC Advances, 2015, 5, 50813-50820.	1.7	26
255	Ervatamines Aâ€“I, Anti-inflammatory Monoterpenoid Indole Alkaloids with Diverse Skeletons from Ervatamia hainanensis. Journal of Natural Products, 2015, 78, 1253-1261.	1.5	68
256	A Nearâ€Infrared Fluorescence Probe for Thiols Based on Analyteâ€Specific Cleavage of Carbamate and Its Application in Bioimaging. European Journal of Organic Chemistry, 2015, 2015, 1711-1718.	1.2	27
257	Effects of the A117V mutation on the folding and aggregation of palindromic sequences (PrP113â€“120) in prion: insights from replica exchange molecular dynamics simulations. Molecular BioSystems, 2015, 11, 647-655.	2.9	11
258	HBT-based chemosensors for the detection of fluoride through deprotonation process: experimental and DFT studies. RSC Advances, 2015, 5, 19983-19988.	1.7	8
259	Direct dynamics study on hydrogen abstraction reaction of morpholine with hydroxyl radical. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	3
260	Characterization of the binding of shikonin to human immunoglobulin using scanning electron microscope, molecular modeling and multi-spectroscopic methods. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2015, 150, 514-522.	2.0	6
261	Near-Infrared and Naked-Eye Fluorescence Probe for Direct and Highly Selective Detection of Cysteine and Its Application in Living Cells. Analytical Chemistry, 2015, 87, 4856-4863.	3.2	194
262	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
263	Naked-Eye and Near-Infrared Fluorescence Probe for Hydrazine and Its Applications in In Vitro and In Vivo Bioimaging. Analytical Chemistry, 2015, 87, 9101-9107.	3.2	185
264	Computational insights into the inhibition and destabilization of morin on the oligomer of full-length human islet amyloid polypeptide. Physical Chemistry Chemical Physics, 2015, 17, 29103-29112.	1.3	20
265	Unveiling the molecular mechanism of brassinosteroids: Insights from structure-based molecular modeling studies. Steroids, 2015, 104, 111-117.	0.8	12
266	New nor-ursane type triterpenoids from Gelsemium elegans. FÃ¬toterapÃ¬Ã¢, 2015, 106, 175-183.	1.1	11
267	Molecular Mechanism of the Inhibition and Remodeling of Human Islet Amyloid Polypeptide (hIAPP_{1â€“37}) Oligomer by Resveratrol from Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2015, 119, 15-24.	1.2	51
268	Interaction of erucic acid with bovine serum albumin using a multi-spectroscopic method and molecular docking technique. Food Chemistry, 2015, 173, 31-37.	4.2	95
269	Computational Study on the Inhibitor Binding Mode and Allosteric Regulation Mechanism in Hepatitis C Virus NS3/4A Protein. PLoS ONE, 2014, 9, e87077.	1.1	19
270	Structural Diversity and Initial Oligomerization of PrP106â€“126 Studied by Replica-Exchange and Conventional Molecular Dynamics Simulations. PLoS ONE, 2014, 9, e87266.	1.1	13

#	Article	IF	Citations
271	Molecular Modeling Study on the Allosteric Inhibition Mechanism of HIV-1 Integrase by LEDGF/p75 Binding Site Inhibitors. PLoS ONE, 2014, 9, e90799.	1.1	16
272	Exploring the Influence of EGCG on the Î²-Sheet-Rich Oligomers of Human Islet Amyloid Polypeptide (hIAPP1â€“37) and Identifying Its Possible Binding Sites from Molecular Dynamics Simulation. PLoS ONE, 2014, 9, e94796.	1.1	40
273	Search for Î²2 Adrenergic Receptor Ligands by Virtual Screening via Grid Computing and Investigation of Binding Modes by Docking and Molecular Dynamics Simulations. PLoS ONE, 2014, 9, e107837.	1.1	13
274	Prediction on the Inhibition Ratio of Pyrrolidine Derivatives on Matrix Metalloproteinase Based on Gene Expression Programming. BioMed Research International, 2014, 2014, 1-8.	0.9	3
275	Dioxasampsones A and B, Two Polycyclic Polyprenylated Acylphloroglucinols with Unusual Epoxy-Ring-Fused Skeleton from Hypericum sampsonii. Organic Letters, 2014, 16, 6346-6349.	2.4	37
276	Phenolic Compounds from Liquidambar formosana Fruits as Monoamine Oxidase Inhibitors. Chemistry of Natural Compounds, 2014, 50, 1118-1119.	0.2	5
277	New clerodane diterpenoid glycosides from the aerial parts of Nannoglottis carpesioides. FÃ¬toterapÃ¬Ã¢, 2014, 93, 39-46.	1.1	11
278	Theoretical investigation of phenothiazineâ€“triphenylamine-based organic dyes with different Ïâ€ spacers for dye-sensitized solar cells. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 123, 282-289.	2.0	25
279	Stabilities and structures of islet amyloid polypeptide (IAPP22â€“28) oligomers: From dimer to 16-mer. Biochimica Et Biophysica Acta - General Subjects, 2014, 1840, 357-366.	1.1	24
280	Synthesis and structureâ€“activity relationship of nuciferine derivatives as potential acetylcholinesterase inhibitors. Medicinal Chemistry Research, 2014, 23, 3178-3186.	1.1	25
281	A coumarin-derived fluorescent chemosensor for selectively detecting Cu2+: Synthesis, DFT calculations and cell imaging applications. Talanta, 2014, 124, 139-145.	2.9	29
282	Molecular modeling study on the dynamical structural features of human smoothened receptor and binding mechanism of antagonist LY2940680 by metadynamics simulation and free energy calculation. Biochimica Et Biophysica Acta - General Subjects, 2014, 1840, 2128-2138.	1.1	29
283	A rhodamine B-based â€œturn-onâ€•fluorescent sensor for detecting Cu2+ and sulfur anions in aqueous media. RSC Advances, 2014, 4, 5718.	1.7	59
284	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
285	The adsorption mechanism and induced conformational changes of three typical proteins with different secondary structural features on graphene. RSC Advances, 2014, 4, 9953.	1.7	54
286	Computational study on the interaction between CCR5 and HIV-1 entry inhibitor maraviroc: insight from accelerated molecular dynamics simulation and free energy calculation. Physical Chemistry Chemical Physics, 2014, 16, 24332-24338.	1.3	25
287	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
288	Indoleacetic acid derivatives from the seeds of Ziziphus jujuba var. spinosa. FÃ¬toterapÃ¬Ã¢, 2014, 99, 48-55.	1.1	21

#	Article	IF	Citations
289	Novel polycyclic polyprenylated acylphloroglucinols from Hypericum sampsonii. Tetrahedron, 2014, 70, 7912-7916.	1.0	30
290	Norsampsones Aâ€“D, Four New Decarbonyl Polycyclic Polyprenylated Acylphloroglucinols from Hypericum sampsonii. Organic Letters, 2014, 16, 3448-3451.	2.4	55
291	Molecular modeling and residue interaction network studies on the mechanism of binding and resistance of the HCV NS5B polymerase mutants to VX-222 and ANA598. Antiviral Research, 2014, 104, 40-51.	1.9	35
292	A Novel Strategy of Structural Similarity Based Consensus Modeling. Molecular Informatics, 2013, 32, 599-608.	1.4	10
293	Exploring the Molecular Mechanism of Cross-Resistance to HIV-1 Integrase Strand Transfer Inhibitors by Molecular Dynamics Simulation and Residue Interaction Network Analysis. Journal of Chemical Information and Modeling, 2013, 53, 210-222.	2.5	75
294	Influence of Interface Structure on the Properties of ZnO/Graphene Composites: A Theoretical Study by Density Functional Theory Calculations. Journal of Physical Chemistry C, 2013, 117, 10536-10544.	1.5	76
295	Synthesis, Biological Activity Evaluation and Molecular Modeling Study on the New Isoconessimine Derivatives as Acetylcholinesterase Inhibitors. Chinese Journal of Chemistry, 2013, 31, 1228-1233.	2.6	2
296	Exploring the Influence of Carbon Nanoparticles on the Formation of Î²-Sheet-Rich Oligomers of IAPP22â€“28 Peptide by Molecular Dynamics Simulation. PLoS ONE, 2013, 8, e65579.	1.1	48
297	Understanding the molecular basis of MK2â€“p38Î± signaling complex assembly: insights into proteinâ€“protein interaction by molecular dynamics and free energy studies. Molecular BioSystems, 2012, 8, 2106.	2.9	46
298	Molecular dynamics and free energy studies on Aurora kinase A and its mutant bound with MLN8054: insight into molecular mechanism of subtype selectivity. Molecular BioSystems, 2012, 8, 3049.	2.9	24
299	Discrimination ofRadix Angelicae SinensisAccording to Harvest Time and Geographical Origin with Midinfrared Diffuse Reflectance Spectroscopy and Chemometric Methods. Spectroscopy Letters, 2012, 45, 430-437.	0.5	5
300	Exploring structural and thermodynamic stabilities of human prion protein pathogenic mutants D202N, E211Q and Q217R. Journal of Structural Biology, 2012, 178, 225-232.	1.3	24
301	Influence of the pathogenic mutations T188K/R/A on the structural stability and misfolding of human prion protein: Insight from molecular dynamics simulations. Biochimica Et Biophysica Acta - General Subjects, 2012, 1820, 116-123.	1.1	32
302	Quantitative Near-Infrared Spectrum-Active Blood Efficacy Relationship of Compound Danshen Tablet with Genetic Algorithmâ€“Multiple Linear Regression. Spectroscopy Letters, 2012, 45, 167-174.	0.5	1
303	The molecular basis of IGF-II/IGF2R recognition: a combined molecular dynamics simulation, free-energy calculation and computational alanine scanning study. Journal of Molecular Modeling, 2012, 18, 1421-1430.	0.8	21
304	Molecular modeling study on the resistance mechanism of HCV NS3/4A serine protease mutants R155K, A156V and D168A to TMC435. Antiviral Research, 2012, 93, 126-137.	1.9	79
305	Molecular mechanism of HIVâ€1 integraseâ€“vDNA interactions and strand transfer inhibitor action: A molecular modeling perspective. Journal of Computational Chemistry, 2012, 33, 527-536.	1.5	36
306	Structure-property relationships in conjugated donorâ€“acceptor systems functionalized with tetrathiafulvalene. New Journal of Chemistry, 2011, 35, 1876.	1.4	8

#	Article	IF	Citations
307	A nanocontainer that releases a fluorescence sensor for cadmium ions in water and its biological applications. Journal of Materials Chemistry, 2011, 21, 10298.	6.7	18
308	A Highly Zinc(II)â€Selective Fluorescent Sensor Based on 8â€Aminoquinoline and Its Application in Biological Imaging. European Journal of Inorganic Chemistry, 2011, 2011, 2927-2931.	1.0	25
309	Molecular Basis of the Interaction for an Essential Subunit PAâ˜PB1 in Influenza Virus RNA Polymerase: Insights from Molecular Dynamics Simulation and Free Energy Calculation. Molecular Pharmaceutics, 2010, 7, 75-85.	2.3	78
310	Facile and Efficient Synthesis of Benzoxazoles and Benzimidazoles: The Application of Hantzsch Ester 1,4â€Dihydropyridines in Reductive Cyclization Reactions. European Journal of Organic Chemistry, 2010, 2010, 6627-6632.	1.2	34
311	In Silico Identification of the Potential Drug Resistance Sites over 2009 Influenza A (H1N1) Virus Neuraminidase. Molecular Pharmaceutics, 2010, 7, 894-904.	2.3	57
312	Interaction Study of 2,6â€Bis[4â€(4â€aminoâ€2â€trifluoromethyl phenoxy)benzoyl] Pyridine with Human Immunoglobulin by Optical Spectroscopy and Molecular Modeling. Chinese Journal of Chemistry, 2009, 27, 324-330.	2.6	2
313	QSPR Study on the Melting Points of a Diverse Set of Potential Ionic Liquids by Projection Pursuit Regression. QSAR and Combinatorial Science, 2009, 28, 1237-1244.	1.5	21
314	In Silico Prediction of Inhibition Activity of Pyrazineâ€“Pyridine Biheteroaryls as VEGFR-2 Inhibitors Based on Least Squares Support Vector Machines. QSAR and Combinatorial Science, 2008, 27, 157-164.	1.5	7
315	QSAR Models for the Dermal Penetration of Polycyclic Aromatic Hydrocarbons Based on Gene Expression Programming. QSAR and Combinatorial Science, 2008, 27, 913-921.	1.5	4
316	Accurate Prediction of Aquatic Toxicity of Aromatic Compounds Based on Genetic Algorithm and Least Squares Support Vector Machines. QSAR and Combinatorial Science, 2008, 27, 850-865.	1.5	12
317	Accurate and Validated Quantitative Structureâ€“Activity Relationship Model of Caspaseâ€mediated Apoptosisâ€inducing Activity of Phenolic Compounds Using Density Functional Theory Calculation and Genetic Algorithmâ€“Multiple Linear Regression. QSAR and Combinatorial Science, 2008, 27, 1318-1325.	1.5	4
318	Investigation of the Interaction between Adenosine and Human Serum Albumin by Fluorescent Spectroscopy and Molecular Modeling. Chinese Journal of Chemistry, 2008, 26, 661-665.	2.6	7
319	QSAR study of malonylâ€CoA decarboxylase inhibitors using GAâ€MLR and a new strategy of consensus modeling. Journal of Computational Chemistry, 2008, 29, 2636-2647.	1.5	46
320	Prediction of nematic transition temperatures in thermotropic liquid crystals by a heuristic method. Liquid Crystals, 2007, 34, 1291-1297.	0.9	6
321	Study on the Structure-Activity Relationship of New Anti-HIV Nucleoside Derivatives Based on the Support Vector Machine Method. QSAR and Combinatorial Science, 2007, 26, 161-172.	1.5	6
322	Quantitative Structureâ€“Activity Relationship Study on a Series of Novel Ligands Binding to Central Benzodiazepine Receptor By Using the Combination of Heuristic Method and Support Vector Machines. QSAR and Combinatorial Science, 2007, 26, 443-451.	1.5	11
323	Interaction of aloe-emodin with human serum albumin. Science Bulletin, 2007, 52, 200-204.	1.7	0
324	Molecular modeling and spectroscopic studies on the binding of guaiacol to human immunoglobulin. Science in China Series B: Chemistry, 2006, 49, 550-559.	0.8	1

#	Article	IF	Citations
325	Interaction of APT with BSA or HSA. Science Bulletin, 2006, 51, 2201-2207.	1.7	29
326	QSAR and Classification Study of 1,4-Dihydropyridine Calcium Channel Antagonists Based on Least Squares Support Vector Machines. Molecular Pharmaceutics, 2005, 2, 348-356.	2.3	52
327	Quantitative structure property relationship models for the prediction of liquid heat capacity. QSAR and Combinatorial Science, 2003, 22, 29-48.	1.5	14
328	Correlation between molecular structures and relative electrophoretic mobility in capillary electrophoresis: Alkylpyridines. Chinese Journal of Chemistry, 2003, 21, 1247-1251.	2.6	1
329	Prediction of gas chromatographic retention indices by the use of radial basis function neural networks. Talanta, 2002, 57, 297-306.	2.9	29
330	Radial basis function neural network based QSPR for the prediction of critical pressures of substituted benzenes. Computers & Chemistry, 2002, 26, 159-169.	1.2	23
331	Radial Basis Function Neural Networks Based QSPR for the Prediction of log P. Chinese Journal of Chemistry, 2002, 20, 722-730.	2.6	2
332	THE APPLICATION OF THE RESONANCE ENHANCED RAYLEIGH LIGHT-SCATTERING TECHNIQUE FOR THE DETERMINATION OF GOLD(III) WITH A NEW TRIAZENE REAGENT. Analytical Letters, 2001, 34, 773-784.	1.0	3
333	Application of artificial neural networks for the simultaneous determination of a mixture of fluorescent dyes by synchronous fluorescence. Analyst, The, 2000, 125, 2049-2053.	1.7	46
334	Self-Assembled Hydrophobic Molecule-Based Surface Modification: A Strategy to Improve Efficiency and Stability of Perovskite Solar Cells. ACS Sustainable Chemistry and Engineering, 0, , .	3.2	2
335	Exploring Low-Toxicity Chemical Space with Deep Learning for Molecular Generation. Journal of Chemical Information and Modeling, 0, , .	2.5	5