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	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
2	Molecular dynamics simulations and novel drug discovery. Expert Opinion on Drug Discovery, 2018, 13, 23-37.	2.5	292
3	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
4	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
5	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
6	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
7	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
8	Nrf2: a dark horse in Alzheimer's disease treatment. Ageing Research Reviews, 2020, 64, 101206.	5.0	131
9	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
10	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
11	Early lung cancer diagnostic biomarker discovery by machine learning methods. Translational Oncology, 2021, 14, 100907.	1.7	99
12	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
13	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
14	Comprehensive Evaluation of Fourteen Docking Programs on Proteinâ€“Peptide Complexes. Journal of Chemical Theory and Computation, 2020, 16, 3959-3969.	2.3	90
15	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
16	Identification of metabolic vulnerabilities of receptor tyrosine kinases-driven cancer. Nature Communications, 2019, 10, 2701.	5.8	82
17	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
18	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

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19	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
20	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
21	Hernandezine, a novel AMPK activator induces autophagic cell death in drug-resistant cancers. Oncotarget, 2016, 7, 8090-8104.	0.8	74
22	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
23	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
24	Nobiletin enhances the efficacy of chemotherapeutic agents in ABCB1 overexpression cancer cells. Scientific Reports, 2015, 5, 18789.	1.6	70
25	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
26	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
27	SCD1 is associated with tumor promotion, late stage and poor survival in lung adenocarcinoma. Oncotarget, 2016, 7, 39970-39979.	0.8	69
28	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
29	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
30	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
31	Definition and classification system of glacial lake for inventory and hazards study. Journal of Chinese Geography, 2018, 28, 193-205.	1.5	66
32	Cordycepin Inhibits Drug-resistance Non-small Cell Lung Cancer Progression by Activating AMPK Signaling Pathway. Pharmacological Research, 2019, 144, 79-89.	3.1	66
33	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
34	Suppressing mPGES-1 expression by sinomenine ameliorates inflammation and arthritis. Biochemical Pharmacology, 2017, 142, 133-144.	2.0	60
35	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
36	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

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37	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
38	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
39	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
40	Norsampsones Aâ€“D, Four New Decarbonyl Polycyclic Polyprenylated Acylphloroglucinols from Hypericum sampsonii. Organic Letters, 2014, 16, 3448-3451.	2.4	55
41	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
42	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
43	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
44	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
45	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
46	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
47	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
48	Understanding the molecular basis of MK2â€“p38Îº signaling complex assembly: insights into proteinâ€“protein interaction by molecular dynamics and free energy studies. Molecular BioSystems, 2012, 8, 2106.	2.9	46
49	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
50	Computer-Aided Formulation Design for a Highly Soluble Luteinâ€“Cyclodextrin Multiple-Component Delivery System. Molecular Pharmaceutics, 2018, 15, 1664-1673.	2.3	46
51	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
52	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
53	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
54	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

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55	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
56	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
57	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
58	RetroPrime: A Diverse, plausible and Transformer-based method for Single-Step retrosynthesis predictions. Chemical Engineering Journal, 2021, 420, 129845.	6.6	44
59	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
60	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
61	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
62	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
63	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
64	Dimeric Cadinane Sesquiterpenoid Derivatives from Artemisia annua. Organic Letters, 2018, 20, 453-456.	2.4	39
65	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
66	(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
67	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
68	Sesquiterpenoids and tirucallane triterpenoids from the roots of Scorzonera divaricata. Phytochemistry, 2016, 124, 86-98.	1.4	38
69	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
70	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
71	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
72	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

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73	RELATION: A Deep Generative Model for Structure-Based De Novo Drug Design. Journal of Medicinal Chemistry, 2022, 65, 9478-9492.	2.9	36
74	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
75	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
76	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
77	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
78	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
79	An efficient and hydrophobic molecular doping in perovskite solar cells. Nano Energy, 2021, 82, 105751.	8.2	35
80	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
81	Identification of a New Potent Inhibitor Targeting KRAS in Non-small Cell Lung Cancer Cells. Frontiers in Pharmacology, 2017, 8, 823.	1.6	34
82	Xanthatin Promotes Apoptosis via Inhibiting Thioredoxin Reductase and Eliciting Oxidative Stress. Molecular Pharmaceutics, 2018, 15, 3285-3296.	2.3	34
83	Thalidezine, a novel AMPK activator, eliminates apoptosis-resistant cancer cells through energy-mediated autophagic cell death. Oncotarget, 2017, 8, 30077-30091.	0.8	34
84	Resistance looms for KRAS G12C inhibitors and rational tackling strategies. , 2022, 229, 108050.		34
85	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
86	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
87	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
88	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
89	Tangeretin, a citrus pentamethoxyflavone, antagonizes ABCB1-mediated multidrug resistance by inhibiting its transport function. Pharmacological Research, 2016, 110, 193-204.	3.1	31
90	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

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91	Novel polycyclic polyprenylated acylphloroglucinols from Hypericum sampsonii. Tetrahedron, 2014, 70, 7912-7916.	1.0	30
92	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
93	Prediction of gas chromatographic retention indices by the use of radial basis function neural networks. Talanta, 2002, 57, 297-306.	2.9	29
94	Interaction of APT with BSA or HSA. Science Bulletin, 2006, 51, 2201-2207.	1.7	29
95	A coumarin-derived fluorescent chemosensor for selectively detecting Cu2+: Synthesis, DFT calculations and cell imaging applications. Talanta, 2014, 124, 139-145.	2.9	29
96	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
97	Aggreganoids Aâ€“F, Carbon-Bridged Sesquiterpenoid Dimers and Trimers from Lindera aggregata. Organic Letters, 2019, 21, 5753-5756.	2.4	29
98	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
99	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
100	TrimNet: learning molecular representation from triplet messages for biomedicine. Briefings in Bioinformatics, 2021, 22, .	3.2	28
101	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
102	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
103	Mutation of cysteine 46 in IKK-beta increases inflammatory responses. Oncotarget, 2015, 6, 31805-31819.	0.8	26
104	Dithiafulvenylâ€triphenylamine organic dyes with alkyl chains for efficient coadsorbent-free dye-sensitized solar cells. RSC Advances, 2015, 5, 50813-50820.	1.7	26
105	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
106	Fluorophore-Dependent Cleavage of Disulfide Bond Leading to a Highly Selective Fluorescent Probe of Thioredoxin. Analytical Chemistry, 2019, 91, 8524-8531.	3.2	26
107	Network pharmacological approach for elucidating the mechanisms of traditional Chinese medicine in treating COVID-19 patients. Pharmacological Research, 2020, 159, 105043.	3.1	26
108	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

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109	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
110	Theoretical investigation of phenothiazineâ€“triphenylamine-based organic dyes with different Ï€ spacers for dye-sensitized solar cells. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2014, 123, 282-289.	2.0	25
111	Synthesis and structureâ€“activity relationship of nuciferine derivatives as potential acetylcholinesterase inhibitors. Medicinal Chemistry Research, 2014, 23, 3178-3186.	1.1	25
112	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
113	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
114	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
115	Subtype-selective mechanisms of negative allosteric modulators binding to group I metabotropic glutamate receptors. Acta Pharmacologica Sinica, 2021, 42, 1354-1367.	2.8	25
116	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
117	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
118	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
119	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
120	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
121	Prediction of the Antioxidant Response Elements' Response of Compound by Deep Learning. Frontiers in Chemistry, 2019, 7, 385.	1.8	24
122	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
123	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
124	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
125	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
126	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

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127	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
128	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
129	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
130	Indoleacetic acid derivatives from the seeds of Ziziphus jujuba var. spinosa. FÃ¬toterapÃ¬Ã¢, 2014, 99, 48-55.	1.1	21
131	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
132	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
133	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
134	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
135	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
136	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
137	Linderalides Aâ€“D, Disesquiterpenoidâ€“Geranylbenzofuranone Conjugates from Lindera aggregata. Journal of Organic Chemistry, 2019, 84, 8242-8247.	1.7	21
138	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
139	Emodin induces apoptosis and suppresses non-small-cell lung cancer growth via downregulation of sPLA2-IIa. Phytomedicine, 2022, 95, 153786.	2.3	21
140	Novel direct AMPK activator suppresses non-small cell lung cancer through inhibition of lipid metabolism. Oncotarget, 2017, 8, 96089-96102.	0.8	21
141	Andrographolide suppresses non-small-cell lung cancer progression through induction of autophagy and antitumor immune response. Pharmacological Research, 2022, 179, 106198.	3.1	21
142	A Highly Efficient Gene Expression Programming (GEP) Model for Auxiliary Diagnosis of Small Cell Lung Cancer. PLoS ONE, 2015, 10, e0125517.	1.1	20
143	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
144	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

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145	Identification of potential genetic causal variants for rheumatoid arthritis by whole-exome sequencing. Oncotarget, 2017, 8, 111119-111129.	0.8	20
146	Gossypol Inhibits Non-small Cell Lung Cancer Cells Proliferation by Targeting EGFRL858R/T790M. Frontiers in Pharmacology, 2018, 9, 728.	1.6	20
147	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
148	Hypersampsones Sâ€“W, new polycyclic polyprenylated acylphloroglucinols from Hypericum sampsonii. RSC Advances, 2016, 6, 50887-50894.	1.7	19
149	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
150	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
151	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
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