Yun Tang

List of Publications by Year
in descending order

160 papers	8,593 citations	66343 42 h-index	49909 87 g-index
170 all docs	170 docs citations	170 times ranked	9411 citing authors

#	Article	IF	Citations
1	admetSAR: A Comprehensive Source and Free Tool for Assessment of Chemical ADMET Properties. Journal of Chemical Information and Modeling, 2012, 52, 3099-3105.	5.4	1,439
2	admetSAR 2.0: web-service for prediction and optimization of chemical ADMET properties. Bioinformatics, 2019, 35, 1067-1069.	4.1	753
3	Prediction of Drug-Target Interactions and Drug Repositioning via Network-Based Inference. PLoS Computational Biology, 2012, 8, e1002503.	3.2	674
4	SoNar, a Highly Responsive NAD+/NADH Sensor, Allows High-Throughput Metabolic Screening of Anti-tumor Agents. Cell Metabolism, 2015, 21, 777-789.	16.2	311
5	ADMET-score â€“ a comprehensive scoring function for evaluation of chemical drug-likeness. MedChemComm, 2019, 10, 148-157.	3.4	295
6	Estimation of ADME Properties with Substructure Pattern Recognition. Journal of Chemical Information and Modeling, 2010, 50, 1034-1041.	5.4	266
7	In Silico ADMET Prediction: Recent Advances, Current Challenges and Future Trends. Current Topics in Medicinal Chemistry, 2013, 13, 1273-1289.	2.1	181
8	In silico Prediction of Chemical Ames Mutagenicity. Journal of Chemical Information and Modeling, 2012, 52, 2840-2847.	5.4	163
9	Classification of Cytochrome P450 Inhibitors and Noninhibitors Using Combined Classifiers. Journal of Chemical Information and Modeling, 2011, 51, 996-1011.	5.4	155
10	In Silico Prediction of Chemical Toxicity for Drug Design Using Machine Learning Methods and Structural Alerts. Frontiers in Chemistry, 2018, 6, 30.	3.6	152
11	In Silico Prediction of Chemical Acute Oral Toxicity Using Multi-Classification Methods. Journal of Chemical Information and Modeling, 2014, 54, 1061-1069.	5.4	140
12	Network-Based Methods for Prediction of Drug-Target Interactions. Frontiers in Pharmacology, 2018, 9, 1134.	3.5	131
13	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	6.0	120
14	Association between cigarette smoking and Parkinsonâ€™s disease: A meta-analysis. Archives of Gerontology and Geriatrics, 2015, 61, 510-516.	3.0	119
15	Adverse Drug Events: Database Construction and in Silico Prediction. Journal of Chemical Information and Modeling, 2013, 53, 744-752.	5.4	116
16	In Silico Prediction of Bloodâ€“Brain Barrier Permeability of Compounds by Machine Learning and Resampling Methods. ChemMedChem, 2018, 13, 2189-2201.	3.2	111
17	Performance Evaluation of 2D Fingerprint and 3D Shape Similarity Methods in Virtual Screening. Journal of Chemical Information and Modeling, 2012, 52, 1103-1113.	5.4	106
18	SDTNBI: an integrated network and chemoinformatics tool for systematic prediction of drugâ€“target interactions and drug repositioning. Briefings in Bioinformatics, 2017, 18, bbw012.	6.5	102

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19	Prediction of chemicalâ€“protein interactions: multitarget-QSAR versus computational chemogenomic methods. Molecular BioSystems, 2012, 8, 2373.	2.9	100
20	In Silico Assessment of Chemical Biodegradability. Journal of Chemical Information and Modeling, 2012, 52, 655-669.	5.4	87
21	Prediction of Chemical-Protein Interactions Network with Weighted Network-Based Inference Method. PLoS ONE, 2012, 7, e41064.	2.5	86
22	Prediction of Polypharmacological Profiles of Drugs by the Integration of Chemical, Side Effect, and Therapeutic Space. Journal of Chemical Information and Modeling, 2013, 53, 753-762.	5.4	86
23	New technologies in computer-aided drug design: Toward target identification and new chemical entity discovery. Drug Discovery Today: Technologies, 2006, 3, 307-313.	4.0	85
24	Network-based identification of microRNAs as potential pharmacogenomic biomarkers for anticancer drugs. Oncotarget, 2016, 7, 45584-45596.	1.8	85
25	Quantitative and Systems Pharmacology. 1. In Silico Prediction of Drugâ€“Target Interactions of Natural Products Enables New Targeted Cancer Therapy. Journal of Chemical Information and Modeling, 2017, 57, 2657-2671.	5.4	76
26	In silico prediction of Tetrahymena pyriformis toxicity for diverse industrial chemicals with substructure pattern recognition and machine learning methods. Chemosphere, 2011, 82, 1636-1643.	8.2	75
27	In silico Prediction of Drug Induced Liver Toxicity Using Substructure Pattern Recognition Method. Molecular Informatics, 2016, 35, 136-144.	2.5	75
28	In silico prediction of chemical mechanism of action via an improved networkâ€based inference method. British Journal of Pharmacology, 2016, 173, 3372-3385.	5.4	73
29	CATMoS: Collaborative Acute Toxicity Modeling Suite. Environmental Health Perspectives, 2021, 129, 47013.	6.0	63
30	In Silico Prediction of Compounds Binding to Human Plasma Proteins by QSAR Models. ChemMedChem, 2018, 13, 572-581.	3.2	62
31	Insights into Molecular Basis of Cytochrome P450 Inhibitory Promiscuity of Compounds. Journal of Chemical Information and Modeling, 2011, 51, 2482-2495.	5.4	60
32	Discovery of novel propargylamine-modified 4-aminoalkyl imidazole substituted pyrimidinylthiourea derivatives as multifunctional agents for the treatment of Alzheimer's disease. European Journal of Medicinal Chemistry, 2018, 143, 33-47.	5.5	60
33	ADMETopt: A Web Server for ADMET Optimization in Drug Design via Scaffold Hopping. Journal of Chemical Information and Modeling, 2018, 58, 2051-2056.	5.4	60
34	Evaluation of Different Methods for Identification of Structural Alerts Using Chemical Ames Mutagenicity Data Set as a Benchmark. Chemical Research in Toxicology, 2017, 30, 1355-1364.	3.3	53
35	Computational prediction of microRNA networks incorporating environmental toxicity and disease etiology. Scientific Reports, 2014, 4, 5576.	3.3	51
36	Computational models to predict endocrine-disrupting chemical binding with androgen or oestrogen receptors. Ecotoxicology and Environmental Safety, 2014, 110, 280-287.	6.0	50

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37	The Acute-Phase Protein Orosomucoid Regulates Food Intake and Energy Homeostasis via Leptin Receptor Signaling Pathway. Diabetes, 2016, 65, 1630-1641.	0.6	50
38	In silico prediction of hERG potassium channel blockage by chemical category approaches. Toxicology Research, 2016, 5, 570-582.	2.1	50
39	An Unusual (R)â€Selective Epoxide Hydrolase with High Activity for Facile Preparation of Enantiopure Glycidyl Ethers. Advanced Synthesis and Catalysis, 2011, 353, 1510-1518.	4.3	46
40	Computational Approaches to Identify Structural Alerts and Their Applications in Environmental Toxicology and Drug Discovery. Chemical Research in Toxicology, 2020, 33, 1312-1322.	3.3	46
41	Discovery of Potent Ligands for Estrogen Receptor Î² by Structure-Based Virtual Screening. Journal of Medicinal Chemistry, 2010, 53, 5361-5365.	6.4	44
42	FXR antagonism of NSAIDs contributes to drug-induced liver injury identified by systems pharmacology approach. Scientific Reports, 2015, 5, 8114.	3.3	44
43	A Computational Systems Pharmacology Approach to Investigate Molecular Mechanisms of Herbal Formula Tian-Ma-Gou-Teng-Yin for Treatment of Alzheimerâ€™s Disease. Frontiers in Pharmacology, 2018, 9, 668.	3.5	43
44	In Silico Estimation of Chemical Carcinogenicity with Binary and Ternary Classification Methods. Molecular Informatics, 2015, 34, 228-235.	2.5	42
45	In silico prediction of chemical toxicity on avian species using chemical category approaches. Chemosphere, 2015, 122, 280-287.	8.2	41
46	Predicting Meridian in Chinese traditional medicine using machine learning approaches. PLoS Computational Biology, 2019, 15, e1007249.	3.2	41
47	In silico prediction of serious eye irritation or corrosion potential of chemicals. RSC Advances, 2017, 7, 6697-6703.	3.6	37
48	Design, synthesis and evaluation of diosgenin carbamate derivatives as multitarget anti-Alzheimerâ€™s disease agents. European Journal of Medicinal Chemistry, 2020, 187, 111913.	5.5	36
49	In silico prediction of chemical reproductive toxicity using machine learning. Journal of Applied Toxicology, 2019, 39, 844-854.	2.8	34
50	In Silico Prediction of Chemicals Binding to Aromatase with Machine Learning Methods. Chemical Research in Toxicology, 2017, 30, 1209-1218.	3.3	33
51	In silico prediction of chemical genotoxicity using machine learning methods and structural alerts. Toxicology Research, 2018, 7, 211-220.	2.1	33
52	Network pharmacological mechanisms of Vernonia anthelmintica (L.) in the treatment of vitiligo: Isorhamnetin induction of melanogenesis via up-regulation of melanin-biosynthetic genes. BMC Systems Biology, 2017, 11, 103.	3.0	32
53	Microwave-assisted construction of triazole-linked amino acidâ€“glucoside conjugates as novel PTP1B inhibitors. New Journal of Chemistry, 2011, 35, 622.	2.8	31
54	Drug Repurposing of Histone Deacetylase Inhibitors That Alleviate Neutrophilic Inflammation in Acute Lung Injury and Idiopathic Pulmonary Fibrosis via Inhibiting Leukotriene A4 Hydrolase and Blocking LTB4 Biosynthesis. Journal of Medicinal Chemistry, 2017, 60, 1817-1828.	6.4	30

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55	Insights into the molecular mechanisms of Polygonum multiflorum Thunb-induced liver injury: a computational systems toxicology approach. Acta Pharmacologica Sinica, 2017, 38, 719-732.	6.1	30
56	In silico prediction of pesticide aquatic toxicity with chemical category approaches. Toxicology Research, 2017, 6, 831-842.	2.1	30
57	A genetically encoded biosensor for in vitro and in vivo detection of NADP+. Biosensors and Bioelectronics, 2016, 77, 901-906.	10.1	29
58	Design, synthesis and biological evaluation of chalcones as reversers of P-glycoprotein-mediated multidrug resistance. European Journal of Medicinal Chemistry, 2019, 180, 350-366.	5.5	29
59	In silico prediction of chemical aquatic toxicity with chemical category approaches and substructural alerts. Toxicology Research, 2015, 4, 452-463.	2.1	28
60	Biomarker-based drug safety assessment in the age of systems pharmacology: from foundational to regulatory science. Biomarkers in Medicine, 2015, 9, 1241-1252.	1.4	28
61	Quantitative and systems pharmacology 2. In silico polypharmacology of G protein-coupled receptor ligands via network-based approaches. Pharmacological Research, 2018, 129, 400-413.	7.1	28
62	Drug repositioning by prediction of drugâ€™s anatomical therapeutic chemical code via network-based inference approaches. Briefings in Bioinformatics, 2021, 22, 2058-2072.	6.5	25
63	Research progress in cation-Ï€ interactions. Science in China Series B: Chemistry, 2008, 51, 709-717.	0.8	24
64	A novel derivative of artemisinin inhibits cell proliferation and metastasis via down-regulation of cathepsin K in breast cancer. European Journal of Pharmacology, 2019, 858, 172382.	3.5	23
65	NetInfer: A Web Server for Prediction of Targets and Therapeutic and Adverse Effects via Network-Based Inference Methods. Journal of Chemical Information and Modeling, 2020, 60, 3687-3691.	5.4	23
66	A novel multistage antiplasmodial inhibitor targeting Plasmodium falciparum histone deacetylase 1. Cell Discovery, 2020, 6, 93.	6.7	23
67	In silico prediction of mitochondrial toxicity of chemicals using machine learning methods. Journal of Applied Toxicology, 2021, 41, 1518-1526.	2.8	23
68	Reduced Catalytic Activity of P450 2A6 Mutants with Coumarin: A Computational Investigation. Journal of Chemical Theory and Computation, 2009, 5, 1411-1420.	5.3	22
69	Discovery of new non-steroidal FXR ligands via a virtual screening workflow based on Phase shape and induced fit docking. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 6848-6853.	2.2	22
70	Computational insights into the G-protein-biased activation and inactivation mechanisms of the Î¼ opioid receptor. Acta Pharmacologica Sinica, 2018, 39, 154-164.	6.1	22
71	In Silico Prediction of Endocrine Disrupting Chemicals Using Single-Label and Multilabel Models. Journal of Chemical Information and Modeling, 2019, 59, 973-982.	5.4	22
72	In SilicoPrediction of Bloodâ€“Brain Partitioning Using a Chemometric Method Called Genetic Algorithm Based Variable Selection. QSAR and Combinatorial Science, 2008, 27, 704-717.	1.4	21

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73	Computational Prediction of Site of Metabolism for UGT-Catalyzed Reactions. Journal of Chemical Information and Modeling, 2019, 59, 1085-1095.	5.4	21
74	In silico prediction of chemical aquatic toxicity for marine crustaceans via machine learning. Toxicology Research, 2019, 8, 341-352.	2.1	20
75	Molecular switches of the Î¤ opioid receptor triggered by 6â€²-GNTI and 5â€²-GNTI. Scientific Reports, 2016, 6, 18913.	3.3	19
76	Discovery, mechanism and metabolism studies of 2,3-difluorophenyl-linker-containing PARP1 inhibitors with enhanced inÂvivo efficacy for cancer therapy. European Journal of Medicinal Chemistry, 2017, 138, 514-531.	5.5	18
77	In silico prediction of chemical neurotoxicity using machine learning. Toxicology Research, 2020, 9, 164-172.	2.1	18
78	Residues remote from the binding pocket control the antagonist selectivity towards the corticotropin-releasing factor receptor-1. Scientific Reports, 2015, 5, 8066.	3.3	17
79	Prediction of the skin sensitising potential and potency of compounds via mechanism-based binary and ternary classification models. Toxicology in Vitro, 2019, 59, 204-214.	2.4	17
80	Strategy for Efficient Discovery of Cocrystals via a Network-Based Recommendation Model. Crystal Growth and Design, 2020, 20, 6820-6830.	3.0	17
81	Homotropic Cooperativity of Midazolam Metabolism by Cytochrome P450 3A4: Insight from Computational Studies. Journal of Chemical Information and Modeling, 2021, 61, 2418-2426.	5.4	17
82	Effects of protein flexibility on the site of metabolism prediction for CYP2A6 substrates. Journal of Molecular Graphics and Modelling, 2014, 54, 90-99.	2.4	16
83	Prediction of Farnesoid X Receptor Disruptors with Machine Learning Methods. Chemical Research in Toxicology, 2018, 31, 1128-1137.	3.3	16
84	In silicoestimation of chemical aquatic toxicity on crustaceans using chemical category methods. Environmental Sciences: Processes and Impacts, 2018, 20, 1234-1243.	3.5	16
85	Multiclassification Prediction of Enzymatic Reactions for Oxidoreductases and Hydrolases Using Reaction Fingerprints and Machine Learning Methods. Journal of Chemical Information and Modeling, 2018, 58, 1169-1181.	5.4	16
86	Identification of Nontoxic Substructures: A New Strategy to Avoid Potential Toxicity Risk. Toxicological Sciences, 2018, 165, 396-407.	3.1	16
87	In Silico Prediction of Human Renal Clearance of Compounds Using Quantitative Structure-Pharmacokinetic Relationship Models. Chemical Research in Toxicology, 2020, 33, 640-650.	3.3	16
88	Structure-based ensemble-QSAR model: a novel approach to the study of the EGFR tyrosine kinase and its inhibitors. Acta Pharmacologica Sinica, 2014, 35, 301-310.	6.1	15
89	Selective ligands of estrogen receptor Î² discovered using pharmacophore mapping and structure-based virtual screening. Acta Pharmacologica Sinica, 2014, 35, 1333-1341.	6.1	15
90	In silico prediction of chemical subcellular localization via multi-classification methods. MedChemComm, 2017, 8, 1225-1234.	3.4	15

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91	Effects of protein flexibility and active site water molecules on the prediction of sites of metabolism for cytochrome P450 2C19 substrates. Molecular BioSystems, 2016, 12, 868-878.	2.9	14
92	Development of Novel N-hydroxypyridone Derivatives as Potential Anti-Ischemic Stroke Agents. Journal of Medicinal Chemistry, 2020, 63, 1051-1067.	6.4	14
93	2-Arylbenzo[b]furan derivatives as potent human lipoxygenase inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 98-105.	5.2	13
94	Computational Investigation of Ligand Binding to the Peripheral Site in CYP3A4: Conformational Dynamics and Inhibitor Discovery. Journal of Chemical Information and Modeling, 2017, 57, 616-626.	5.4	13
95	Insights into mechanisms and severity of drug-induced liver injury via computational systems toxicology approach. Toxicology Letters, 2019, 312, 22-33.	0.8	13
96	In silico prediction of chemical acute contact toxicity on honey bees via machine learning methods. Toxicology in Vitro, 2021, 72, 105089.	2.4	13
97	Catalytic Mechanism of Cytochrome P450 2D6 for 4â€Hydroxylation of Aripiprazole: A QM/MM Study. Chinese Journal of Chemistry, 2013, 31, 1219-1227.	4.9	12
98	Discovery of new antimalarial agents: Second-generation dual inhibitors against FP-2 and PfDHFR via fragments assembely. Bioorganic and Medicinal Chemistry, 2017, 25, 6467-6478.	3.0	12
99	wSDTNBI: a novel network-based inference method for virtual screening. Chemical Science, 2022, 13, 1060-1079.	7.4	11
100	Cation sitting in aromatic cages:ab initio computational studies on tetramethylammoniumâ€“(benzene)n (n=3â€“4) complexes. Journal of Physical Organic Chemistry, 2007, 20, 448-453.	1.9	10
101	Computational Insights into Ligand Selectivity of Estrogen Receptors from Pharmacophore Modeling. Molecular Informatics, 2011, 30, 539-549.	2.5	10
102	In Silico Prediction of CYP2C8 Inhibition with Machine-Learning Methods. Chemical Research in Toxicology, 2021, 34, 1850-1859.	3.3	10
103	A multitask GNN-based interpretable model for discovery of selective JAK inhibitors. Journal of Cheminformatics, 2022, 14, 16.	6.1	10
104	Synthesis and evaluation of Î¹-opioid receptor agonistic activity and antinociceptive effect of novel morphine analogues, 7Î±-phenyl-6Î±,14Î±-endo-etheno-tetrahydrothebaine with substituted o-, m- and p-amino group. Medicinal Chemistry Research, 2011, 20, 1364-1370.	2.4	9
105	Computational insights into the different catalytic activities of <scp>CYP</scp>3A4 and <scp>CYP</scp>3A5 toward schisantherin E. Chemical Biology and Drug Design, 2019, 93, 854-864.	3.2	9
106	Computational Insights into Molecular Activation and Positive Cooperative Mechanisms of FFAR1 Modulators. Journal of Chemical Information and Modeling, 2020, 60, 3214-3230.	5.4	9
107	Artificial neural network cascade identifies multi-P450 inhibitors in natural compounds. PeerJ, 2015, 3, e1524.	2.0	9
108	IDL-PPBopt: A Strategy for Prediction and Optimization of Human Plasma Protein Binding of Compounds via an Interpretable Deep Learning Method. Journal of Chemical Information and Modeling, 2022, 62, 2788-2799.	5.4	9

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109	Computational insights into inhibitory mechanism of azole compounds against human aromatase. RSC Advances, 2015, 5, 90871-90880.	3.6	8
110	Identifying the structural features and diversifying the chemical domain of peripherally acting CB1 receptor antagonists using molecular modeling techniques. RSC Advances, 2016, 6, 1466-1483.	3.6	8
111	Improving the physicochemical properties of bicalutamide by complex formation with bovine serum albumin. European Journal of Pharmaceutical Sciences, 2017, 106, 381-392.	4.0	8
112	Computational Insight Into Vitamin K1 Ï‰-Hydroxylation by Cytochrome P450 4F2. Frontiers in Pharmacology, 2018, 9, 1065.	3.5	8
113	Computational insights into the interaction mechanisms of estrogenâ€related receptor alpha with endogenous ligand cholesterol. Chemical Biology and Drug Design, 2019, 94, 1316-1329.	3.2	8
114	MetaADEDB 2.0: a comprehensive database on adverse drug events. Bioinformatics, 2021, 37, 2221-2222.	4.1	8
115	Insights into the mechanism of Arnebia euchroma on leukemia via network pharmacology approach. BMC Complementary Medicine and Therapies, 2020, 20, 322.	2.7	8
116	Insights into the Molecular Mechanisms of Liuwei Dihuang Decoction via Network Pharmacology. Chemical Research in Toxicology, 2021, 34, 91-102.	3.3	8
117	Pathway-Based Drug Repurposing with DPNetinfer: A Method to Predict Drugâ€“Pathway Associations via Network-Based Approaches. Journal of Chemical Information and Modeling, 2021, 61, 2475-2485.	5.4	8
118	MPSM-DTI: prediction of drugâ€“target interaction via machine learning based on the chemical structure and protein sequence. , 2022, 1, 115-126.		8
119	In silico prediction of potential drugâ€induced nephrotoxicity with machine learning methods. Journal of Applied Toxicology, 2022, 42, 1639-1650.	2.8	8
120	Interactions of omeprazole-based analogues with cytochrome P450 2C19: a computational study. Molecular BioSystems, 2016, 12, 1913-1921.	2.9	7
121	In Silico Prediction of Metabolic Epoxidation for Drugâ€like Molecules via Machine Learning Methods. Molecular Informatics, 2020, 39, e1900178.	2.5	7
122	Extracts from Chinese herbs with anti-amyloid and neuroprotective activities. International Journal of Biological Macromolecules, 2021, 179, 475-484.	7.5	7
123	Discovery of Natural Products Targeting NQO1 via an Approach Combining Network-Based Inference and Identification of Privileged Substructures. Journal of Chemical Information and Modeling, 2021, 61, 2486-2498.	5.4	7
124	Mechanistic Insights into the Regioâ€•and Stereoselectivities of Testosterone and Dihydrotestosterone Hydroxylation Catalyzed by CYP3A4 and CYP19A1. Chemistry - A European Journal, 2020, 26, 6214-6223.	3.3	7
125	The open-close mechanism of M2 channel protein in influenza A virus: A computational study on the hydrogen bonds and cation-Ï€ interactions among His37 and Trp41. Science in China Series B: Chemistry, 2008, 51, 768-775.	0.8	6
126	The role of benzoic acid in prolineâ€catalyzed asymmetric michael addition: A density functional theory study. International Journal of Quantum Chemistry, 2013, 113, 1339-1348.	2.0	6

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127	Computational investigation of the interaction mechanism between the estrogen related receptor Î± and its agonists. RSC Advances, 2016, 6, 94119-94127.	3.6	6
128	Computational insight into conformational states of glucagon-like peptide-1 receptor (GLP-1R) and its binding mode with GLP-1. RSC Advances, 2016, 6, 13490-13497.	3.6	6
129	Prediction of the allergic mechanism of haptens via a reaction-substructure-compound-target-pathway network system. Toxicology Letters, 2019, 317, 68-81.	0.8	6
130	Dissecting the Structural Plasticity and Dynamics of Cytochrome P450 2B4 by Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2020, 60, 5026-5035.	5.4	6
131	In silico prediction of chemical respiratory toxicity via machine learning. Computational Toxicology, 2021, 18, 100155.	3.3	6
132	Computational Insight into the Allosteric Activation Mechanism of Farnesoid X Receptor. Journal of Chemical Information and Modeling, 2020, 60, 1540-1550.	5.4	5
133	SMINBR: An Integrated Network and Chemoinformatics Tool Specialized for Prediction of Two-Component Crystal Formation. Journal of Chemical Information and Modeling, 2021, 61, 4290-4302.	5.4	5
134	Pharmacophore modeling and 3D-QSAR study for the design of novel Î±-synuclein aggregation inhibitors. Journal of Molecular Modeling, 2021, 27, 260.	1.8	5
135	Development of a Multi-Target Strategy for the Treatment of Vitiligo via Machine Learning and Network Analysis Methods. Frontiers in Pharmacology, 2021, 12, 754175.	3.5	5
136	Discovery of New Estrogen-Related Receptor Î± Agonists via a Combination Strategy Based on Shape Screening and Ensemble Docking. Journal of Chemical Information and Modeling, 2022, 62, 486-497.	5.4	5
137	In silico prediction of UGT-mediated metabolism in drug-like molecules via graph neural network. Journal of Cheminformatics, 2022, 14, .	6.1	5
138	Refinement and 3Dâ€QSAR Studies of Inhibitors of Cyclophilin A Containing Amide Linker. QSAR and Combinatorial Science, 2009, 28, 183-193.	1.4	4
139	ADENet: a novel network-based inference method for prediction of drug adverse events. Briefings in Bioinformatics, 2022, 23, .	6.5	4
140	An Improved Practical Route to (Â±)â€Epibatidine through Lâ€Proline Catalyzed Intramolecular Michael Addition. Chinese Journal of Chemistry, 2012, 30, 1305-1309.	4.9	3
141	Quantitative Regression Models for the Prediction of Chemical Properties by an Efficient Workflow. Molecular Informatics, 2015, 34, 679-688.	2.5	3
142	Computational insights into different inhibition modes of the Î¼-opioid receptor with antagonists LY2456302 and JDTic. RSC Advances, 2016, 6, 13626-13635.	3.6	3
143	Insights into the interaction mechanisms of estrogen-related receptor alpha (ERRÎ±) with ligands via molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2020, 38, 3867-3878.	3.5	3
144	Assessment of CYP2C9 Structural Models for Site of Metabolism Prediction. ChemMedChem, 2021, 16, 1755-1764.	3.2	3

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145	Twin drug design, synthesis and evaluation of diosgenin derivatives as multitargeted agents for the treatment of vascular dementia. Bioorganic and Medicinal Chemistry, 2021, 37, 116109.	3.0	3
146	In Silico Prediction of Potential Drug Combinations for Type 2 Diabetes Mellitus by an Integrated Network and Transcriptome Analysis. ChemMedChem, 2022, 17, .	3.2	3
147	Drug Repurposing for Newly Emerged Diseases via Networkâ€based Inference on a Geneâ€diseaseâ€drug Network. Molecular Informatics, 2022, 41, .	2.5	3
148	In silico prediction of chemical aquatic toxicity by multiple machine learning and deep learning approaches. Journal of Applied Toxicology, 2022, 42, 1766-1776.	2.8	3
149	Inhibitors of HIVâ€1 Integraseâ€Human LEDGF/p75 Interaction Identified from Natural Products via Virtual Screening. Chinese Journal of Chemistry, 2012, 30, 2752-2758.	4.9	2
150	Comparative pharmacophore modeling of human adenosine receptor A1 and A3 antagonists. Science China Chemistry, 2012, 55, 2407-2418.	8.2	2
151	Structural features of GABAA receptor antagonists: pharmacophore modeling and 3D-QSAR studies. Medicinal Chemistry Research, 2013, 22, 5961-5972.	2.4	2
152	Theoretical and NMR investigations on the conformations of (Ââ^'Â)-meptazinol hydrochloride in solution. Molecular Simulation, 2013, 39, 1065-1069.	2.0	2
153	Computational insights into the subtype selectivity and â€œmessage-address-efficacyâ€•mechanisms of opioid receptors through JDTic binding and unbinding. Acta Pharmacologica Sinica, 2018, 39, 482-491.	6.1	2
154	Design, synthesis and biological evaluation of novel indone derivatives as selective ERÎ² modulators. Medicinal Chemistry Research, 2019, 28, 1010-1026.	2.4	2
155	Insights into the molecular mechanisms of Huangqi decoction on liver fibrosis via computational systems pharmacology approaches. Chinese Medicine, 2021, 16, 59.	4.0	2
156	Insights into the antineoplastic mechanism of Chelidonium majus via systems pharmacology approach. Quantitative Biology, 2019, 7, 42-53.	0.5	1
157	Predicting Meridian in Chinese traditional medicine using machine learning approaches. , 2019, 15, e1007249.		0
158	Predicting Meridian in Chinese traditional medicine using machine learning approaches. , 2019, 15, e1007249.		0
159	Predicting Meridian in Chinese traditional medicine using machine learning approaches. , 2019, 15, e1007249.		0
160	Predicting Meridian in Chinese traditional medicine using machine learning approaches. , 2019, 15, e1007249.		0