Zengrui Wu

List of Publications by Year
in descending order

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50 papers	2,962 citations	394286 19 h-index	197736 49 g-index
53 all docs	53 docs citations	53 times ranked	3843 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.	2.5	1,439
2	In Silico Prediction of Chemical Acute Oral Toxicity Using Multi-Classification Methods. Journal of Chemical Information and Modeling, 2014, 54, 1061-1069.	2.5	140
3	Network-Based Methods for Prediction of Drug-Target Interactions. Frontiers in Pharmacology, 2018, 9, 1134.	1.6	131
4	Adverse Drug Events: Database Construction and in Silico Prediction. Journal of Chemical Information and Modeling, 2013, 53, 744-752.	2.5	116
5	In Silico Prediction of Bloodâ€“Brain Barrier Permeability of Compounds by Machine Learning and Resampling Methods. ChemMedChem, 2018, 13, 2189-2201.	1.6	111
6	SDTNBI: an integrated network and chemoinformatics tool for systematic prediction of drugâ€“target interactions and drug repositioning. Briefings in Bioinformatics, 2017, 18, bbw012.	3.2	102
7	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.	2.5	86
8	Network-based identification of microRNAs as potential pharmacogenomic biomarkers for anticancer drugs. Oncotarget, 2016, 7, 45584-45596.	0.8	85
9	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.	2.5	76
10	In silico prediction of chemical mechanism of action via an improved networkâ€based inference method. British Journal of Pharmacology, 2016, 173, 3372-3385.	2.7	73
11	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.	1.7	53
12	Computational prediction of microRNA networks incorporating environmental toxicity and disease etiology. Scientific Reports, 2014, 4, 5576.	1.6	51
13	In silico prediction of hERG potassium channel blockage by chemical category approaches. Toxicology Research, 2016, 5, 570-582.	0.9	50
14	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.	1.6	43
15	In Silico Estimation of Chemical Carcinogenicity with Binary and Ternary Classification Methods. Molecular Informatics, 2015, 34, 228-235.	1.4	42
16	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.	2.9	30
17	Quantitative and systems pharmacology 2. In silico polypharmacology of G protein-coupled receptor ligands via network-based approaches. Pharmacological Research, 2018, 129, 400-413.	3.1	28
18	Drug repositioning by prediction of drugâ€™s anatomical therapeutic chemical code via network-based inference approaches. Briefings in Bioinformatics, 2021, 22, 2058-2072.	3.2	25

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19	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.	2.5	23
20	In silico prediction of mitochondrial toxicity of chemicals using machine learning methods. Journal of Applied Toxicology, 2021, 41, 1518-1526.	1.4	23
21	Strategy for Efficient Discovery of Cocrystals via a Network-Based Recommendation Model. Crystal Growth and Design, 2020, 20, 6820-6830.	1.4	17
22	Prediction of Farnesoid X Receptor Disruptors with Machine Learning Methods. Chemical Research in Toxicology, 2018, 31, 1128-1137.	1.7	16
23	In Silico Prediction of Human Renal Clearance of Compounds Using Quantitative Structure-Pharmacokinetic Relationship Models. Chemical Research in Toxicology, 2020, 33, 640-650.	1.7	16
24	Development of Novel N-hydroxypyridone Derivatives as Potential Anti-Ischemic Stroke Agents. Journal of Medicinal Chemistry, 2020, 63, 1051-1067.	2.9	14
25	Insights into mechanisms and severity of drug-induced liver injury via computational systems toxicology approach. Toxicology Letters, 2019, 312, 22-33.	0.4	13
26	In silico prediction of chemical acute contact toxicity on honey bees via machine learning methods. Toxicology in Vitro, 2021, 72, 105089.	1.1	13
27	wSDTNBI: a novel network-based inference method for virtual screening. Chemical Science, 2022, 13, 1060-1079.	3.7	11
28	A multitask GNN-based interpretable model for discovery of selective JAK inhibitors. Journal of Cheminformatics, 2022, 14, 16.	2.8	10
29	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.	1.5	9
30	Computational Insights into Molecular Activation and Positive Cooperative Mechanisms of FFAR1 Modulators. Journal of Chemical Information and Modeling, 2020, 60, 3214-3230.	2.5	9
31	MetaADEDB 2.0: a comprehensive database on adverse drug events. Bioinformatics, 2021, 37, 2221-2222.	1.8	8
32	Insights into the mechanism of Arnebia euchroma on leukemia via network pharmacology approach. BMC Complementary Medicine and Therapies, 2020, 20, 322.	1.2	8
33	Insights into the Molecular Mechanisms of Liuwei Dihuang Decoction via Network Pharmacology. Chemical Research in Toxicology, 2021, 34, 91-102.	1.7	8
34	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.	2.5	8
35	MPSM-DTI: prediction of drugâ€“target interaction via machine learning based on the chemical structure and protein sequence. , 2022, 1, 115-126.		8
36	In silico prediction of potential drugâ€induced nephrotoxicity with machine learning methods. Journal of Applied Toxicology, 2022, 42, 1639-1650.	1.4	8

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37	Interactions of omeprazole-based analogues with cytochrome P450 2C19: a computational study. Molecular BioSystems, 2016, 12, 1913-1921.	2.9	7
38	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.	2.5	7
39	Prediction of the allergic mechanism of haptens via a reaction-substructure-compound-target-pathway network system. Toxicology Letters, 2019, 317, 68-81.	0.4	6
40	Computational Insight into the Allosteric Activation Mechanism of Farnesoid X Receptor. Journal of Chemical Information and Modeling, 2020, 60, 1540-1550.	2.5	5
41	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.	2.5	5
42	Development of a Multi-Target Strategy for the Treatment of Vitiligo via Machine Learning and Network Analysis Methods. Frontiers in Pharmacology, 2021, 12, 754175.	1.6	5
43	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.	2.5	5
44	ADENet: a novel network-based inference method for prediction of drug adverse events. Briefings in Bioinformatics, 2022, 23, .	3.2	4
45	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.	2.0	3
46	Assessment of CYP2C9 Structural Models for Site of Metabolism Prediction. ChemMedChem, 2021, 16, 1755-1764.	1.6	3
47	In Silico Prediction of Potential Drug Combinations for Type 2 Diabetes Mellitus by an Integrated Network and Transcriptome Analysis. ChemMedChem, 2022, 17, .	1.6	3
48	Drug Repurposing for Newly Emerged Diseases via Networkâ€based Inference on a Geneâ€diseaseâ€drug Network. Molecular Informatics, 2022, 41, .	1.4	3
49	Insights into the molecular mechanisms of Huangqi decoction on liver fibrosis via computational systems pharmacology approaches. Chinese Medicine, 2021, 16, 59.	1.6	2
50	Insights into the antineoplastic mechanism of Chelidonium majus via systems pharmacology approach. Quantitative Biology, 2019, 7, 42-53.	0.3	1