Zengrui Wu

List of Publications by Year
in descending order

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50 papers	2,962 citations	393982 19 h-index	197535 49 g-index
53 all docs	53 docs citations	53 times ranked	3843 citing authors

#	Article	IF	Citations
1	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
2	ADENet: a novel network-based inference method for prediction of drug adverse events. Briefings in Bioinformatics, 2022, 23, .	3.2	4
3	wSDTNBI: a novel network-based inference method for virtual screening. Chemical Science, 2022, 13, 1060-1079.	3.7	11
4	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
5	MPSM-DTI: prediction of drugâ€“target interaction via machine learning based on the chemical structure and protein sequence. , 2022, 1, 115-126.		8
6	A multitask GNN-based interpretable model for discovery of selective JAK inhibitors. Journal of Cheminformatics, 2022, 14, 16.	2.8	10
7	Drug Repurposing for Newly Emerged Diseases via Networkâ€based Inference on a Geneâ€diseaseâ€drug Network. Molecular Informatics, 2022, 41, .	1.4	3
8	In silico prediction of potential drugâ€induced nephrotoxicity with machine learning methods. Journal of Applied Toxicology, 2022, 42, 1639-1650.	1.4	8
9	MetaADEDB 2.0: a comprehensive database on adverse drug events. Bioinformatics, 2021, 37, 2221-2222.	1.8	8
10	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
11	Insights into the Molecular Mechanisms of Liuwei Dihuang Decoction via Network Pharmacology. Chemical Research in Toxicology, 2021, 34, 91-102.	1.7	8
12	In silico prediction of mitochondrial toxicity of chemicals using machine learning methods. Journal of Applied Toxicology, 2021, 41, 1518-1526.	1.4	23
13	Assessment of CYP2C9 Structural Models for Site of Metabolism Prediction. ChemMedChem, 2021, 16, 1755-1764.	1.6	3
14	In silico prediction of chemical acute contact toxicity on honey bees via machine learning methods. Toxicology in Vitro, 2021, 72, 105089.	1.1	13
15	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
16	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
17	Insights into the molecular mechanisms of Huangqi decoction on liver fibrosis via computational systems pharmacology approaches. Chinese Medicine, 2021, 16, 59.	1.6	2
18	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

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19	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
20	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
21	Development of Novel N-hydroxypyridone Derivatives as Potential Anti-Ischemic Stroke Agents. Journal of Medicinal Chemistry, 2020, 63, 1051-1067.	2.9	14
22	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
23	Insights into the mechanism of Arnebia euchroma on leukemia via network pharmacology approach. BMC Complementary Medicine and Therapies, 2020, 20, 322.	1.2	8
24	Strategy for Efficient Discovery of Cocrystals via a Network-Based Recommendation Model. Crystal Growth and Design, 2020, 20, 6820-6830.	1.4	17
25	Computational Insight into the Allosteric Activation Mechanism of Farnesoid X Receptor. Journal of Chemical Information and Modeling, 2020, 60, 1540-1550.	2.5	5
26	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
27	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
28	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
29	Insights into mechanisms and severity of drug-induced liver injury via computational systems toxicology approach. Toxicology Letters, 2019, 312, 22-33.	0.4	13
30	Insights into the antineoplastic mechanism of Chelidonium majus via systems pharmacology approach. Quantitative Biology, 2019, 7, 42-53.	0.3	1
31	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
32	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
33	Network-Based Methods for Prediction of Drug-Target Interactions. Frontiers in Pharmacology, 2018, 9, 1134.	1.6	131
34	Prediction of Farnesoid X Receptor Disruptors with Machine Learning Methods. Chemical Research in Toxicology, 2018, 31, 1128-1137.	1.7	16
35	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
36	In Silico Prediction of Bloodâ€“Brain Barrier Permeability of Compounds by Machine Learning and Resampling Methods. ChemMedChem, 2018, 13, 2189-2201.	1.6	111

#	Article	IF	Citations
37	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
38	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
39	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
40	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
41	Interactions of omeprazole-based analogues with cytochrome P450 2C19: a computational study. Molecular BioSystems, 2016, 12, 1913-1921.	2.9	7
42	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
43	In silico prediction of hERG potassium channel blockage by chemical category approaches. Toxicology Research, 2016, 5, 570-582.	0.9	50
44	Network-based identification of microRNAs as potential pharmacogenomic biomarkers for anticancer drugs. Oncotarget, 2016, 7, 45584-45596.	0.8	85
45	In Silico Estimation of Chemical Carcinogenicity with Binary and Ternary Classification Methods. Molecular Informatics, 2015, 34, 228-235.	1.4	42
46	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
47	Computational prediction of microRNA networks incorporating environmental toxicity and disease etiology. Scientific Reports, 2014, 4, 5576.	1.6	51
48	Adverse Drug Events: Database Construction and in Silico Prediction. Journal of Chemical Information and Modeling, 2013, 53, 744-752.	2.5	116
49	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
50	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