Mingyue Zheng

List of Publications by Year
in descending order

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174	5,873	87888 38	114465 63
papers	citations	h-index	g-index

190	190	190	7019
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Pushing the Boundaries of Molecular Representation for Drug Discovery with the Graph Attention Mechanism. Journal of Medicinal Chemistry, 2020, 63, 8749-8760.	6.4	402
2	In silicoADME/T modelling for rational drug design. Quarterly Reviews of Biophysics, 2015, 48, 488-515.	5.7	250
3	Preclinical characterization of anlotinib, a highly potent and selective vascular endothelial growth factor receptorâ€2 inhibitor. Cancer Science, 2018, 109, 1207-1219.	3.9	233
4	TransformerCPI: improving compoundâ€“protein interaction prediction by sequence-based deep learning with self-attention mechanism and label reversal experiments. Bioinformatics, 2020, 36, 4406-4414.	4.1	190
5	Artificial intelligence in drug design. Science China Life Sciences, 2018, 61, 1191-1204.	4.9	145
6	Optimization of metabolomic data processing using NOREVA. Nature Protocols, 2022, 17, 129-151.	12.0	114
7	Syntheses of triazole-modified zanamivir analogues via click chemistry and anti-AIV activities. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 5009-5013.	2.2	104
8	Astemizole Arrests the Proliferation of Cancer Cells by Disrupting the EZH2-EED Interaction of Polycomb Repressive Complex 2. Journal of Medicinal Chemistry, 2014, 57, 9512-9521.	6.4	96
9	Identifying Novel Selective Non-Nucleoside DNA Methyltransferase 1 Inhibitors through Docking-Based Virtual Screening. Journal of Medicinal Chemistry, 2014, 57, 9028-9041.	6.4	96
10	Regulating Glucose Metabolism with Prodrug Nanoparticles for Promoting Photoimmunotherapy of Pancreatic Cancer. Advanced Science, 2021, 8, 2002746.	11.2	96
11	Aspirin Inhibits Cancer Metastasis and Angiogenesis via Targeting Heparanase. Clinical Cancer Research, 2017, 23, 6267-6278.	7.0	94
12	Identification of Drug-Drug Interactions Using Chemical Interactions. Current Bioinformatics, 2017, 12, .	1.5	92
13	Discovery of Highly Potent, Selective, and Orally Efficacious p300/CBP Histone Acetyltransferases Inhibitors. Journal of Medicinal Chemistry, 2020, 63, 1337-1360.	6.4	85
14	Analysis and prediction of drugâ€“drug interaction by minimum redundancy maximum relevance and incremental feature selection. Journal of Biomolecular Structure and Dynamics, 2017, 35, 312-329.	3.5	81
15	Site of metabolism prediction for six biotransformations mediated by cytochromes P450. Bioinformatics, 2009, 25, 1251-1258.	4.1	72
16	Generative Models for De Novo Drug Design. Journal of Medicinal Chemistry, 2021, 64, 14011-14027.	6.4	72
17	Graph neural networks for automated de novo drug design. Drug Discovery Today, 2021, 26, 1382-1393.	6.4	71
18	Computational methods for drug design and discovery: focus on China. Trends in Pharmacological Sciences, 2013, 34, 549-559.	8.7	70

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19	Focused Combinatorial Library Design Based on Structural Diversity, Druglikeness and Binding Affinity Score. ACS Combinatorial Science, 2005, 7, 398-406.	3.3	69
20	Recent Advances in Neuraminidase Inhibitor Development as Antiâ€influenza Drugs. ChemMedChem, 2012, 7, 1527-1536.	3.2	62
21	Identification of compoundâ€“protein interactions through the analysis of gene ontology, KEGG enrichment for proteins and molecular fragments of compounds. Molecular Genetics and Genomics, 2016, 291, 2065-2079.	2.1	62
22	Molecular Basis of NDM-1, a New Antibiotic Resistance Determinant. PLoS ONE, 2011, 6, e23606.	2.5	62
23	Computational Screening for Active Compounds Targeting Protein Sequences: Methodology and Experimental Validation. Journal of Chemical Information and Modeling, 2011, 51, 2821-2828.	5.4	61
24	Novel thiophene derivatives as PTP1B inhibitors with selectivity and cellular activity. Bioorganic and Medicinal Chemistry, 2010, 18, 1773-1782.	3.0	59
25	Discovery and Optimization of Novel, Selective Histone Methyltransferase SET7 Inhibitors by Pharmacophore- and Docking-Based Virtual Screening. Journal of Medicinal Chemistry, 2015, 58, 8166-8181.	6.4	59
26	Deep Learning Enhancing Kinome-Wide Polypharmacology Profiling: Model Construction and Experiment Validation. Journal of Medicinal Chemistry, 2020, 63, 8723-8737.	6.4	58
27	Novel Bayesian classification models for predicting compounds blocking hERG potassium channels. Acta Pharmacologica Sinica, 2014, 35, 1093-1102.	6.1	53
28	TarPred: a web application for predicting therapeutic and side effect targets of chemical compounds. Bioinformatics, 2015, 31, 2049-2051.	4.1	52
29	Synthesis and antitumor evaluation of a novel series of triaminotriazine derivatives. Bioorganic and Medicinal Chemistry, 2007, 15, 1815-1827.	3.0	51
30	Graph neural network approaches for drug-target interactions. Current Opinion in Structural Biology, 2022, 73, 102327.	5.7	51
31	Structure-Based Design and Synthesis of C-1- and C-4-Modified Analogs of Zanamivir as Neuraminidase Inhibitors. Journal of Medicinal Chemistry, 2013, 56, 671-684.	6.4	50
32	Rapid and selective access to three distinct sets of indole-based heterocycles from a single set of Ugi-adducts under microwave heating. Chemical Communications, 2013, 49, 2894.	4.1	48
33	In Silicotarget fishing: addressing a â€œBig Dataâ€•problem by ligand-based similarity rankings with data fusion. Journal of Cheminformatics, 2014, 6, 33.	6.1	48
34	Discovering Potent Inhibitors Against the Î²-Hydroxyacyl-Acyl Carrier Protein Dehydratase (FabZ) of Helicobacter pylori: Structure-Based Design, Synthesis, Bioassay, and Crystal Structure Determination. Journal of Medicinal Chemistry, 2009, 52, 2465-2481.	6.4	46
35	Identification and synthesis of Nâ€²-(2-oxoindolin-3-ylidene)hydrazide derivatives against c-Met kinase. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 3749-3754.	2.2	45
36	SNX10 (sorting nexin 10) inhibits colorectal cancer initiation and progression by controlling autophagic degradation of SRC. Autophagy, 2020, 16, 735-749.	9.1	43

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37	Catalytic Mechanism Investigation of Lysine-Specific Demethylase 1 (LSD1): A Computational Study. PLoS ONE, 2011, 6, e25444.	2.5	42
38	AST1306, A Novel Irreversible Inhibitor of the Epidermal Growth Factor Receptor 1 and 2, Exhibits Antitumor Activity Both In Vitro and In Vivo. PLoS ONE, 2011, 6, e21487.	2.5	40
39	Machine-Learning-Assisted Approach for Discovering Novel Inhibitors Targeting Bromodomain-Containing Protein 4. Journal of Chemical Information and Modeling, 2017, 57, 1677-1690.	5.4	40
40	An effective docking strategy for virtual screening based on multi-objective optimization algorithm. BMC Bioinformatics, 2009, 10, 58.	2.6	39
41	Computational chemical biology and drug design: Facilitating protein structure, function, and modulation studies. Medicinal Research Reviews, 2018, 38, 914-950.	10.5	38
42	Mechanism of the All-Î± to All-Î² Conformational Transition of RfaH-CTD: Molecular Dynamics Simulation and Markov State Model. Journal of Chemical Theory and Computation, 2014, 10, 2255-2264.	5.3	37
43	Cytoplasmic DNA sensing by KU complex in aged CD4+ TÂcell potentiates TÂcell activation and aging-related autoimmune inflammation. Immunity, 2021, 54, 632-647.e9.	14.3	37
44	Toward understanding the molecular basis for chemical allosteric modulator design. Journal of Molecular Graphics and Modelling, 2012, 38, 324-333.	2.4	36
45	A quantum mechanics/molecular mechanics study on the hydrolysis mechanism of New Delhi metallo-Î²-lactamase-1. Journal of Computer-Aided Molecular Design, 2013, 27, 247-256.	2.9	36
46	Discovery of the First-in-Class Agonist-Based SOS1 PROTACs Effective in Human Cancer Cells Harboring Various KRAS Mutations. Journal of Medicinal Chemistry, 2022, 65, 3923-3942.	6.4	36
47	Aldehyde Oxidase Mediated Metabolism in Drug-like Molecules: A Combined Computational and Experimental Study. Journal of Medicinal Chemistry, 2017, 60, 2973-2982.	6.4	34
48	Discovery of novel BET inhibitors by drug repurposing of nitroxoline and its analogues. Organic and Biomolecular Chemistry, 2017, 15, 9352-9361.	2.8	34
49	Improving the Virtual Screening Ability of Target-Specific Scoring Functions Using Deep Learning Methods. Frontiers in Pharmacology, 2019, 10, 924.	3.5	34
50	Knowledge-Based Scoring Functions in Drug Design. 1. Developing a Target-Specific Method for Kinaseâ^'Ligand Interactions. Journal of Chemical Information and Modeling, 2010, 50, 1378-1386.	5.4	33
51	Non-Covalent Interactions with Aromatic Rings: Current Understanding and Implications for Rational Drug Design. Current Pharmaceutical Design, 2013, 19, 6522-6533.	1.9	33
52	Using support vector regression coupled with the genetic algorithm for predicting acute toxicity to the fathead minnow. SAR and QSAR in Environmental Research, 2010, 21, 559-570.	2.2	32
53	Sorting Nexin 10 Mediates Metabolic Reprogramming of Macrophages in Atherosclerosis Through the Lyn-Dependent TFEB Signaling Pathway. Circulation Research, 2020, 127, 534-549.	4.5	32
54	Diversified strategy for the synthesis of DNA-encoded oxindole libraries. Chemical Science, 2021, 12, 2841-2847.	7.4	32

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55	Knowledge-Based Scoring Functions in Drug Design: 2. Can the Knowledge Base Be Enriched?. Journal of Chemical Information and Modeling, 2011, 51, 386-397.	5.4	31
56	Discovery of Pyrazolo[3,4-d]pyridazinone Derivatives as Selective DDR1 Inhibitors via Deep Learning Based Design, Synthesis, and Biological Evaluation. Journal of Medicinal Chemistry, 2022, 65, 103-119.	6.4	31
57	Identification of pentacyclic triterpenes derivatives as potent inhibitors against glycogen phosphorylase based on 3D-QSAR studies. European Journal of Medicinal Chemistry, 2011, 46, 2011-2021.	5.5	30
58	Rapid Generation of Privileged Substructure-Based Compound Libraries with Structural Diversity and Drug-Likeness. ACS Combinatorial Science, 2014, 16, 184-191.	3.8	30
59	Estimation of acute oral toxicity in rat using local lazy learning. Journal of Cheminformatics, 2014, 6, 26.	6.1	30
60	Applying high-performance computing in drug discovery and molecular simulation. National Science Review, 2016, 3, 49-63.	9.5	30
61	Identification of new candidate drugs for lung cancer using chemicalâ€“chemical interactions, chemicalâ€“protein interactions and a K-means clustering algorithm. Journal of Biomolecular Structure and Dynamics, 2016, 34, 906-917.	3.5	30
62	Indole derivatives as potent inhibitors of 5-lipoxygenase: Design, synthesis, biological evaluation, and molecular modeling. Bioorganic and Medicinal Chemistry Letters, 2007, 17, 2414-2420.	2.2	29
63	Prediction of Effective Drug Combinations by Chemical Interaction, Protein Interaction and Target Enrichment of KEGG Pathways. BioMed Research International, 2013, 2013, 1-10.	1.9	29
64	Cholesterolâ€î²₁AR interaction versus cholesterolâ€î²₂AR interaction. Proteins: Structure, Function and Bioinformatics, 2014, 82, 760-770.	2.6	29
65	In silico site of metabolism prediction for human UGT-catalyzed reactions. Bioinformatics, 2014, 30, 398-405.	4.1	29
66	Mutagenic probability estimation of chemical compounds by a novel molecular electrophilicity vector and support vector machine. Bioinformatics, 2006, 22, 2099-2106.	4.1	28
67	Design, Synthesis, and Pharmacological Evaluation of Monocyclic Pyrimidinones as Novel Inhibitors of PDE5. Journal of Medicinal Chemistry, 2012, 55, 10540-10550.	6.4	28
68	Catalytic Mechanism of Histone Acetyltransferase p300: From the Proton Transfer to Acetylation Reaction. Journal of Physical Chemistry B, 2014, 118, 2009-2019.	2.6	28
69	Identification of novel candidate drivers connecting different dysfunctional levels for lung adenocarcinoma using protein-protein interactions and a shortest path approach. Scientific Reports, 2016, 6, 29849.	3.3	28
70	Discovery and optimization of selective inhibitors of protein arginine methyltransferase 5 by docking-based virtual screening. Organic and Biomolecular Chemistry, 2017, 15, 3648-3661.	2.8	28
71	Discovery and Development of a Series of Pyrazolo[3,4-d]pyridazinone Compounds as the Novel Covalent Fibroblast Growth Factor Receptor Inhibitors by the Rational Drug Design. Journal of Medicinal Chemistry, 2019, 62, 7473-7488.	6.4	28
72	Ligand-Promoted Alkynylation of Aryl Ketones: A Practical Tool for Structural Diversity in Drugs and Natural Products. ACS Catalysis, 2021, 11, 1758-1764.	11.2	28

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73	(+)-Rutamarin as a Dual Inducer of Both GLUT4 Translocation and Expression Efficiently Ameliorates Glucose Homeostasis in Insulin-Resistant Mice. PLoS ONE, 2012, 7, e31811.	2.5	28
74	Virtual screening and biological evaluation of novel small molecular inhibitors against protein arginine methyltransferase 1 (PRMT1). Organic and Biomolecular Chemistry, 2014, 12, 9665-9673.	2.8	27
75	Estimation of elimination half-lives of organic chemicals in humans using gradient boosting machine. Biochimica Et Biophysica Acta - General Subjects, 2016, 1860, 2664-2671.	2.4	27
76	Identification of Novel Disruptor of Telomeric Silencing 1-like (DOT1L) Inhibitors through Structure-Based Virtual Screening and Biological Assays. Journal of Chemical Information and Modeling, 2016, 56, 527-534.	5.4	27
77	Combinatorial Pharmacophore-Based 3D-QSAR Analysis and Virtual Screening of FGFR1 Inhibitors. International Journal of Molecular Sciences, 2015, 16, 13407-13426.	4.1	26
78	Water PMF for predicting the properties of water molecules in protein binding site. Journal of Computational Chemistry, 2013, 34, 583-592.	3.3	25
79	Predicting Chemical Toxicity Effects Based on Chemical-Chemical Interactions. PLoS ONE, 2013, 8, e56517.	2.5	25
80	Automated design and optimization of multitarget schizophrenia drug candidates by deep learning. European Journal of Medicinal Chemistry, 2020, 204, 112572.	5.5	25
81	Drug repurposing against breast cancer by integrating drug-exposure expression profiles and drugâ€“drug links based on graph neural network. Bioinformatics, 2021, 37, 2930-2937.	4.1	25
82	KinomeX: a web application for predicting kinome-wide polypharmacology effect of small molecules. Bioinformatics, 2019, 35, 5354-5356.	4.1	24
83	Essential structural profile of a dual functional inhibitor against cyclooxygenase-2 (COX-2) and 5-lipoxygenase (5-LOX): Molecular docking and 3D-QSAR analyses on DHDMBF analogues. Bioorganic and Medicinal Chemistry, 2006, 14, 3428-3437.	3.0	23
84	Predicting Drugs Side Effects Based on Chemical-Chemical Interactions and Protein-Chemical Interactions. BioMed Research International, 2013, 2013, 1-8.	1.9	23
85	A Genetic Algorithm Based Support Vector Machine Model for Blood-Brain Barrier Penetration Prediction. BioMed Research International, 2015, 2015, 1-13.	1.9	23
86	DrugSpaceX: a large screenable and synthetically tractable database extending drug space. Nucleic Acids Research, 2021, 49, D1170-D1178.	14.5	23
87	Unbinding Pathways of GW4064 from Human Farnesoid X Receptor As Revealed by Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2012, 52, 3043-3052.	5.4	22
88	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
89	Discovery of a new series of imidazo[1,2-a]pyridine compounds as selective c-Met inhibitors. Acta Pharmacologica Sinica, 2016, 37, 698-707.	6.1	22
90	Discovery of Novel Inhibitors Targeting the Menin-Mixed Lineage Leukemia Interface Using Pharmacophore- and Docking-Based Virtual Screening. Journal of Chemical Information and Modeling, 2016, 56, 1847-1855.	5.4	22

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91	Discovery of Novel Disruptor of Silencing Telomeric 1-Like (DOT1L) Inhibitors using a Target-Specific Scoring Function for the (S)-Adenosyl-<scp>l</scp>-methionine (SAM)-Dependent Methyltransferase Family. Journal of Medicinal Chemistry, 2017, 60, 2026-2036.	6.4	22
92	SNX10â€mediated LPS sensing causes intestinal barrier dysfunction via a caspaseâ€5â€dependent signaling cascade. EMBO Journal, 2021, 40, e108080.	7.8	22
93	QSAR analyses on avian influenza virus neuraminidase inhibitors using CoMFA, CoMSIA, and HQSAR. Journal of Computer-Aided Molecular Design, 2006, 20, 549-566.	2.9	21
94	Combinatorial Pharmacophore Modeling of Organic Cation Transporter 2 (OCT2) Inhibitors: Insights into Multiple Inhibitory Mechanisms. Molecular Pharmaceutics, 2013, 10, 4611-4619.	4.6	21
95	Characterizing the binding of annexin V to a lipid bilayer using molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2014, 82, 312-322.	2.6	21
96	Discovery of Novel Inhibitors of Indoleamine 2,3-Dioxygenase 1 Through Structure-Based Virtual Screening. Frontiers in Pharmacology, 2018, 9, 277.	3.5	21
97	Optimizing chemical reaction conditions using deep learning: a case study for the Suzukiâ€“Miyaura cross-coupling reaction. Organic Chemistry Frontiers, 2020, 7, 2269-2277.	4.5	21
98	Development of a novel class of B-RafV600E-selective inhibitors through virtual screening and hierarchical hit optimization. Organic and Biomolecular Chemistry, 2012, 10, 7402.	2.8	20
99	An integrated drug-likeness study for bicyclic privileged structures: from physicochemical properties to in vitro ADME properties. Molecular Diversity, 2011, 15, 857-876.	3.9	19
100	Design, Synthesis, and Pharmacological Evaluation of Novel Multisubstituted Pyridin-3-amine Derivatives as Multitargeted Protein Kinase Inhibitors for the Treatment of Non-Small Cell Lung Cancer. Journal of Medicinal Chemistry, 2017, 60, 6018-6035.	6.4	19
101	Investigation of the remote acyl group participation in glycosylation from conformational perspectives by using trichloroacetimidate as the acetyl surrogate. Organic Chemistry Frontiers, 2020, 7, 1606-1615.	4.5	19
102	Multi-instance learning of graph neural networks for aqueous pKa prediction. Bioinformatics, 2022, 38, 792-798.	4.1	19
103	3D-QSAR study of 20 (S)-camptothecin analogs. Acta Pharmacologica Sinica, 2007, 28, 307-314.	6.1	18
104	Metabolomics Analysis of L-Arginine Induced Gastrointestinal Motility Disorder in Rats Using UPLC-MS After Magnolol Treatment. Frontiers in Pharmacology, 2019, 10, 183.	3.5	18
105	A hybrid framework for improving uncertainty quantification in deep learning-based QSAR regression modeling. Journal of Cheminformatics, 2021, 13, 69.	6.1	18
106	Drug target inference by mining transcriptional data using a novel graph convolutional network framework. Protein and Cell, 2022, 13, 281-301.	11.0	18
107	Knowledge-Based Scoring Functions in Drug Design: 3. A Two-Dimensional Knowledge-Based Hydrogen-Bonding Potential for the Prediction of Proteinâ€“Ligand Interactions. Journal of Chemical Information and Modeling, 2011, 51, 2994-3004.	5.4	17
108	Identifying Chemicals with Potential Therapy of HIV Based on Protein-Protein and Protein-Chemical Interaction Network. PLoS ONE, 2013, 8, e65207.	2.5	17

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109	Design, synthesis and biological evaluation of isoquinoline-based derivatives as novel histone deacetylase inhibitors. Bioorganic and Medicinal Chemistry, 2015, 23, 5881-5890.	3.0	17
110	Discovery of novel glyceraldehyde-3-phosphate dehydrogenase inhibitor via docking-based virtual screening. Bioorganic Chemistry, 2020, 96, 103620.	4.1	17
111	Facing small and biased data dilemma in drug discovery with enhanced federated learning approaches. Science China Life Sciences, 2022, 65, 529-539.	4.9	17
112	Design, synthesis and biological evaluation of pyrazolo[3,4-d]pyridazinone derivatives as covalent FGFR inhibitors. Acta Pharmaceutica Sinica B, 2021, 11, 781-794.	12.0	16
113	Estimation of Carcinogenicity Using Molecular Fragments Tree. Journal of Chemical Information and Modeling, 2012, 52, 1994-2003.	5.4	15
114	Combinatorial Pharmacophore Modeling of Multidrug and Toxin Extrusion Transporter 1 Inhibitors: a Theoretical Perspective for Understanding Multiple Inhibitory Mechanisms. Scientific Reports, 2015, 5, 13684.	3.3	15
115	Structure-Based Virtual Screening and Identification of Potential Inhibitors of SARS-CoV-2 S-RBD and ACE2 Interaction. Frontiers in Chemistry, 2021, 9, 740702.	3.6	15
116	Towards discovering dual functional inhibitors against both wild type and K103N mutant HIV-1 reverse transcriptases: molecular docking and QSAR studies on 4,1-benzoxazepinone analogues. Journal of Computer-Aided Molecular Design, 2006, 20, 281-293.	2.9	14
117	Selective Synthesis of 5,6â€Ðihydroindolo[1,2â€a]quinoxalines and 6,7â€Ðihydroindolo[2,3â€c]quinolines by Orthogonal Copper and Palladium Catalysis. European Journal of Organic Chemistry, 2013, 2013, 5710-5715.	2.4	14
118	Prediction of Cancer Drugs by Chemical-Chemical Interactions. PLoS ONE, 2014, 9, e87791.	2.5	14
119	Metadynamics Simulation Study on the Conformational Transformation of HhaI Methyltransferase: An Induced-Fit Base-Flipping Hypothesis. BioMed Research International, 2014, 2014, 1-13.	1.9	14
120	Machine Learning-Based Modeling of Drug Toxicity. Methods in Molecular Biology, 2018, 1754, 247-264.	0.9	14
121	Discovery of novel trimethoxy-ring BRD4 bromodomain inhibitors: AlphaScreen assay, crystallography and cell-based assay. MedChemComm, 2017, 8, 1322-1331.	3.4	13
122	Rational design of 5-((1H-imidazol-1-yl)methyl)quinolin-8-ol derivatives as novel bromodomain-containing protein 4 inhibitors. European Journal of Medicinal Chemistry, 2019, 163, 281-294.	5.5	13
123	Solution-Phase DNA-Compatible Pictet-Spengler Reaction Aided by Machine Learning Building Block Filtering. IScience, 2020, 23, 101142.	4.1	13
124	Identification of Novel Small Molecules as Inhibitors of Hepatitis C Virus by Structure-Based Virtual Screening. International Journal of Molecular Sciences, 2013, 14, 22845-22856.	4.1	12
125	Anthraquinone Derivatives as Potent Inhibitors of c-Met Kinase and the Extracellular Signaling Pathway. ACS Medicinal Chemistry Letters, 2013, 4, 408-413.	2.8	12
126	Characterization of covalent binding of tyrosine kinase inhibitors to plasma proteins. Drug Metabolism and Pharmacokinetics, 2020, 35, 456-465.	2.2	12

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127	Active Learning for Drug Design: A Case Study on the Plasma Exposure of Orally Administered Drugs. Journal of Medicinal Chemistry, 2021, 64, 16838-16853.	6.4	12
128	Structural optimization and biological evaluation of 1,5-disubstituted pyrazole-3-carboxamines as potent inhibitors of human 5-lipoxygenase. Acta Pharmaceutica Sinica B, 2016, 6, 32-45.	12.0	11
129	Wedelolactone metabolism in rats through regioselective glucuronidation catalyzed by uridine diphosphate-glucuronosyltransferases 1As (UGT1As). Phytomedicine, 2016, 23, 340-349.	5.3	11
130	Bloodâ€“brain barrier penetration prediction enhanced by uncertainty estimation. Journal of Cheminformatics, 2022, 14, .	6.1	11
131	Dynamic Mechanism of Fatty Acid Transport across Cellular Membranes through FadL: Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2008, 112, 13070-13078.	2.6	10
132	Fragment-based prediction of skin sensitization using recursive partitioning. Journal of Computer-Aided Molecular Design, 2011, 25, 885-893.	2.9	10
133	Development and evaluation of a novel series of Nitroxoline-derived BET inhibitors with antitumor activity in renal cell carcinoma. Oncogenesis, 2018, 7, 83.	4.9	10
134	Deep Neural Network Classifier for Virtual Screening Inhibitors of (S)-Adenosyl-L-Methionine (SAM)-Dependent Methyltransferase Family. Frontiers in Chemistry, 2019, 7, 324.	3.6	10
135	Revisiting Aldehyde Oxidase Mediated Metabolism in Drug-like Molecules: An Improved Computational Model. Journal of Medicinal Chemistry, 2020, 63, 6523-6537.	6.4	10
136	In Silico Prediction of Cytochrome P450-Mediated Site of Metabolism (SOM). Protein and Peptide Letters, 2013, 20, 279-289.	0.9	10
137	Interaction Between DNA/histone Methyltransferases and their Inhibitors. Current Medicinal Chemistry, 2014, 22, 360-372.	2.4	10
138	In Silico Prediction of Chemical Toxicity Profile Using Local Lazy Learning. Combinatorial Chemistry and High Throughput Screening, 2017, 20, 346-353.	1.1	10
139	New <scp>Cembraneâ€Type</scp> Diterpenoids from the South China Sea Soft Coral Sinularia nanolobata. Chinese Journal of Chemistry, 2022, 40, 28-38.	4.9	10
140	Dynamic monitoring of Î²-cell injury with impedance and rescue by glucagon-like peptide-1. Analytical Biochemistry, 2012, 423, 61-69.	2.4	9
141	Enantioselective drugâ€“protein interaction between mexiletine and plasma protein. Journal of Pharmacy and Pharmacology, 2012, 64, 792-801.	2.4	9
142	Binding sensitivity of adefovir to the polymerase from different genotypes of HBV: molecular modeling, docking and dynamics simulation studies. Acta Pharmacologica Sinica, 2013, 34, 319-328.	6.1	9
143	Discovery of novel BRD4 inhibitors by high-throughput screening, crystallography, and cell-based assays. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 2003-2009.	2.2	9
144	Conformation and dynamics of the C-terminal region in human phosphoglycerate mutase 1. Acta Pharmacologica Sinica, 2017, 38, 1673-1682.	6.1	9

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145	The Use of Chemical-Chemical Interaction and Chemical Structure to Identify New Candidate Chemicals Related to Lung Cancer. PLoS ONE, 2015, 10, e0128696.	2.5	9
146	An inductive graph neural network model for compoundâ€“protein interaction prediction based on a homogeneous graph. Briefings in Bioinformatics, 2022, 23, .	6.5	9
147	Computational Models for Predicting Interactions with Membrane Transporters. Current Medicinal Chemistry, 2013, 20, 2118-2136.	2.4	8
148	Repair of methyl lesions in RNA by oxidative demethylation. MedChemComm, 2014, 5, 1797-1803.	3.4	7
149	Crowdsourced identification of multi-target kinase inhibitors for RET- and TAU- based disease: The Multi-Targeting Drug DREAM Challenge. PLoS Computational Biology, 2021, 17, e1009302.	3.2	7
150	A Triad of Lys12, Lys41, Arg78 Spatial Domain, a Novel Identified Heparin Binding Site on Tat Protein, Facilitates Tat-Driven Cell Adhesion. PLoS ONE, 2008, 3, e2662.	2.5	7
151	Hydrolytic Metabolism of Cyanopyrrolidine DPP-4 Inhibitors Mediated by Dipeptidyl Peptidases. Drug Metabolism and Disposition, 2019, 47, 238-248.	3.3	6
152	Discovery and characterization of natural products as novel indoleamine 2,3-dioxygenase 1 inhibitors through high-throughput screening. Acta Pharmacologica Sinica, 2020, 41, 423-431.	6.1	6
153	Pharmacologic characterization of SHR8443, a novel dual inhibitor of phosphatidylinositol 3-kinase and mammalian target of rapamycin. Oncotarget, 2017, 8, 107977-107990.	1.8	6
154	Discovery of triazoloquinoxaline as novel STING agonists via structure-based virtual screening. Bioorganic Chemistry, 2020, 100, 103958.	4.1	6
155	RD-Metabolizer: an integrated and reaction types extensive approach to predict metabolic sites and metabolites of drug-like molecules. Chemistry Central Journal, 2017, 11, 65.	2.6	5
156	Discovery of a potent, selective, and covalent ZAP-70 kinase inhibitor. European Journal of Medicinal Chemistry, 2021, 219, 113393.	5.5	5
157	Discovery of ARF1-targeting inhibitor demethylzeylasteral as a potential agent against breast cancer. Acta Pharmaceutica Sinica B, 2022, 12, 2619-2622.	12.0	5
158	Predicting Hepatotoxicity of Drug Metabolites Via an Ensemble Approach Based on Support Vector Machine. Combinatorial Chemistry and High Throughput Screening, 2018, 20, 839-849.	1.1	4
159	AutoGGN: A gene graph network AutoML tool for multi-omics research. Artificial Intelligence in the Life Sciences, 2021, 1, 100019.	2.2	4
160	Prediction of Drug Indications Based on Chemical Interactions and Chemical Similarities. BioMed Research International, 2015, 2015, 1-14.	1.9	3
161	Targeting sorting nexin 10 improves mouse colitis via inhibiting PIKfyve-mediated TBK1/c-Rel signaling activation. Pharmacological Research, 2021, 169, 105679.	7.1	3
162	Current status of active learning for drug discovery. Artificial Intelligence in the Life Sciences, 2021, 1, 100023.	2.2	3

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