Ting-Jun Hou

List of Publications by Year
in descending order

373	23,519	9234	12233
papers	citations	74 h-index	133 g-index

383	383	383	20225
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Assessing the Performance of the MM/PBSA and MM/GBSA Methods. 1. The Accuracy of Binding Free Energy Calculations Based on Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2011, 51, 69-82.	2.5	2,005
2	End-Point Binding Free Energy Calculation with MM/PBSA and MM/GBSA: Strategies and Applications in Drug Design. Chemical Reviews, 2019, 119, 9478-9508.	23.0	1,064
3	ADMETlab 2.0: an integrated online platform for accurate and comprehensive predictions of ADMET properties. Nucleic Acids Research, 2021, 49, W5-W14.	6.5	915
4	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
5	Assessing the performance of the molecular mechanics/Poisson Boltzmann surface area and molecular mechanics/generalized Born surface area methods. II. The accuracy of ranking poses generated from docking. Journal of Computational Chemistry, 2011, 32, 866-877.	1.5	615
6	Assessing the performance of MM/PBSA and MM/GBSA methods. 4. Accuracies of MM/PBSA and MM/GBSA methodologies evaluated by various simulation protocols using PDBbind data set. Physical Chemistry Chemical Physics, 2014, 16, 16719-16729.	1.3	586
7	Assessing the performance of MM/PBSA and MM/GBSA methods. 5. Improved docking performance using high solute dielectric constant MM/GBSA and MM/PBSA rescoring. Physical Chemistry Chemical Physics, 2014, 16, 22035-22045.	1.3	432
8	Assessing the Performance of MM/PBSA and MM/GBSA Methods. 3. The Impact of Force Fields and Ligand Charge Models. Journal of Physical Chemistry B, 2013, 117, 8408-8421.	1.2	419
9	Assessing the performance of the MM/PBSA and MM/GBSA methods. 6. Capability to predict proteinâ€“protein binding free energies and re-rank binding poses generated by proteinâ€“protein docking. Physical Chemistry Chemical Physics, 2016, 18, 22129-22139.	1.3	350
10	HawkDock: a web server to predict and analyze the proteinâ€“protein complex based on computational docking and MM/GBSA. Nucleic Acids Research, 2019, 47, W322-W330.	6.5	329
11	The application of in silico drug-likeness predictions in pharmaceutical research. Advanced Drug Delivery Reviews, 2015, 86, 2-10.	6.6	306
12	Recent Advances in Free Energy Calculations with a Combination of Molecular Mechanics and Continuum Models. Current Computer-Aided Drug Design, 2006, 2, 287-306.	0.8	300
13	Molecular Dynamics and Free Energy Studies on the Wild-type and Double Mutant HIV-1 Protease Complexed with Amprenavir and Two Amprenavir-Related Inhibitors:â€‰ Mechanism for Binding and Drug Resistance. Journal of Medicinal Chemistry, 2007, 50, 1177-1188.	2.9	251
14	Janus Structures of Transition Metal Dichalcogenides as the Heterojunction Photocatalysts for Water Splitting. Journal of Physical Chemistry C, 2018, 122, 3123-3129.	1.5	246
15	Assessing the performance of MM/PBSA and MM/GBSA methods. 7. Entropy effects on the performance of end-point binding free energy calculation approaches. Physical Chemistry Chemical Physics, 2018, 20, 14450-14460.	1.3	243
16	Could graph neural networks learn better molecular representation for drug discovery? A comparison study of descriptor-based and graph-based models. Journal of Cheminformatics, 2021, 13, 12.	2.8	214
17	ADME Evaluation in Drug Discovery. 4. Prediction of Aqueous Solubility Based on Atom Contribution Approach. Journal of Chemical Information and Computer Sciences, 2004, 44, 266-275.	2.8	213
18	Characterization of Domainâ€“Peptide Interaction Interface: A Case Study on the Amphiphysin-1 SH3 Domain. Journal of Molecular Biology, 2008, 376, 1201-1214.	2.0	194

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19	Characterization of Domainâ€“Peptide Interaction Interface: Prediction of SH3 Domain-Mediated Proteinâ€“Protein Interaction Network in Yeast by Generic Structure-Based Models. Journal of Proteome Research, 2012, 11, 2982-2995.	1.8	194
20	Recent Development and Application of Virtual Screening in Drug Discovery: An Overview. Current Pharmaceutical Design, 2004, 10, 1011-1033.	0.9	185
21	ADME Evaluation in Drug Discovery. 7. Prediction of Oral Absorption by Correlation and Classification. Journal of Chemical Information and Modeling, 2007, 47, 208-218.	2.5	171
22	Recent Advances in Computational Prediction of Drug Absorption and Permeability in Drug Discovery. Current Medicinal Chemistry, 2006, 13, 2653-2667.	1.2	167
23	ADME Evaluation in Drug Discovery. 5. Correlation of Caco-2 Permeation with Simple Molecular Properties. Journal of Chemical Information and Computer Sciences, 2004, 44, 1585-1600.	2.8	157
24	ADME Evaluation in Drug Discovery. 6. Can Oral Bioavailability in Humans Be Effectively Predicted by Simple Molecular Property-Based Rules?. Journal of Chemical Information and Modeling, 2007, 47, 460-463.	2.5	155
25	Allosite: a method for predicting allosteric sites. Bioinformatics, 2013, 29, 2357-2359.	1.8	153
26	ADME Evaluation in Drug Discovery. 10. Predictions of P-Glycoprotein Inhibitors Using Recursive Partitioning and Naive Bayesian Classification Techniques. Molecular Pharmaceutics, 2011, 8, 889-900.	2.3	148
27	Computational Analysis and Prediction of the Binding Motif and Protein Interacting Partners of the Abl SH3 Domain. PLoS Computational Biology, 2006, 2, e1.	1.5	145
28	From machine learning to deep learning: Advances in scoring functions for proteinâ€“ligand docking. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1429.	6.2	142
29	Development of Polarizable Models for Molecular Mechanical Calculations I: Parameterization of Atomic Polarizability. Journal of Physical Chemistry B, 2011, 115, 3091-3099.	1.2	137
30	ADMET Evaluation in Drug Discovery. 12. Development of Binary Classification Models for Prediction of hERG Potassium Channel Blockage. Molecular Pharmaceutics, 2012, 9, 996-1010.	2.3	137
31	Application of molecular dynamics simulations in molecular property prediction II: Diffusion coefficient. Journal of Computational Chemistry, 2011, 32, 3505-3519.	1.5	135
32	Potential Application of Novel Boron-Doped Graphene Nanoribbon as Oxygen Reduction Reaction Catalyst. Journal of Physical Chemistry C, 2016, 120, 17427-17434.	1.5	131
33	PROTAC-DB: an online database of PROTACs. Nucleic Acids Research, 2021, 49, D1381-D1387.	6.5	127
34	Two-dimensional germanium monochalcogenide photocatalyst for water splitting under ultraviolet, visible to near-infrared light. Nanoscale, 2017, 9, 8608-8615.	2.8	124
35	Atomistic Origins of Surface Defects in CH₃NH₃PbBr₃ Perovskite and Their Electronic Structures. ACS Nano, 2017, 11, 2060-2065.	7.3	123
36	Computational models for predicting substrates or inhibitors of P-glycoprotein. Drug Discovery Today, 2012, 17, 343-351.	3.2	122

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37	Structure â€“ ADME relationship: still a long way to go?. Expert Opinion on Drug Metabolism and Toxicology, 2008, 4, 759-770.	1.5	120
38	ADME evaluation in drug discovery. Journal of Molecular Modeling, 2002, 8, 337-349.	0.8	116
39	ADME Evaluation in Drug Discovery. 8. The Prediction of Human Intestinal Absorption by a Support Vector Machine. Journal of Chemical Information and Modeling, 2007, 47, 2408-2415.	2.5	114
40	ADME Evaluation in Drug Discovery. 9. Prediction of Oral Bioavailability in Humans Based on Molecular Properties and Structural Fingerprints. Molecular Pharmaceutics, 2011, 8, 841-851.	2.3	114
41	Application of Molecular Dynamics Simulations in Molecular Property Prediction. 1. Density and Heat of Vaporization. Journal of Chemical Theory and Computation, 2011, 7, 2151-2165.	2.3	114
42	CaFE: a tool for binding affinity prediction using end-point free energy methods. Bioinformatics, 2016, 32, 2216-2218.	1.8	114
43	ADME Evaluation in Drug Discovery. 3. Modeling Blood-Brain Barrier Partitioning Using Simple Molecular Descriptors. Journal of Chemical Information and Computer Sciences, 2003, 43, 2137-2152.	2.8	113
44	Evaluating the potency of HIVâ€1 protease drugs to combat resistance. Proteins: Structure, Function and Bioinformatics, 2008, 71, 1163-1174.	1.5	110
45	Development of Reliable Aqueous Solubility Models and Their Application in Druglike Analysis. Journal of Chemical Information and Modeling, 2007, 47, 1395-1404.	2.5	103
46	Recent Advances on Aqueous Solubility Prediction. Combinatorial Chemistry and High Throughput Screening, 2011, 14, 328-338.	0.6	102
47	ADMET evaluation in drug discovery: 15. Accurate prediction of rat oral acute toxicity using relevance vector machine and consensus modeling. Journal of Cheminformatics, 2016, 8, 6.	2.8	102
48	Develop and Test a Solvent Accessible Surface Area-Based Model in Conformational Entropy Calculations. Journal of Chemical Information and Modeling, 2012, 52, 1199-1212.	2.5	99
49	Two-Dimensional MnO₂ as a Better Cathode Material for Lithium Ion Batteries. Journal of Physical Chemistry C, 2015, 119, 28783-28788.	1.5	98
50	Characterization of Domain-Peptide Interaction Interface. Molecular and Cellular Proteomics, 2009, 8, 639-649.	2.5	96
51	Drug and Drug Candidate Building Block Analysis. Journal of Chemical Information and Modeling, 2010, 50, 55-67.	2.5	96
52	Drug-likeness Analysis of Traditional Chinese Medicines: Prediction of Drug-likeness Using Machine Learning Approaches. Molecular Pharmaceutics, 2012, 9, 2875-2886.	2.3	96
53	ADMET Evaluation in Drug Discovery. 13. Development of in Silico Prediction Models for P-Glycoprotein Substrates. Molecular Pharmaceutics, 2014, 11, 716-726.	2.3	96
54	Assessing an Ensemble Docking-Based Virtual Screening Strategy for Kinase Targets by Considering Protein Flexibility. Journal of Chemical Information and Modeling, 2014, 54, 2664-2679.	2.5	96

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55	Assessing the performance of MM/PBSA and MM/GBSA methods. 9. Prediction reliability of binding affinities and binding poses for proteinâ€“peptide complexes. Physical Chemistry Chemical Physics, 2019, 21, 10135-10145.	1.3	96
56	Mechanism of Graphene Oxide as an Enzyme Inhibitor from Molecular Dynamics Simulations. ACS Applied Materials & Interfaces, 2014, 6, 7153-7163.	4.0	95
57	ADMET Evaluation in Drug Discovery. 16. Predicting hERG Blockers by Combining Multiple Pharmacophores and Machine Learning Approaches. Molecular Pharmaceutics, 2016, 13, 2855-2866.	2.3	90
58	Peptide-Tethered Hydrogel Scaffold Promotes Recovery from Spinal Cord Transection via Synergism with Mesenchymal Stem Cells. ACS Applied Materials & Interfaces, 2017, 9, 3330-3342.	4.0	90
59	Comprehensive Evaluation of Fourteen Docking Programs on Proteinâ€“Peptide Complexes. Journal of Chemical Theory and Computation, 2020, 16, 3959-3969.	2.3	90
60	New Ti-decorated B40 fullerene as a promising hydrogen storage material. Scientific Reports, 2015, 5, 9952.	1.6	89
61	InteractionGraphNet: A Novel and Efficient Deep Graph Representation Learning Framework for Accurate Proteinâ€“Ligand Interaction Predictions. Journal of Medicinal Chemistry, 2021, 64, 18209-18232.	2.9	87
62	P-loop Conformation Governed Crizotinib Resistance in G2032R-Mutated ROS1 Tyrosine Kinase: Clues from Free Energy Landscape. PLoS Computational Biology, 2014, 10, e1003729.	1.5	86
63	A unified drugâ€“target interaction prediction framework based on knowledge graph and recommendation system. Nature Communications, 2021, 12, 6775.	5.8	86
64	A 3D Structure Database of Components from Chinese Traditional Medicinal Herbs. Journal of Chemical Information and Computer Sciences, 2002, 42, 481-489.	2.8	85
65	Insight into Crizotinib Resistance Mechanisms Caused by Three Mutations in ALK Tyrosine Kinase using Free Energy Calculation Approaches. Journal of Chemical Information and Modeling, 2013, 53, 2376-2389.	2.5	85
66	ADMET Evaluation in Drug Discovery. 19. Reliable Prediction of Human Cytochrome P450 Inhibition Using Artificial Intelligence Approaches. Journal of Chemical Information and Modeling, 2019, 59, 4587-4601.	2.5	85
67	Assessing the performance of MM/PBSA and MM/GBSA methods. 8. Predicting binding free energies and poses of proteinâ€“RNA complexes. Rna, 2018, 24, 1183-1194.	1.6	84
68	Combined strategies in structure-based virtual screening. Physical Chemistry Chemical Physics, 2020, 22, 3149-3159.	1.3	83
69	Predictions of Binding of a Diverse Set of Ligands to Gelatinase-A by a Combination of Molecular Dynamics and Continuum Solvent Models. Journal of Physical Chemistry B, 2002, 106, 5527-5535.	1.2	82
70	Detecting and understanding combinatorial mutation patterns responsible for HIV drug resistance. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 1321-1326.	3.3	82
71	Current developments of macrophage migration inhibitory factor (MIF) inhibitors. Drug Discovery Today, 2013, 18, 592-600.	3.2	81
72	Assessing the performance of the MM/PBSA and MM/GBSA methods. 10. Impacts of enhanced sampling and variable dielectric model on proteinâ€“protein Interactions. Physical Chemistry Chemical Physics, 2019, 21, 18958-18969.	1.3	80

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73	Drug Discovery Targeting Anaplastic Lymphoma Kinase (ALK). Journal of Medicinal Chemistry, 2019, 62, 10927-10954.	2.9	80
74	Predicting drug resistance of the HIVâ€1 protease using molecular interaction energy components. Proteins: Structure, Function and Bioinformatics, 2009, 74, 837-846.	1.5	78
75	Mapping the Binding Site of a Large Set of Quinazoline Type EGF-R Inhibitors Using Molecular Field Analyses and Molecular Docking Studies. Journal of Chemical Information and Computer Sciences, 2003, 43, 273-287.	2.8	76
76	Heptazine-based graphitic carbon nitride as an effective hydrogen purification membrane. RSC Advances, 2016, 6, 52377-52383.	1.7	76
77	Molybdenum disulfide as a highly efficient adsorbent for non-polar gases. Physical Chemistry Chemical Physics, 2015, 17, 11700-11704.	1.3	75
78	Stable and metallic borophene nanoribbons from first-principles calculations. Journal of Materials Chemistry C, 2016, 4, 6380-6385.	2.7	75
79	Recent Developments of In Silico Predictions of Intestinal Absorption and Oral Bioavailability. Combinatorial Chemistry and High Throughput Screening, 2009, 12, 497-506.	0.6	74
80	Multi-constraint molecular generation based on conditional transformer, knowledge distillation and reinforcement learning. Nature Machine Intelligence, 2021, 3, 914-922.	8.3	73
81	Revealing the favorable dissociation pathway of type II kinase inhibitors via enhanced sampling simulations and two-end-state calculations. Scientific Reports, 2015, 5, 8457.	1.6	72
82	B40 fullerene: An efficient material for CO2 capture, storage and separation. Current Applied Physics, 2015, 15, 1084-1089.	1.1	71
83	Prediction of Binding Affinities between the Human Amphiphysin-1 SH3 Domain and Its Peptide Ligands Using Homology Modeling, Molecular Dynamics and Molecular Field Analysis. Journal of Proteome Research, 2006, 5, 32-43.	1.8	70
84	Discovery and optimization of triazine derivatives as ROCK1 inhibitors: molecular docking, molecular dynamics simulations and free energy calculations. Molecular BioSystems, 2013, 9, 361.	2.9	70
85	SiC₇siligraphene: a novel donor material with extraordinary sunlight absorption. Nanoscale, 2016, 8, 6994-6999.	2.8	70
86	Monolayer graphitic germanium carbide (g-GeC): the promising cathode catalyst for fuel cell and lithiumâ€“oxygen battery applications. Journal of Materials Chemistry A, 2018, 6, 2212-2218.	5.2	70
87	Do we need different machine learning algorithms for QSAR modeling? A comprehensive assessment of 16 machine learning algorithms on 14 QSAR data sets. Briefings in Bioinformatics, 2021, 22, .	3.2	70
88	Prediction of peptides binding to the PKA RIIÎ± subunit using a hierarchical strategy. Bioinformatics, 2011, 27, 1814-1821.	1.8	67
89	Recent Developments in Computational Prediction of hERG Blockage. Current Topics in Medicinal Chemistry, 2013, 13, 1317-1326.	1.0	67
90	Development and Evaluation of an Integrated Virtual Screening Strategy by Combining Molecular Docking and Pharmacophore Searching Based on Multiple Protein Structures. Journal of Chemical Information and Modeling, 2013, 53, 2743-2756.	2.5	66

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91	Discovery of Novel Inhibitors Targeting the Macrophage Migration Inhibitory Factor via Structure-Based Virtual Screening and Bioassays. Journal of Medicinal Chemistry, 2014, 57, 3737-3745.	2.9	66
92	ADMET Evaluation in Drug Discovery. 18. Reliable Prediction of Chemical-Induced Urinary Tract Toxicity by Boosting Machine Learning Approaches. Molecular Pharmaceutics, 2017, 14, 3935-3953.	2.3	66
93	Fast Approaches for Molecular Polarizability Calculations. Journal of Physical Chemistry A, 2007, 111, 4443-4448.	1.1	65
94	Advances in the development of Rho-associated protein kinase (ROCK) inhibitors. Drug Discovery Today, 2013, 18, 1323-1333.	3.2	64
95	Theoretical investigations on novel SiC5 siligraphene as gas sensor for air pollutants. Carbon, 2017, 113, 114-121.	5.4	64
96	Applications of Genetic Algorithms on the Structureâ^'Activity Relationship Analysis of Some Cinnamamides. Journal of Chemical Information and Computer Sciences, 1999, 39, 775-781.	2.8	63
97	Theoretical Studies on the Susceptibility of Oseltamivir against Variants of 2009 A/H1N1 Influenza Neuraminidase. Journal of Chemical Information and Modeling, 2012, 52, 2715-2729.	2.5	63
98	Drug-likeness analysis of traditional Chinese medicines: 1. property distributions of drug-like compounds, non-drug-like compounds and natural compounds from traditional Chinese medicines. Journal of Cheminformatics, 2012, 4, 31.	2.8	63
99	Metformin activates chaperone-mediated autophagy and improves disease pathologies in an Alzheimer disease mouse model. Protein and Cell, 2021, 12, 769-787.	4.8	63
100	ADMET Evaluation in Drug Discovery. 11. PharmacoKinetics Knowledge Base (PKKB): A Comprehensive Database of Pharmacokinetic and Toxic Properties for Drugs. Journal of Chemical Information and Modeling, 2012, 52, 1132-1137.	2.5	62
101	MG-BERT: leveraging unsupervised atomic representation learning for molecular property prediction. Briefings in Bioinformatics, 2021, 22, .	3.2	62
102	Aqueous Solubility Prediction Based on Weighted Atom Type Counts and Solvent Accessible Surface Areas. Journal of Chemical Information and Modeling, 2009, 49, 571-581.	2.5	61
103	Constructing and Validating High-Performance MIEC-SVM Models in Virtual Screening for Kinases: A Better Way for Actives Discovery. Scientific Reports, 2016, 6, 24817.	1.6	59
104	ADMET Evaluation in Drug Discovery. Part 17: Development of Quantitative and Qualitative Prediction Models for Chemical-Induced Respiratory Toxicity. Molecular Pharmaceutics, 2017, 14, 2407-2421.	2.3	59
105	farPPI: a webserver for accurate prediction of protein-ligand binding structures for small-molecule PPI inhibitors by MM/PB(GB)SA methods. Bioinformatics, 2019, 35, 1777-1779.	1.8	59
106	Morphology and Performance of Polymer Solar Cell Characterized by DPD Simulation and Graph Theory. Scientific Reports, 2015, 5, 16854.	1.6	57
107	Theoretical investigations on SiC2 siligraphene as promising metal-free catalyst for oxygen reduction reaction. Journal of Power Sources, 2015, 299, 371-379.	4.0	57
108	MoS₂ supported single platinum atoms and their superior catalytic activity for CO oxidation: a density functional theory study. Journal of Materials Chemistry A, 2015, 3, 23113-23119.	5.2	56

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109	The Tricyclic Antidepressant Amitriptyline Inhibits d-Cyclin Transactivation and Induces Myeloma Cell Apoptosis by Inhibiting Histone Deacetylases: In Vitro and In Silico Evidence. Molecular Pharmacology, 2011, 79, 672-680.	1.0	54
110	Deep learning approaches for de novo drug design: An overview. Current Opinion in Structural Biology, 2022, 72, 135-144.	2.6	54
111	Monolayer group IVA monochalcogenides as potential and efficient catalysts for the oxygen reduction reaction from first-principles calculations. Journal of Materials Chemistry A, 2017, 5, 1734-1741.	5.2	53
112	Characterizing Drugâ€“Target Residence Time with Metadynamics: How To Achieve Dissociation Rate Efficiently without Losing Accuracy against Time-Consuming Approaches. Journal of Chemical Information and Modeling, 2017, 57, 1895-1906.	2.5	53
113	ARIH1 signaling promotes anti-tumor immunity by targeting PD-L1 for proteasomal degradation. Nature Communications, 2021, 12, 2346.	5.8	52
114	Structural Diversity of Ligand-Binding Androgen Receptors Revealed by Microsecond Long Molecular Dynamics Simulations and Enhanced Sampling. Journal of Chemical Theory and Computation, 2016, 12, 4611-4619.	2.3	51
115	Integrative Modeling of PROTAC-Mediated Ternary Complexes. Journal of Medicinal Chemistry, 2021, 64, 16271-16281.	2.9	51
116	Structural basis of GABAB receptorâ€“Gi protein coupling. Nature, 2021, 594, 594-598.	13.7	50
117	Discovery of Rho-kinase inhibitors by docking-based virtual screening. Molecular BioSystems, 2013, 9, 1511.	2.9	49
118	Can machine learning consistently improve the scoring power of classical scoring functions? Insights into the role of machine learning in scoring functions. Briefings in Bioinformatics, 2021, 22, 497-514.	3.2	49
119	Automated docking of peptides and proteins by using a genetic algorithm combined with a tabu search. Protein Engineering, Design and Selection, 1999, 12, 639-648.	1.0	48
120	New Use for an Old Drug: Inhibiting ABCG2 with Sorafenib. Molecular Cancer Therapeutics, 2012, 11, 1693-1702.	1.9	48
121	Importance of protein flexibility in ranking inhibitor affinities: modeling the binding mechanisms of piperidine carboxamides as Type I1/2 ALK inhibitors. Physical Chemistry Chemical Physics, 2015, 17, 6098-6113.	1.3	48
122	HawkRank: a new scoring function for proteinâ€“protein docking based on weighted energy terms. Journal of Cheminformatics, 2017, 9, 66.	2.8	48
123	The inflammatory cytokine IL-6 induces FRA1 deacetylation promoting colorectal cancer stem-like properties. Oncogene, 2019, 38, 4932-4947.	2.6	48
124	The structure of erastin-bound xCTâ€“4F2hc complexÂreveals molecular mechanisms underlying erastin-induced ferroptosis. Cell Research, 2022, 32, 687-690.	5.7	48
125	Farnesyltransferase and geranylgeranyltransferase I: structures, mechanism, inhibitors and molecular modeling. Drug Discovery Today, 2015, 20, 267-276.	3.2	47
126	Simulation of the Phase Behavior of the (EO)13(PO)30(EO)13(Pluronic L64)/Water/p-Xylene System Using MesoDyn. Journal of Physical Chemistry B, 2002, 106, 11397-11403.	1.2	46

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127	Improving the Alkaline Stability of Imidazolium Cations by Substitution. ChemPhysChem, 2014, 15, 3006-3014.	1.0	46
128	DNA methyltransferases: emerging targets for the discovery of inhibitors as potent anticancer drugs. Drug Discovery Today, 2019, 24, 2323-2331.	3.2	46
129	ADME Evaluation in Drug Discovery. 2. Prediction of Partition Coefficient by Atom-Additive Approach Based on Atom-Weighted Solvent Accessible Surface Areas. Journal of Chemical Information and Computer Sciences, 2003, 43, 1058-1067.	2.8	45
130	Discovery of Novel and Selective Adenosine A_{2A} Receptor Antagonists for Treating Parkinsonâ€™s Disease through Comparative Structure-Based Virtual Screening. Journal of Chemical Information and Modeling, 2017, 57, 1474-1487.	2.5	45
131	Cheminformatic Insight into the Differences between Terrestrial and Marine Originated Natural Products. Journal of Chemical Information and Modeling, 2018, 58, 1182-1193.	2.5	45
132	ADMET evaluation in drug discovery. 20. Prediction of breast cancer resistance protein inhibition through machine learning. Journal of Cheminformatics, 2020, 12, 16.	2.8	45
133	Computational Modeling of Structure-Function of G Protein-Coupled Receptors with Applications for Drug Design. Current Medicinal Chemistry, 2010, 17, 1167-1180.	1.2	44
134	Computational Simulation of Drug Delivery at Molecular Level. Current Medicinal Chemistry, 2010, 17, 4482-4491.	1.2	44
135	A magic drug target: Androgen receptor. Medicinal Research Reviews, 2019, 39, 1485-1514.	5.0	44
136	Discovery of selective phosphatidylinositol 3-kinase inhibitors to treat hematological malignancies. Drug Discovery Today, 2015, 20, 988-994.	3.2	43
137	Photophysical Studies on the Mono- and Dichromophoric Hemicyanine Dyes I. Photoelectric Conversion from the Dye Modified ITO Electrodes. Journal of Physical Chemistry B, 2002, 106, 10020-10030.	1.2	42
138	Combating Drug-Resistant Mutants of Anaplastic Lymphoma Kinase with Potent and Selective Type-I^{1/2} Inhibitors by Stabilizing Unique DFG-Shifted Loop Conformation. ACS Central Science, 2017, 3, 1208-1220.	5.3	42
139	CovalentInDB: a comprehensive database facilitating the discovery of covalent inhibitors. Nucleic Acids Research, 2021, 49, D1122-D1129.	6.5	42
140	The Antiparasitic Clioquinol Induces Apoptosis in Leukemia and Myeloma Cells by Inhibiting Histone Deacetylase Activity. Journal of Biological Chemistry, 2013, 288, 34181-34189.	1.6	41
141	Directly Binding Rather than Induced-Fit Dominated Binding Affinity Difference in (S)- and (R)-Crizotinib Bound MTH1. Journal of Chemical Theory and Computation, 2016, 12, 851-860.	2.3	41
142	Structural Analysis and Identification of Colloidal Aggregators in Drug Discovery. Journal of Chemical Information and Modeling, 2019, 59, 3714-3726.	2.5	41
143	Increased gene copy number of DEFA1/DEFA3 worsens sepsis by inducing endothelial pyroptosis. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 3161-3170.	3.3	41
144	Molecular Principle of Topotecan Resistance by Topoisomerase I Mutations through Molecular Modeling Approaches. Journal of Chemical Information and Modeling, 2013, 53, 997-1006.	2.5	40

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145	Two-dimensional siligraphenes as cathode catalysts for nonaqueous lithium-oxygen batteries. Carbon, 2018, 126, 580-587.	5.4	40
146	Improving Docking-Based Virtual Screening Ability by Integrating Multiple Energy Auxiliary Terms from Molecular Docking Scoring. Journal of Chemical Information and Modeling, 2020, 60, 4216-4230.	2.5	40
147	Empirical Aqueous Solvation Models Based on Accessible Surface Areas with Implicit Electrostatics. Journal of Physical Chemistry B, 2002, 106, 11295-11304.	1.2	39
148	Studies on the Interactions between Î²₂ Adrenergic Receptor and Gs Protein by Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2012, 52, 1005-1014.	2.5	39
149	Structural basis of the interactions between CXCR4 and CXCL12/SDF-1 revealed by theoretical approaches. Molecular BioSystems, 2013, 9, 2107.	2.9	39
150	Modeling Compoundâ€“Target Interaction Network of Traditional Chinese Medicines for Type II Diabetes Mellitus: Insight for Polypharmacology and Drug Design. Journal of Chemical Information and Modeling, 2013, 53, 1787-1803.	2.5	39
151	Inhibition of macrophage migration inhibitory factor (<scp>MIF</scp>) tautomerase activity suppresses microgliaâ€mediated inflammatory responses. Clinical and Experimental Pharmacology and Physiology, 2016, 43, 1134-1144.	0.9	39
152	B₄₀fullerene as a highly sensitive molecular device for NH₃detection at low bias: a first-principles study. Nanotechnology, 2016, 27, 075501.	1.3	39
153	Insight into the selective binding mechanism of DNMT1 and DNMT3A inhibitors: a molecular simulation study. Physical Chemistry Chemical Physics, 2019, 21, 12931-12947.	1.3	39
154	Beware of the generic machine learning-based scoring functions in structure-based virtual screening. Briefings in Bioinformatics, 2021, 22, .	3.2	39
155	Mining Toxicity Information from Large Amounts of Toxicity Data. Journal of Medicinal Chemistry, 2021, 64, 6924-6936.	2.9	39
156	Targeting the Phosphatidylinositol 3-Kinase/AKT Pathway for the Treatment of Multiple Myeloma. Current Medicinal Chemistry, 2014, 21, 3173-3187.	1.2	39
157	Recent Developments of In Silico Predictions of Oral Bioavailability. Combinatorial Chemistry and High Throughput Screening, 2011, 14, 362-374.	0.6	38
158	Binding Affinities for a Series of Selective Inhibitors of Gelatinase-A Using Molecular Dynamics with a Linear Interaction Energy Approach. Journal of Physical Chemistry B, 2001, 105, 5304-5315.	1.2	37
159	Structural stability and O2 dissociation on nitrogen-doped graphene with transition metal atoms embedded: A first-principles study. AIP Advances, 2015, 5, .	0.6	37
160	Molecular Dynamics Simulations Revealed the Regulation of Ligands to the Interactions between Androgen Receptor and Its Coactivator. Journal of Chemical Information and Modeling, 2018, 58, 1652-1661.	2.5	37
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