List of Publications by Year in descending order

263 papers	20,213 citations	12322 69 h-index	13758 129 g-index
268 all docs	268 docs citations	268 times ranked	16724 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	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
18	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

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19	Recent Development and Application of Virtual Screening in Drug Discovery: An Overview. Current Pharmaceutical Design, 2004, 10, 1011-1033.	0.9	185
20	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
21	Recent Advances in Computational Prediction of Drug Absorption and Permeability in Drug Discovery. Current Medicinal Chemistry, 2006, 13, 2653-2667.	1.2	167
22	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
23	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
24	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
25	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
26	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
27	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
28	Application of molecular dynamics simulations in molecular property prediction II: Diffusion coefficient. Journal of Computational Chemistry, 2011, 32, 3505-3519.	1.5	135
29	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
30	PROTAC-DB: an online database of PROTACs. Nucleic Acids Research, 2021, 49, D1381-D1387.	6.5	127
31	Two-dimensional germanium monochalcogenide photocatalyst for water splitting under ultraviolet, visible to near-infrared light. Nanoscale, 2017, 9, 8608-8615.	2.8	124
32	Computational models for predicting substrates or inhibitors of P-glycoprotein. Drug Discovery Today, 2012, 17, 343-351.	3.2	122
33	Structure â€“ ADME relationship: still a long way to go?. Expert Opinion on Drug Metabolism and Toxicology, 2008, 4, 759-770.	1.5	120
34	ADME evaluation in drug discovery. Journal of Molecular Modeling, 2002, 8, 337-349.	0.8	116
35	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
36	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

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37	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
38	CaFE: a tool for binding affinity prediction using end-point free energy methods. Bioinformatics, 2016, 32, 2216-2218.	1.8	114
39	Evaluating the potency of HIVâ€1 protease drugs to combat resistance. Proteins: Structure, Function and Bioinformatics, 2008, 71, 1163-1174.	1.5	110
40	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
41	Recent Advances on Aqueous Solubility Prediction. Combinatorial Chemistry and High Throughput Screening, 2011, 14, 328-338.	0.6	102
42	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
43	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
44	Two-Dimensional MnO₂ as a Better Cathode Material for Lithium Ion Batteries. Journal of Physical Chemistry C, 2015, 119, 28783-28788.	1.5	98
45	Characterization of Domain-Peptide Interaction Interface. Molecular and Cellular Proteomics, 2009, 8, 639-649.	2.5	96
46	Drug and Drug Candidate Building Block Analysis. Journal of Chemical Information and Modeling, 2010, 50, 55-67.	2.5	96
47	Drug-likeness Analysis of Traditional Chinese Medicines: Prediction of Drug-likeness Using Machine Learning Approaches. Molecular Pharmaceutics, 2012, 9, 2875-2886.	2.3	96
48	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
49	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
50	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
51	Mechanism of Graphene Oxide as an Enzyme Inhibitor from Molecular Dynamics Simulations. ACS Applied Materials & Interfaces, 2014, 6, 7153-7163.	4.0	95
52	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
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58	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
59	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
60	Combined strategies in structure-based virtual screening. Physical Chemistry Chemical Physics, 2020, 22, 3149-3159.	1.3	83
61	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
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63	Current developments of macrophage migration inhibitory factor (MIF) inhibitors. Drug Discovery Today, 2013, 18, 592-600.	3.2	81
64	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
65	Drug Discovery Targeting Anaplastic Lymphoma Kinase (ALK). Journal of Medicinal Chemistry, 2019, 62, 10927-10954.	2.9	80
66	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
67	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
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71	B40 fullerene: An efficient material for CO2 capture, storage and separation. Current Applied Physics, 2015, 15, 1084-1089.	1.1	71
72	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

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75	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
76	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
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82	Fast Approaches for Molecular Polarizability Calculations. Journal of Physical Chemistry A, 2007, 111, 4443-4448.	1.1	65
83	Advances in the development of Rho-associated protein kinase (ROCK) inhibitors. Drug Discovery Today, 2013, 18, 1323-1333.	3.2	64
84	Theoretical investigations on novel SiC5 siligraphene as gas sensor for air pollutants. Carbon, 2017, 113, 114-121.	5.4	64
85	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
86	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
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88	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
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97	Integrative Modeling of PROTAC-Mediated Ternary Complexes. Journal of Medicinal Chemistry, 2021, 64, 16271-16281.	2.9	51
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99	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
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105	DNA methyltransferases: emerging targets for the discovery of inhibitors as potent anticancer drugs. Drug Discovery Today, 2019, 24, 2323-2331.	3.2	46
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110	A magic drug target: Androgen receptor. Medicinal Research Reviews, 2019, 39, 1485-1514.	5.0	44
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118	Empirical Aqueous Solvation Models Based on Accessible Surface Areas with Implicit Electrostatics. Journal of Physical Chemistry B, 2002, 106, 11295-11304.	1.2	39
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122	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
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128	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
129	DDInter: an online drugâ€“drug interaction database towards improving clinical decision-making and patient safety. Nucleic Acids Research, 2022, 50, D1200-D1207.	6.5	37
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