Huiyong Sun

List of Publications by Year
in descending order

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81 papers	6,478 citations	117453 34 h-index	69108 77 g-index
85 all docs	85 docs citations	85 times ranked	6051 citing authors

#	Article	IF	Citations
1	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
2	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
3	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
4	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
5	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
6	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
7	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
8	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
9	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
10	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
11	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
12	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
13	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
14	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
15	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
16	Combined strategies in structure-based virtual screening. Physical Chemistry Chemical Physics, 2020, 22, 3149-3159.	1.3	83
17	Current developments of macrophage migration inhibitory factor (MIF) inhibitors. Drug Discovery Today, 2013, 18, 592-600.	3.2	81
18	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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19	Drug Discovery Targeting Anaplastic Lymphoma Kinase (ALK). Journal of Medicinal Chemistry, 2019, 62, 10927-10954.	2.9	80
20	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
21	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
22	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
23	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
24	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
25	A molecular dynamics investigation on the crizotinib resistance mechanism of C1156Y mutation in ALK. Biochemical and Biophysical Research Communications, 2012, 423, 319-324.	1.0	58
26	Discovery of Small-Molecule Inhibitors of the PD-1/PD-L1 Axis That Promote PD-L1 Internalization and Degradation. Journal of Medicinal Chemistry, 2022, 65, 3879-3893.	2.9	55
27	Deep learning approaches for de novo drug design: An overview. Current Opinion in Structural Biology, 2022, 72, 135-144.	2.6	54
28	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
29	HawkRank: a new scoring function for proteinâ€“protein docking based on weighted energy terms. Journal of Cheminformatics, 2017, 9, 66.	2.8	48
30	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
31	The impact of interior dielectric constant and entropic change on HIV-1 complex binding free energy prediction. Structural Dynamics, 2018, 5, 064101.	0.9	44
32	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
33	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
34	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
35	Structural basis of the interactions between CXCR4 and CXCL12/SDF-1 revealed by theoretical approaches. Molecular BioSystems, 2013, 9, 2107.	2.9	39
36	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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37	Voltage-gated sodium channels: structures, functions, and molecular modeling. Drug Discovery Today, 2019, 24, 1389-1397.	3.2	36
38	fastDRH: a webserver to predict and analyze proteinâ€“ligand complexes based on molecular docking and MM/PB(GB)SA computation. Briefings in Bioinformatics, 2022, 23, .	3.2	34
39	Discovery of Novel Androgen Receptor Ligands by Structure-based Virtual Screening and Bioassays. Genomics, Proteomics and Bioinformatics, 2018, 16, 416-427.	3.0	32
40	Communication between the Ligand-Binding Pocket and the Activation Function-2 Domain of Androgen Receptor Revealed by Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2019, 59, 842-857.	2.5	30
41	Gasdermin E-derived caspase-3 inhibitors effectively protect mice from acute hepatic failure. Acta Pharmacologica Sinica, 2021, 42, 68-76.	2.8	30
42	The competitive binding between inhibitors and substrates of HCV NS3/4A protease: A general mechanism of drug resistance. Antiviral Research, 2014, 103, 60-70.	1.9	29
43	VAD-MM/GBSA: A Variable Atomic Dielectric MM/GBSA Model for Improved Accuracy in Proteinâ€“Ligand Binding Free Energy Calculations. Journal of Chemical Information and Modeling, 2021, 61, 2844-2856.	2.5	29
44	Discovery of Novel ROCK1 Inhibitors via Integrated Virtual Screening Strategy and Bioassays. Scientific Reports, 2015, 5, 16749.	1.6	27
45	Prediction of luciferase inhibitors by the high-performance MIEC-GBDT approach based on interaction energetic patterns. Physical Chemistry Chemical Physics, 2017, 19, 10163-10176.	1.3	27
46	Structure-Based Drug Design and Identification of H₂O-Soluble and Low Toxic Hexacyclic Camptothecin Derivatives with Improved Efficacy in Cancer and Lethal Inflammation Models in Vivo. Journal of Medicinal Chemistry, 2018, 61, 8613-8624.	2.9	27
47	Structureâ€based discovery of CZL80, a caspaseâ€1 inhibitor with therapeutic potential for febrile seizures and later enhanced epileptogenic susceptibility. British Journal of Pharmacology, 2020, 177, 3519-3534.	2.7	26
48	Structural and Energetic Analyses of SNPs in Drug Targets and Implications for Drug Therapy. Journal of Chemical Information and Modeling, 2013, 53, 3343-3351.	2.5	25
49	Comparative analyses of structural features and scaffold diversity for purchasable compound libraries. Journal of Cheminformatics, 2017, 9, 25.	2.8	25
50	Development and Evaluation of MM/GBSA Based on a Variable Dielectric GB Model for Predicting Proteinâ€“Ligand Binding Affinities. Journal of Chemical Information and Modeling, 2020, 60, 5353-5365.	2.5	25
51	Recent Advances in Protein-Protein Docking. Current Drug Targets, 2016, 17, 1586-1594.	1.0	25
52	Aggregated Single-Walled Carbon Nanotubes Absorb and Deform Dopamine-Related Proteins Based on Molecular Dynamics Simulations. ACS Applied Materials & Interfaces, 2017, 9, 32452-32462.	4.0	24
53	Exploring the binding mechanisms of MIF to CXCR2 using theoretical approaches. Physical Chemistry Chemical Physics, 2015, 17, 3370-3382.	1.3	23
54	Importance of protein flexibility in molecular recognition: a case study on Type-I1/2 inhibitors of ALK. Physical Chemistry Chemical Physics, 2018, 20, 4851-4863.	1.3	22

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55	Molecular principle of the cyclin-dependent kinase selectivity of 4-(thiazol-5-yl)-2-(phenylamino) pyrimidine-5-carbonitrile derivatives revealed by molecular modeling studies. Physical Chemistry Chemical Physics, 2016, 18, 2034-2046.	1.3	21
56	Finding chemical drugs for genetic diseases. Drug Discovery Today, 2014, 19, 1836-1840.	3.2	20
57	<scp>2â€Diphenylphosphinoyl</scp>â€acetyl as a Remote Directing Group for the Highly Stereoselective Synthesis of <scp>Î²â€Glycosides</scp>. Chinese Journal of Chemistry, 2022, 40, 443-452.	2.6	18
58	Exploring resistance mechanisms of HCV NS3/4A protease mutations to MK5172: insight from molecular dynamics simulations and free energy calculations. Molecular BioSystems, 2015, 11, 2568-2578.	2.9	17
59	How Does the L884P Mutation Confer Resistance to Type-II Inhibitors of JAK2 Kinase: A Comprehensive Molecular Modeling Study. Scientific Reports, 2017, 7, 9088.	1.6	16
60	DeepAtomicCharge: a new graph convolutional network-based architecture for accurate prediction of atomic charges. Briefings in Bioinformatics, 2021, 22, .	3.2	16
61	TEPP-46-Based AIE Fluorescent Probe for Detection and Bioimaging of PKM2 in Living Cells. Analytical Chemistry, 2021, 93, 12682-12689.	3.2	15
62	Unraveling the conformational determinants of LARP7 and 7SK small nuclear RNA by theoretical approaches. Molecular BioSystems, 2016, 12, 2613-2621.	2.9	13
63	Benchmark Study Based on 2P2I_{DB} to Gain Insights into the Discovery of Small-Molecule PPI Inhibitors. Journal of Physical Chemistry B, 2018, 122, 2544-2555.	1.2	12
64	Identification of novel and selective non-peptide inhibitors targeting the polo-box domain of polo-like kinase 1. Bioorganic Chemistry, 2018, 81, 278-288.	2.0	12
65	More than a Leaving Group: Nâ€Phenyltrifluoroacetimidate as a Remote Directing Group for Highly Î±â€Selective 1,2â€cis Glycosylation. Angewandte Chemie - International Edition, 2022, 61, .	7.2	12
66	Fullerene derivatives act as inhibitors of leukocyte common antigen based on molecular dynamics simulations. RSC Advances, 2018, 8, 13997-14008.	1.7	10
67	Subresidue-Resolution Footprinting of Ligandâ€“Protein Interactions by Carbene Chemistry and Ion Mobilityâ€“Mass Spectrometry. Analytical Chemistry, 2020, 92, 947-956.	3.2	10
68	Characterizing the stabilization effects of stabilizers in proteinâ€“protein systems with end-point binding free energy calculations. Briefings in Bioinformatics, 2022, 23, .	3.2	10
69	Identification and Preliminary SAR Analysis of Novel Type-I Inhibitors of TIE-2 via Structure-Based Virtual Screening and Biological Evaluation in in vitro Models. Journal of Chemical Information and Modeling, 2015, 55, 2693-2704.	2.5	9
70	Fast and accurate prediction of partial charges using Atom-Path-Descriptor-based machine learning. Bioinformatics, 2020, 36, 4721-4728.	1.8	9
71	Comprehensive assessment of deep generative architectures for de novo drug design. Briefings in Bioinformatics, 2022, 23, .	3.2	9
72	Discovery of N-(4-(Benzyloxy)-phenyl)-sulfonamide Derivatives as Novel Antagonists of the Human Androgen Receptor Targeting the Activation Function 2. Journal of Medicinal Chemistry, 2022, 65, 2507-2521.	2.9	8

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73	Discovery of novel nonpeptide small-molecule NRP1 antagonists: Virtual screening, molecular simulation and structural modification. Bioorganic and Medicinal Chemistry, 2020, 28, 115183.	1.4	7
74	Out-of-the-box deep learning prediction of quantum-mechanical partial charges by graph representation and transfer learning. Briefings in Bioinformatics, 2022, 23, .	3.2	7
75	Improving the Efficiency of Non-equilibrium Sampling in the Aqueous Environment via Implicit-Solvent Simulations. Journal of Chemical Theory and Computation, 2017, 13, 1827-1836.	2.3	6
76	Prediction of fibril formation by early-stage amyloid peptide aggregation. Journal of Pharmaceutical Analysis, 2020, 10, 194-199.	2.4	6
77	Exploring PI3KÎ³ binding preference with Eganelisib, Duvelisib, and Idelalisib via energetic, pharmacophore and dissociation pathway analyses. Computers in Biology and Medicine, 2022, 147, 105642.	3.9	6
78	In Silico Exploration for Novel Type-I Inhibitors of Tie-2/TEK: The Performance of Different Selection Strategy in Selecting Virtual Screening Candidates. Scientific Reports, 2016, 6, 37628.	1.6	4
79	DeepChargePredictor: a web server for predicting QM-based atomic charges via state-of-the-art machine-learning algorithms. Bioinformatics, 2021, 37, 4255-4257.	1.8	4
80	Identification of novel peptidomimetics targeting the polo-box domain of polo-like kinase 1. Bioorganic Chemistry, 2019, 91, 103148.	2.0	1
81	More than a Leaving Group: N â€Phenyltrifluoroacetimidate as a Remote Directing Group for Highly Î±â€Selective 1,2â€•cis Glycosylation. Angewandte Chemie, 0, , .	1.6	1