Xibing He

List of Publications by Year in descending order

36 papers	1,712 citations	516710 16 h-index	361022 35 g-index
39 all docs	39 docs citations	39 times ranked	2556 citing authors

#	Article	IF	Citations
1	Recent progress in general force fields of small molecules. Current Opinion in Structural Biology, 2022, 72, 187-193.	5.7	15
2	Development and Evaluation of Geometry Optimization Algorithms in Conjunction with ANI Potentials. Journal of Chemical Theory and Computation, 2022, 18, 978-991.	5.3	2
3	A multiple-step in silico screening protocol to identify allosteric inhibitors of Spikeâ€“hACE2 binding. Physical Chemistry Chemical Physics, 2022, 24, 4305-4316.	2.8	6
4	Joint Computational/Cell-Based Approach for Screening Inhibitors of Tau Oligomerization: A Proof-of-Concept Study. Journal of Alzheimer's Disease, 2022, 89, 107-119.	2.6	2
5	Determination of van der Waals Parameters Using a Double Exponential Potential for Nonbonded Divalent Metal Cations in TIP3P Solvent. Journal of Chemical Theory and Computation, 2021, 17, 1086-1097.	5.3	16
6	Incorporating structural similarity into a scoring function to enhance the prediction of binding affinities. Journal of Cheminformatics, 2021, 13, 11.	6.1	1
7	Machine learning on ligand-residue interaction profiles to significantly improve binding affinity prediction. Briefings in Bioinformatics, 2021, 22, .	6.5	17
8	In silico binding profile characterization of SARS-CoV-2 spike protein and its mutants bound to human ACE2 receptor. Briefings in Bioinformatics, 2021, 22, .	6.5	22
9	Effects of All-Atom Molecular Mechanics Force Fields on Amyloid Peptide Assembly: The Case of PHF6 Peptide of Tau Protein. Journal of Chemical Theory and Computation, 2021, 17, 6458-6471.	5.3	23
10	How Well Does the Extended Linear Interaction Energy Method Perform in Accurate Binding Free Energy Calculations?. Journal of Chemical Information and Modeling, 2020, 60, 6624-6633.	5.4	9
11	A fast and high-quality charge model for the next generation general AMBER force field. Journal of Chemical Physics, 2020, 153, 114502.	3.0	195
12	Prediction of the Binding Affinities and Selectivity for CB1 and CB2 Ligands Using Homology Modeling, Molecular Docking, Molecular Dynamics Simulations, and MM-PBSA Binding Free Energy Calculations. ACS Chemical Neuroscience, 2020, 11, 1139-1158.	3.5	38
13	Fast, Accurate, and Reliable Protocols for Routine Calculations of Proteinâ€“Ligand Binding Affinities in Drug Design Projects Using AMBER GPU-TI with ff14SB/GAFF. ACS Omega, 2020, 5, 4611-4619.	3.5	74
14	Introducing Virtual Oligomerization Inhibition to Identify Potent Inhibitors of AÎ² Oligomerization. Journal of Chemical Theory and Computation, 2020, 16, 3920-3935.	5.3	7
15	Molecular Mechanism and Kinetics of Amyloid-Î²₄₂ Aggregate Formation: A Simulation Study. ACS Chemical Neuroscience, 2019, 10, 4643-4658.	3.5	13
16	Prediction of Drugâ€“Drug Interactions Between Opioids and Overdosed Benzodiazepines Using Physiologically Based Pharmacokinetic (PBPK) Modeling and Simulation. Drugs in R and D, 2019, 19, 297-305.	2.2	17
17	Significantly different effects of tetrahydroberberrubine enantiomers on dopamine D1/D2 receptors revealed by experimental study and integrated in silico simulation. Journal of Computer-Aided Molecular Design, 2019, 33, 447-459.	2.9	6
18	Insight of Captagon Abuse by Chemogenomics Knowledgebase-guided Systems Pharmacology Target Mapping Analyses. Scientific Reports, 2019, 9, 2268.	3.3	10

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19	New application of in silico methods in identifying mechanisms of action and key components of anti-cancer herbal formulation YIV-906 (PHY906). Physical Chemistry Chemical Physics, 2019, 21, 23501-23513.	2.8	9
20	Calculate proteinâ€“ligand binding affinities with the extended linear interaction energy method: application on the Cathepsin S set in the D3R Grand Challenge 3. Journal of Computer-Aided Molecular Design, 2019, 33, 105-117.	2.9	27
21	Computational systems pharmacology analysis of cannabidiol: a combination of chemogenomics-knowledgebase network analysis and integrated in silico modeling and simulation. Acta Pharmacologica Sinica, 2019, 40, 374-386.	6.1	34
22	Effects of All-Atom Molecular Mechanics Force Fields on Amyloid Peptide Assembly: The Case of Aî²_{16â€“22} Dimer. Journal of Chemical Theory and Computation, 2019, 15, 1440-1452.	5.3	102
23	An insight into paracetamol and its metabolites using molecular docking and molecular dynamics simulation. Journal of Molecular Modeling, 2018, 24, 243.	1.8	14
24	Drude polarizable force field for aliphatic ketones and aldehydes, and their associated acyclic carbohydrates. Journal of Computer-Aided Molecular Design, 2017, 31, 349-363.	2.9	16
25	Drude Polarizable Force Field for Molecular Dynamics Simulations of Saturated and Unsaturated Zwitterionic Lipids. Journal of Chemical Theory and Computation, 2017, 13, 4535-4552.	5.3	90
26	Entropy and Polarity Control the Partition and Transportation of Drug-like Molecules in Biological Membrane. Scientific Reports, 2017, 7, 17749.	3.3	21
27	Polarizable Empirical Force Field for Hexopyranose Monosaccharides Based on the Classical Drude Oscillator. Journal of Physical Chemistry B, 2015, 119, 637-652.	2.6	67
28	Development of a Polarizable Force Field for Macromolecules Based on the Classical Drude Oscillator. Biophysical Journal, 2014, 106, 43a.	0.5	0
29	Bifurcated Hydrogen Bonding and Asymmetric Fluctuations in a Carbohydrate Crystal Studied via X-ray Crystallography and Computational Analysis. Journal of Physical Chemistry B, 2013, 117, 7546-7553.	2.6	5
30	Polarizable Empirical Force Field for Acyclic Polyalcohols Based on the Classical Drude Oscillator. Biopolymers, 2013, 99, 724-738.	2.4	50
31	A Comparative Kirkwood-Buff Study of Aqueous Methanol Solutions Modeled by the CHARMM Additive and Drude Polarizable Force Fields. Journal of Physical Chemistry B, 2013, 117, 10572-10580.	2.6	13
32	Extension of the CHARMM general force field to sulfonylâ€containing compounds and its utility in biomolecular simulations. Journal of Computational Chemistry, 2012, 33, 2451-2468.	3.3	659
33	Development of a Coarse-Grained Model for the Surfactant Family of Linear Alkylbenzene Sulfonates. Biophysical Journal, 2011, 100, 147a.	0.5	1
34	Paramaterization of a coarse-grained model for linear alkylbenzene sulfonate surfactants and molecular dynamics studies of their self-assembly in aqueous solution. Chemical Physics Letters, 2010, 487, 71-76.	2.6	27
35	Exploring the utility of coarse-grained water models for computational studies of interfacial systems. Molecular Physics, 2010, 108, 2007-2020.	1.7	48
36	Atomistic Simulation Study of Linear Alkylbenzene Sulfonates at the Water/Air Interface. Journal of Physical Chemistry B, 2010, 114, 9787-9794.	2.6	53