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	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
2	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
3	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
4	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
5	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
6	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
7	Atomistic Simulation Study of Linear Alkylbenzene Sulfonates at the Water/Air Interface. Journal of Physical Chemistry B, 2010, 114, 9787-9794.	2.6	53
8	Polarizable Empirical Force Field for Acyclic Polyalcohols Based on the Classical Drude Oscillator. Biopolymers, 2013, 99, 724-738.	2.4	50
9	Exploring the utility of coarse-grained water models for computational studies of interfacial systems. Molecular Physics, 2010, 108, 2007-2020.	1.7	48
10	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
11	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
12	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
13	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
14	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
15	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
16	Entropy and Polarity Control the Partition and Transportation of Drug-like Molecules in Biological Membrane. Scientific Reports, 2017, 7, 17749.	3.3	21
17	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
18	Machine learning on ligand-residue interaction profiles to significantly improve binding affinity prediction. Briefings in Bioinformatics, 2021, 22, .	6.5	17

#	Article	IF	Citations
19	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
20	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
21	Recent progress in general force fields of small molecules. Current Opinion in Structural Biology, 2022, 72, 187-193.	5.7	15
22	An insight into paracetamol and its metabolites using molecular docking and molecular dynamics simulation. Journal of Molecular Modeling, 2018, 24, 243.	1.8	14
23	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
24	Molecular Mechanism and Kinetics of Amyloid-Î²₄₂ Aggregate Formation: A Simulation Study. ACS Chemical Neuroscience, 2019, 10, 4643-4658.	3.5	13
25	Insight of Captagon Abuse by Chemogenomics Knowledgebase-guided Systems Pharmacology Target Mapping Analyses. Scientific Reports, 2019, 9, 2268.	3.3	10
26	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
27	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
28	Introducing Virtual Oligomerization Inhibition to Identify Potent Inhibitors of AÎ² Oligomerization. Journal of Chemical Theory and Computation, 2020, 16, 3920-3935.	5.3	7
29	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
30	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
31	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
32	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
33	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
34	Development of a Coarse-Grained Model for the Surfactant Family of Linear Alkylbenzene Sulfonates. Biophysical Journal, 2011, 100, 147a.	0.5	1
35	Incorporating structural similarity into a scoring function to enhance the prediction of binding affinities. Journal of Cheminformatics, 2021, 13, 11.	6.1	1
36	Development of a Polarizable Force Field for Macromolecules Based on the Classical Drude Oscillator. Biophysical Journal, 2014, 106, 43a.	0.5	0