Yifei Qi

List of Publications by Year in descending order

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254	15,318	36271	23514
papers	citations	51 h-index	111 g-index

258	258	258	13175
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	CHARMM-GUI Input Generator for NAMD, GROMACS, AMBER, OpenMM, and CHARMM/OpenMM Simulations Using the CHARMM36 Additive Force Field. Journal of Chemical Theory and Computation, 2016, 12, 405-413.	2.3	2,567
2	CHARMM-GUIMembrane Buildertoward realistic biological membrane simulations. Journal of Computational Chemistry, 2014, 35, 1997-2004.	1.5	1,802
3	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
4	Fullâ€dimensional timeâ€dependent treatment for diatomâ€“diatom reactions: The H2+OH reaction. Journal of Chemical Physics, 1994, 101, 1146-1156.	1.2	422
5	CHARMM-GUI Membrane Builder for Complex Biological Membrane Simulations with Glycolipids and Lipoglycans. Journal of Chemical Theory and Computation, 2019, 15, 775-786.	2.3	388
6	CHARMM-GUI Martini Maker for Coarse-Grained Simulations with the Martini Force Field. Journal of Chemical Theory and Computation, 2015, 11, 4486-4494.	2.3	340
7	Interaction Entropy: A New Paradigm for Highly Efficient and Reliable Computation of Proteinâ€“Ligand Binding Free Energy. Journal of the American Chemical Society, 2016, 138, 5722-5728.	6.6	297
8	Quantum reactive scattering with a deep well: Timeâ€dependent calculation for H+O2reaction and bound state characterization for HO2. Journal of Chemical Physics, 1994, 101, 3671-3678.	1.2	265
9	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
10	CHARMMâ€GUI 10 years for biomolecular modeling and simulation. Journal of Computational Chemistry, 2017, 38, 1114-1124.	1.5	224
11	CHARMM-GUIGlycan Modelerfor modeling and simulation of carbohydrates and glycoconjugates. Glycobiology, 2019, 29, 320-331.	1.3	222
12	CHARMM-GUI PDB Manipulator for Advanced Modeling and Simulations of Proteins Containing Nonstandard Residues. Advances in Protein Chemistry and Structural Biology, 2014, 96, 235-265.	1.0	214
13	Effects of N-glycosylation on protein conformation and dynamics: Protein Data Bank analysis and molecular dynamics simulation study. Scientific Reports, 2015, 5, 8926.	1.6	187
14	Accurate quantum calculation for the benchmark reaction H2+OHâ†'H2O +H in fiveâ€dimensional space: Reaction probabilities for J=0. Journal of Chemical Physics, 1993, 99, 5615-5618.	1.2	175
15	Developing Polarized Protein-Specific Charges for Protein Dynamics: MD Free Energy Calculation of pKa Shifts for Asp26/Asp20 in Thioredoxin. Biophysical Journal, 2008, 95, 1080-1088.	0.2	151
16	CHARMMâ€GUI Martini Maker for modeling and simulation of complex bacterial membranes with lipopolysaccharides. Journal of Computational Chemistry, 2017, 38, 2354-2363.	1.5	150
17	DeepDDG: Predicting the Stability Change of Protein Point Mutations Using Neural Networks. Journal of Chemical Information and Modeling, 2019, 59, 1508-1514.	2.5	146
18	Exact fullâ€dimensional bound state calculations for (HF)2, (DF)2, and HFDF. Journal of Chemical Physics, 1995, 102, 2315-2325.	1.2	132

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19	Effect of mutations on binding of ligands to guanine riboswitch probed by free energy perturbation and molecular dynamics simulations. Nucleic Acids Research, 2019, 47, 6618-6631.	6.5	130
20	LLPSDB: a database of proteins undergoing liquidâ€“liquid phase separation in vitro. Nucleic Acids Research, 2020, 48, D320-D327.	6.5	130
21	Development of Accurate Quantum Dynamical Methods for Tetraatomic Reactions. Journal of Physical Chemistry A, 1997, 101, 2746-2754.	1.1	128
22	Accurate quantum calculations for H2+OHâ†'H2O+H: Reaction probabilities, cross sections, and rate constants. Journal of Chemical Physics, 1994, 100, 2697-2706.	1.2	120
23	Quantum adsorption dynamics of a diatomic molecule on surface: Fourâ€dimensional fixedâ€site model for H2 on Cu(111). Journal of Chemical Physics, 1995, 102, 6280-6289.	1.2	117
24	New Advance in Computational Chemistry:â€‰ Full Quantum Mechanical ab Initio Computation of Streptavidinâ^'Biotin Interaction Energy. Journal of Physical Chemistry B, 2003, 107, 12039-12041.	1.2	117
25	A reactantâ€product decoupling method for stateâ€toâ€state reactive scattering. Journal of Chemical Physics, 1996, 105, 6072-6074.	1.2	114
26	Computational Protein Design with Deep Learning Neural Networks. Scientific Reports, 2018, 8, 6349.	1.6	112
27	Time-Dependent Wave Packet Approach to State-to-State Reactive Scattering and Application to H + O2Reaction. The Journal of Physical Chemistry, 1996, 100, 6898-6903.	2.9	111
28	Complex reaction processes in combustion unraveled by neural network-based molecular dynamics simulation. Nature Communications, 2020, 11, 5713.	5.8	111
29	Quantum calculations of reaction probabilities for HO + COâ†' H + CO2 and bound states of HOCO. Journal of Chemical Physics, 1995, 103, 6512-6519.	1.2	107
30	Hydrogen-bond structure dynamics in bulk water: insights from ab initio simulations with coupled cluster theory. Chemical Science, 2018, 9, 2065-2073.	3.7	98
31	Interaction entropy for protein-protein binding. Journal of Chemical Physics, 2017, 146, 124124.	1.2	92
32	CHARMM-GUI HMMM Builder for Membrane Simulations with the Highly Mobile Membrane-Mimetic Model. Biophysical Journal, 2015, 109, 2012-2022.	0.2	89
33	An accurate free energy estimator: based on MM/PBSA combined with interaction entropy for proteinâ€“ligand binding affinity. Nanoscale, 2020, 12, 10737-10750.	2.8	88
34	An Electrochemical Biosensor with Dual Signal Outputs: Toward Simultaneous Quantification of pH and O₂ in the Brain upon Ischemia and in a Tumor during Cancer Starvation Therapy. Angewandte Chemie - International Edition, 2017, 56, 10471-10475.	7.2	84
35	Interaction Entropy for Computational Alanine Scanning. Journal of Chemical Information and Modeling, 2017, 57, 1112-1122.	2.5	80
36	MolGpka: A Web Server for Small Molecule pK_a Prediction Using a Graph-Convolutional Neural Network. Journal of Chemical Information and Modeling, 2021, 61, 3159-3165.	2.5	79

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37	Calculations of Solvation Free Energy through Energy Reweighting from Molecular Mechanics to Quantum Mechanics. Journal of Chemical Theory and Computation, 2016, 12, 499-511.	2.3	78
38	Computational Alanine Scanning with Interaction Entropy for Proteinâ€“Ligand Binding Free Energies. Journal of Chemical Theory and Computation, 2018, 14, 1772-1780.	2.3	78
39	Automated Fragmentation QM/MM Calculation of Amide Proton Chemical Shifts in Proteins with Explicit Solvent Model. Journal of Chemical Theory and Computation, 2013, 9, 2104-2114.	2.3	73
40	Six-dimensional quantum calculations of vibration-rotation-tunneling levels of Î½1 and Î½2 HCl-stretching excited (HCl)2. Journal of Chemical Physics, 1998, 108, 4804-4816.	1.2	66
41	BamA POTRA Domain Interacts with a Native Lipid Membrane Surface. Biophysical Journal, 2016, 110, 2698-2709.	0.2	65
42	Photofragmentation of HF dimer: Quantum dynamics studies on ab initio potential energy surfaces. Journal of Chemical Physics, 1993, 99, 6624-6633.	1.2	64
43	Symmetry and rotational orientation effects in dissociative adsorption of diatomic molecules on metals: H2 and HD on Cu(111). Journal of Chemical Physics, 1994, 101, 1555-1563.	1.2	64
44	Dynamics and Interactions of OmpF and LPS: Influence on Pore Accessibility and Ion Permeability. Biophysical Journal, 2016, 110, 930-938.	0.2	64
45	Time-dependent quantum dynamics study of the Cl+H2 reaction. Journal of Chemical Physics, 2000, 113, 1434-1440.	1.2	60
46	Quantum Fragment Based ab Initio Molecular Dynamics for Proteins. Journal of Chemical Theory and Computation, 2015, 11, 5897-5905.	2.3	59
47	CHARMM-GUI Supports Hydrogen Mass Repartitioning and Different Protonation States of Phosphates in Lipopolysaccharides. Journal of Chemical Information and Modeling, 2021, 61, 831-839.	2.5	59
48	Accelerated Molecular Dynamics Simulation for Helical Proteins Folding in Explicit Water. Frontiers in Chemistry, 2019, 7, 540.	1.8	56
49	A timeâ€dependent approach to flux calculation in molecular photofragmentation: Vibrational predissociation of HFâ€“DF. Journal of Chemical Physics, 1995, 102, 124-132.	1.2	55
50	Fragment Quantum Mechanical Method for Large-Sized Ionâ€“Water Clusters. Journal of Chemical Theory and Computation, 2017, 13, 2021-2034.	2.3	54
51	Use of negative complex potential as absorbing potential. Journal of Chemical Physics, 1998, 108, 1429-1433.	1.2	52
52	Time-dependent quantum wave packet studies of the F+HCl and F+DCl reactions. Journal of Chemical Physics, 2000, 113, 10105-10113.	1.2	52
53	Quantum computational analysis for drug resistance of HIV-1 reverse transcriptase to nevirapine through point mutations. Proteins: Structure, Function and Bioinformatics, 2005, 61, 423-432.	1.5	52
54	Quantum dynamics studies of adsorption and desorption of hydrogen at a Cu(111) surface. Journal of Chemical Physics, 1993, 99, 1373-1381.	1.2	51

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55	Proteinâ€“Ligand Empirical Interaction Components for Virtual Screening. Journal of Chemical Information and Modeling, 2017, 57, 1793-1806.	2.5	51
56	Interaction entropy for computational alanine scanning in protein-protein binding. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1342.	6.2	51
57	Maturation Mechanism of Severe Acute Respiratory Syndrome (SARS) Coronavirus 3C-like Proteinase. Journal of Biological Chemistry, 2010, 285, 28134-28140.	1.6	50
58	Dissociative chemisorption of H2 on Ni surface: Timeâ€dependent quantum dynamics calculation and comparison with experiment. Journal of Chemical Physics, 1992, 96, 3866-3874.	1.2	49
59	Reactant-product decoupling method for state-to-state reactive scattering: A case study for 3D H+H2 exchange reaction (J=0). Journal of Chemical Physics, 1997, 106, 1742-1748.	1.2	49
60	Timeâ€dependent treatment of vibrational predissociation within the golden rule approximation. Journal of Chemical Physics, 1991, 95, 6449-6455.	1.2	47
61	CHARMM-GUI PACE CG Builder for Solution, Micelle, and Bilayer Coarse-Grained Simulations. Journal of Chemical Information and Modeling, 2014, 54, 1003-1009.	2.5	47
62	Calculation of proteinâ€“ligand binding affinities based on a fragment quantum mechanical method. RSC Advances, 2015, 5, 107020-107030.	1.7	47
63	DenseCPD: Improving the Accuracy of Neural-Network-Based Computational Protein Sequence Design with DenseNet. Journal of Chemical Information and Modeling, 2020, 60, 1245-1252.	2.5	47
64	Identifying Allosteric Binding Sites in Proteins with a Two-State Goì... Model for Novel Allosteric Effector Discovery. Journal of Chemical Theory and Computation, 2012, 8, 2962-2971.	2.3	46
65	DFT Calculations on the Mechanism of Transition-Metal-Catalyzed Reaction of Diazo Compounds with Phenols: Oâ€“H Insertion versus Câ€“H Insertion. Journal of Physical Chemistry A, 2016, 120, 6485-6492.	1.1	45
66	Single Biosensor for Simultaneous Quantification of Glucose and pH in a Rat Brain of Diabetic Model Using Both Current and Potential Outputs. Analytical Chemistry, 2017, 89, 6656-6662.	3.2	45
67	Quantum dynamics study of Li + HF reaction. Theoretical Chemistry Accounts, 1997, 96, 31-38.	0.5	44
68	A New Quantum Calibrated Force Field for Zincâ€“Protein Complex. Journal of Chemical Theory and Computation, 2013, 9, 1788-1798.	2.3	44
69	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
70	DeepBSPâ€”a Machine Learning Method for Accurate Prediction of Proteinâ€“Ligand Docking Structures. Journal of Chemical Information and Modeling, 2021, 61, 2231-2240.	2.5	44
71	Progress of basis optimization techniques in variational calculation of quantum reactive scattering. Journal of Chemical Physics, 1991, 94, 6047-6054.	1.2	43
72	6D quantum calculation of energy levels for HF stretching excited (HF)2. Journal of Chemical Physics, 1995, 103, 2548-2554.	1.2	42

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73	A numerically stable restrained electrostatic potential charge fitting method. Journal of Computational Chemistry, 2013, 34, 847-853.	1.5	42
74	Modeling and simulation of bacterial outer membranes and interactions with membrane proteins. Current Opinion in Structural Biology, 2017, 43, 131-140.	2.6	42
75	CHARMMâ€GUI Nanodisc Builder for modeling and simulation of various nanodisc systems. Journal of Computational Chemistry, 2019, 40, 893-899.	1.5	42
76	Application of Semirigid Vibrating Rotor Target Model to the Reaction of O(3P) + CH4â†' CH3+ OHâ€. Journal of Physical Chemistry A, 2001, 105, 2530-2534.	1.1	41
77	A timeâ€dependent golden rule wave packet calculation for vibrational predissociation of D2HF. Journal of Chemical Physics, 1992, 97, 927-934.	1.2	40
78	Timeâ€dependent spectral calculation of bound and resonance energies of HO2. Journal of Chemical Physics, 1996, 104, 3664-3671.	1.2	40
79	Unfolding of a ClC chloride transporter retains memory of its evolutionary history. Nature Chemical Biology, 2018, 14, 489-496.	3.9	39
80	Preferred Orientations of Phosphoinositides in Bilayers and Their Implications in Protein Recognition Mechanisms. Journal of Physical Chemistry B, 2014, 118, 4315-4325.	1.2	38
81	Electronic Polarization Is Important in Stabilizing the Native Structures of Proteins. Journal of Physical Chemistry B, 2009, 113, 16059-16064.	1.2	37
82	Accurate and Efficient Calculation of Proteinâ€"Protein Binding Free Energy-Interaction Entropy with Residue Type-Specific Dielectric Constants. Journal of Chemical Information and Modeling, 2019, 59, 272-281.	2.5	37
83	Quantum mechanical calculation for photodissociation of hydrogen peroxide. Journal of Chemical Physics, 1993, 98, 6276-6283.	1.2	35
84	A timeâ€dependent calculation for vibrational predissociation of H2HF. Journal of Chemical Physics, 1992, 97, 3149-3156.	1.2	34
85	Preferred conformations ofN-glycan core pentasaccharide in solution and in glycoproteins. Glycobiology, 2016, 26, cwv083.	1.3	34
86	HobPre: accurate prediction of human oral bioavailability for small molecules. Journal of Cheminformatics, 2022, 14, 1.	2.8	32
87	Hybrid QM/MM study of FMO complex with polarized protein-specific charge. Scientific Reports, 2015, 5, 17096.	1.6	30
88	Mechanistic Investigation of Aromatic C(sp²)â€"H and Alkyl C(sp³)â€"H Bond Insertion by Gold Carbenes. Journal of Physical Chemistry A, 2016, 120, 1925-1932.	1.1	29
89	Decoding molecular mechanism of inhibitor bindings to CDK2 using molecular dynamics simulations and binding free energy calculations. Journal of Biomolecular Structure and Dynamics, 2020, 38, 985-996.	2.0	29
90	The origin of the cooperativity in the streptavidin-biotin system: A computational investigation through molecular dynamics simulations. Scientific Reports, 2016, 6, 27190.	1.6	28

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91	Quantum dynamical studies for photodissociation of H2O2 at 248 and 266 nm. Journal of Chemical Physics, 1994, 100, 5631-5638.	1.2	27
92	Quantum dynamics study of the Cl+D2 reaction: Time-dependent wave packet calculations. Journal of Chemical Physics, 2000, 113, 7182-7187.	1.2	27
93	Time-dependent quantum wave packet study of the C+CH reaction. Journal of Chemical Physics, 2001, 115, 731-738.	1.2	27
94	A mixed quantum-classical semirigid vibrating rotor target approach to methane dissociation on Ni surface. Journal of Chemical Physics, 2003, 118, 8954-8959.	1.2	27
95	Accurate quantum mechanical calculation for the N+OH reaction. Journal of Chemical Physics, 2003, 118, 6852-6857.	1.2	27
96	An algebraic variational approach to dissociative adsorption of a diatomic molecule on a smooth metal surface. Journal of Chemical Physics, 1992, 97, 6784-6791.	1.2	26
97	Energy Dependence of State-to-State Reaction Probabilities for H2+ OH â†' H + H2O in Six Dimensions. The Journal of Physical Chemistry, 1996, 100, 13901-13903.	2.9	26
98	Full quantum mechanical study of binding of HIV-1 protease drugs. International Journal of Quantum Chemistry, 2005, 103, 246-257.	1.0	26
99	Anchor-Locker Binding Mechanism of the Coronavirus Spike Protein to Human ACE2: Insights from Computational Analysis. Journal of Chemical Information and Modeling, 2021, 61, 3529-3542.	2.5	26
100	Discovery of Novel Allosteric Effectors Based on the Predicted Allosteric Sites for Escherichia coli D-3-Phosphoglycerate Dehydrogenase. PLoS ONE, 2014, 9, e94829.	1.1	26
101	HergSPred: Accurate Classification of hERG Blockers/Nonblockers with Machine-Learning Models. Journal of Chemical Information and Modeling, 2022, 62, 1830-1839.	2.5	26
102	Vibrational predissociation of HF dimer in Î½HF=1: Influence of initially excited intermolecular vibrations on the fragmentation dynamics. Journal of Chemical Physics, 1995, 102, 4382-4389.	1.2	25
103	CHARMM-GUI MDFF/xMDFF Utilizer for Molecular Dynamics Flexible Fitting Simulations in Various Environments. Journal of Physical Chemistry B, 2017, 121, 3718-3723.	1.2	24
104	Molecular Dynamics Simulation of Zinc Ion in Water with an ab Initio Based Neural Network Potential. Journal of Physical Chemistry A, 2019, 123, 6587-6595.	1.1	24
105	Total and partial decay widths in vibrational predissociation of HF dimer. Journal of Chemical Physics, 1993, 98, 5978-5981.	1.2	23
106	Computational analysis of hot spots and binding mechanism in the PD-1/PD-L1 interaction. RSC Advances, 2019, 9, 14944-14956.	1.7	23
107	Thermodynamic Insights of Base Flipping in TNA Duplex: Force Fields, Salt Concentrations, and Free-Energy Simulation Methods. CCS Chemistry, 2021, 3, 1026-1039.	4.6	23
108	Theoretical model for the dynamics of hydrogen recombination on the Si(100)â€(2Ã—1) surface. Journal of Chemical Physics, 1992, 97, 596-604.	1.2	22

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109	A Coupled Ionization-Conformational Equilibrium Is Required To Understand the Properties of Ionizable Residues in the Hydrophobic Interior of Staphylococcal Nuclease. Journal of the American Chemical Society, 2018, 140, 1639-1648.	6.6	22
110	BARâ€based optimum adaptive steered MD for configurational sampling. Journal of Computational Chemistry, 2019, 40, 1270-1289.	1.5	22
111	Understanding the selectivity of inhibitors toward PI4KIIIÎ± and PI4KIIIÎ² based molecular modeling. Physical Chemistry Chemical Physics, 2019, 21, 22103-22112.	1.3	22
112	Calculation of hot spots for proteinâ€“protein interaction in p53/PMIâ€MDM2/MDMX complexes. Journal of Computational Chemistry, 2019, 40, 1045-1056.	1.5	22
113	Studying the Effect of Site-Specific Hydrophobicity and Polarization on Hydrogen Bond Energy of Protein Using a Polarizable Method. Journal of Chemical Theory and Computation, 2012, 8, 2157-2164.	2.3	21
114	Full QM Calculation of RNA Energy Using Electrostatically Embedded Generalized Molecular Fractionation with Conjugate Caps Method. Journal of Physical Chemistry A, 2017, 121, 2503-2514.	1.1	21
115	Study of SHMT2 Inhibitors and Their Binding Mechanism by Computational Alanine Scanning. Journal of Chemical Information and Modeling, 2019, 59, 3871-3878.	2.5	21
116	Sulfur-substitution-induced base flipping in the DNA duplex. Physical Chemistry Chemical Physics, 2019, 21, 14923-14940.	1.3	21
117	Entropic effect and residue specific entropic contribution to the cooperativity in streptavidinâ€“biotin binding. Nanoscale, 2020, 12, 7134-7145.	2.8	21
118	Time-Dependent Quantum Dynamics Study of the Cl + HD Reactionâ€. Journal of Physical Chemistry A, 2000, 104, 10517-10525.	1.1	20
119	Conformational Flexibility of a Short Loop near the Active Site of the SARS-3CLpro is Essential to Maintain Catalytic Activity. Scientific Reports, 2016, 6, 20918.	1.6	20
120	Effect of polarization on HIV-1protease and fluoro-substituted inhibitors binding energies by large scale molecular dynamics simulations. Scientific Reports, 2017, 7, 42223.	1.6	20
121	An efficient method for computing excess free energy of liquid. Science China Chemistry, 2018, 61, 135-140.	4.2	20
122	Mechanistic Studies of CO2 Cycloaddition Reaction Catalyzed by Amine-Functionalized Ionic Liquids. Frontiers in Chemistry, 2019, 7, 615.	1.8	20
123	Double-Well Ultra-Coarse-Grained Model to Describe Protein Conformational Transitions. Journal of Chemical Theory and Computation, 2020, 16, 6678-6689.	2.3	20
124	Quantum mechanical tunneling through a timeâ€dependent barrier. Journal of Chemical Physics, 1996, 105, 8628-8632.	1.2	19
125	Effect of interprotein polarization on proteinâ€“protein binding energy. Journal of Computational Chemistry, 2012, 33, 1416-1420.	1.5	19
126	Development of an Effective Polarizable Bond Method for Biomolecular Simulation. Journal of Physical Chemistry B, 2013, 117, 14885-14893.	1.2	19

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127	Constructing Optimal Coarse-Grained Sites of Huge Biomolecules by Fluctuation Maximization. Journal of Chemical Theory and Computation, 2016, 12, 2091-2100.	2.3	19
128	An Electrochemical Biosensor with Dual Signal Outputs: Toward Simultaneous Quantification of pH and O₂ in the Brain upon Ischemia and in a Tumor during Cancer Starvation Therapy. Angewandte Chemie, 2017, 129, 10607-10611.	1.6	19
129	Probing the Ion-Specific Effects at the Water/Air Interface and Water-Mediated Ion Pairing in Sodium Halide Solution with Ab Initio Molecular Dynamics. Journal of Physical Chemistry B, 2018, 122, 10202-10209.	1.2	19
130	CHARMMâ€GUI DEER facilitator for spinâ€pair distance distribution calculations and preparation of restrainedâ€ensemble molecular dynamics simulations. Journal of Computational Chemistry, 2020, 41, 415-420.	1.5	19
131	Dissociative Adsorption of O2on Cu(110) and Cu(100):Â Three-Dimensional Quantum Dynamics Studies. The Journal of Physical Chemistry, 1996, 100, 11432-11437.	2.9	18
132	Simulation of the thermodynamics of folding and unfolding of the Trp-cage mini-protein TC5b using different combinations of force fields and solvation models. Science China Chemistry, 2010, 53, 196-201.	4.2	18
133	Insight into Early-Stage Unfolding of GPI-Anchored Human Prion Protein. Biophysical Journal, 2015, 109, 2090-2100.	0.2	18
134	A new algorithm for construction of coarse-grained sites of large biomolecules. Journal of Computational Chemistry, 2016, 37, 795-804.	1.5	18
135	Effect of Substituents in Different Positions of Aminothiazole Hinge-Binding Scaffolds on Inhibitorâ€“CDK2 Association Probed by Interaction Entropy Method. ACS Omega, 2018, 3, 18052-18064.	1.6	18
136	Allosteric sites can be identified based on the residue-residue interaction energy difference. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1375-1384.	1.5	17
137	A Fragment Quantum Mechanical Method for Metalloproteins. Journal of Chemical Theory and Computation, 2019, 15, 1430-1439.	2.3	17
138	Residue-specific free energy analysis in ligand bindings to JAK2. Molecular Physics, 2018, 116, 2633-2641.	0.8	16
139	Binding modes and conformational changes of FK506-binding protein 51 induced by inhibitor bindings: insight into molecular mechanisms based on multiple simulation technologies. Journal of Biomolecular Structure and Dynamics, 2020, 38, 2141-2155.	2.0	16
140	Roles of glycans in interactions between gp120 and HIV broadly neutralizing antibodies. Glycobiology, 2015, 26, cwv101.	1.3	15
141	Functional Loop Dynamics of the Streptavidin-Biotin Complex. Scientific Reports, 2015, 5, 7906.	1.6	15
142	Correct folding of an Î±-helix and a Î²-hairpin using a polarized 2D torsional potential. Scientific Reports, 2015, 5, 10359.	1.6	15
143	A systematic study on RNA NMR chemical shift calculation based on the automated fragmentation QM/MM approach. RSC Advances, 2016, 6, 108590-108602.	1.7	14
144	Exploring the Reasons for Decrease in Binding Affinity of HIV-2 Against HIV-1 Protease Complex Using Interaction Entropy Under Polarized Force Field. Frontiers in Chemistry, 2018, 6, 380.	1.8	14

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145	Automated Fragmentation QM/MM Calculation of NMR Chemical Shifts for Protein-Ligand Complexes. Frontiers in Chemistry, 2018, 6, 150.	1.8	14
146	Developing an effective polarizable bond method for small molecules with application to optimized molecular docking. RSC Advances, 2020, 10, 15530-15540.	1.7	14
147	Immune Escape Mechanisms of SARS-CoV-2 Delta and Omicron Variants against Two Monoclonal Antibodies That Received Emergency Use Authorization. Journal of Physical Chemistry Letters, 2022, 13, 6064-6073.	2.1	14
148	Noiseâ€free spectrum for timeâ€dependent calculation of eigenenergies. Journal of Chemical Physics, 1995, 103, 1491-1497.	1.2	13
149	Folding Simulations of a De Novo Designed Protein with a Î²Î±Î² Fold. Biophysical Journal, 2010, 98, 321-329.	0.2	13
150	Glycosylation Modulates Human CD2-CD58 Adhesion via Conformational Adjustment. Journal of Physical Chemistry B, 2015, 119, 6493-6501.	1.2	13
151	Direct folding simulation of helical proteins using an effective polarizable bond force field. Physical Chemistry Chemical Physics, 2017, 19, 15273-15284.	1.3	13
152	Theoretical understanding of the thermodynamics and interactions in transcriptional regulator TtgRâ€“ligand binding. Physical Chemistry Chemical Physics, 2020, 22, 1511-1524.	1.3	13
153	Molecular Mechanism of Selective Binding of NMS-P118 to PARP-1 and PARP-2: A Computational Perspective. Frontiers in Molecular Biosciences, 2020, 7, 50.	1.6	13
154	Ab initio neural network MD simulation of thermal decomposition of a high energy material CL-20/TNT. Physical Chemistry Chemical Physics, 2022, 24, 11801-11811.	1.3	13
155	Quantification of Drive-Response Relationships Between Residues During Protein Folding. Journal of Chemical Theory and Computation, 2013, 9, 3799-3805.	2.3	12
156	STâ€analyzer: A webâ€based user interface for simulation trajectory analysis. Journal of Computational Chemistry, 2014, 35, 957-963.	1.5	12
157	Replacing Arginine 33 for Alanine in the Hemophore HasA from Pseudomonas aeruginosa Causes Closure of the H32 Loop in the Apo-Protein. Biochemistry, 2016, 55, 2622-2631.	1.2	12
158	PBSA_E: A PBSA-Based Free Energy Estimator for Proteinâ€“Ligand Binding Affinity. Journal of Chemical Information and Modeling, 2016, 56, 854-861.	2.5	12
159	TMFFâ€”A Two-Bead Multipole Force Field for Coarse-Grained Molecular Dynamics Simulation of Protein. Journal of Chemical Theory and Computation, 2016, 12, 6147-6156.	2.3	12
160	Asymmetric Cryo-EM Structure of Anthrax Toxin Protective Antigen Pore with Lethal Factor N-Terminal Domain. Toxins, 2017, 9, 298.	1.5	12
161	A method for efficient calculation of thermal stability of proteins upon point mutations. Physical Chemistry Chemical Physics, 2020, 22, 8461-8466.	1.3	12
162	SVRT calculation for bond-selective reaction H+HODâ†'H2+OD,â€,HD+OH. Journal of Chemical Physics, 2002, 116, 10197-10200.	1.2	11

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163	Folding and thermodynamic studies of Trp-cage based on polarized force field. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	11
164	Direct folding simulation of a long helix in explicit water. Applied Physics Letters, 2013, 102, .	1.5	11
165	Unveiling the gating mechanism of ECF Transporter RibU. Scientific Reports, 2013, 3, 3566.	1.6	11
166	Quantum mechanical calculation of electric fields and vibrational Stark shifts at active site of human aldose reductase. Journal of Chemical Physics, 2015, 143, 184111.	1.2	11
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