John Z H Zhang

List of Publications by Year
in descending order

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166	6,911	66343	74163
papers	citations	42 h-index	75 g-index

168	168	168	5754
all docs	docs citations	times ranked	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.	47.7	1,064
2	Discovery of a Potent and Selective Inhibitor of Cyclin-Dependent Kinase 4/6. Journal of Medicinal Chemistry, 2005, 48, 2388-2406.	6.4	438
3	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.	13.7	297
4	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.	2.8	243
5	Fragment Quantum Mechanical Calculation of Proteins and Its Applications. Accounts of Chemical Research, 2014, 47, 2748-2757.	15.6	173
6	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.	0.5	151
7	DeepDDG: Predicting the Stability Change of Protein Point Mutations Using Neural Networks. Journal of Chemical Information and Modeling, 2019, 59, 1508-1514.	5.4	146
8	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.	14.5	130
9	A new method for direct calculation of total energy of protein. Journal of Chemical Physics, 2005, 122, 031103.	3.0	119
10	A Comparative Insight into Amprenavir Resistance of Mutations V32I, G48V, I50V, I54V, and I84V in HIV-1 Protease Based on Thermodynamic Integration and MM-PBSA Methods. Journal of Chemical Information and Modeling, 2015, 55, 1903-1913.	5.4	118
11	Origins of unique gold-catalysed chemo- and site-selective Câ€“H functionalization of phenols with diazo compounds. Chemical Science, 2016, 7, 1988-1995.	7.4	118
12	Computational Protein Design with Deep Learning Neural Networks. Scientific Reports, 2018, 8, 6349.	3.3	112
13	Complex reaction processes in combustion unraveled by neural network-based molecular dynamics simulation. Nature Communications, 2020, 11, 5713.	12.8	111
14	Electrostatic Polarization Makes a Substantial Contribution to the Free Energy of Avidinâ^'Biotin Binding. Journal of the American Chemical Society, 2010, 132, 5137-5142.	13.7	105
15	Hydrogen-bond structure dynamics in bulk water: insights from ab initio simulations with coupled cluster theory. Chemical Science, 2018, 9, 2065-2073.	7.4	98
16	An efficient approach for ab initio energy calculation of biopolymers. Journal of Chemical Physics, 2005, 122, 184105.	3.0	96
17	Electrostatically Embedded Generalized Molecular Fractionation with Conjugate Caps Method for Full Quantum Mechanical Calculation of Protein Energy. Journal of Physical Chemistry A, 2013, 117, 7149-7161.	2.5	93
18	Interaction entropy for protein-protein binding. Journal of Chemical Physics, 2017, 146, 124124.	3.0	92

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19	The generalized molecular fractionation with conjugate caps/molecular mechanics method for direct calculation of protein energy. Journal of Chemical Physics, 2006, 124, 184703.	3.0	90
20	Folding of a Helix at Room Temperature Is Critically Aided by Electrostatic Polarization of Intraprotein Hydrogen Bonds. Journal of the American Chemical Society, 2010, 132, 11159-11164.	13.7	88
21	An accurate free energy estimator: based on MM/PBSA combined with interaction entropy for proteinâ€“ligand binding affinity. Nanoscale, 2020, 12, 10737-10750.	5.6	88
22	Interaction Entropy for Computational Alanine Scanning. Journal of Chemical Information and Modeling, 2017, 57, 1112-1122.	5.4	80
23	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.	5.4	79
24	Calculations of Solvation Free Energy through Energy Reweighting from Molecular Mechanics to Quantum Mechanics. Journal of Chemical Theory and Computation, 2016, 12, 499-511.	5.3	78
25	Computational Alanine Scanning with Interaction Entropy for Proteinâ€“Ligand Binding Free Energies. Journal of Chemical Theory and Computation, 2018, 14, 1772-1780.	5.3	78
26	Fragment density functional theory calculation of NMR chemical shifts for proteins with implicit solvation. Physical Chemistry Chemical Physics, 2012, 14, 7837-7845.	2.8	74
27	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.	5.3	73
28	Selectivity of Neutral/Weakly Basic P1 Group Inhibitors of Thrombin and Trypsin by a Molecular Dynamics Study. Chemistry - A European Journal, 2008, 14, 8704-8714.	3.3	69
29	Activatable Nearâ€Infrared Probe for Fluorescence Imaging of Î³â€Glutamyl Transpeptidase in Tumor Cells and In Vivo. Chemistry - A European Journal, 2017, 23, 14778-14785.	3.3	69
30	Fragment quantum chemical approach to geometry optimization and vibrational spectrum calculation of proteins. Physical Chemistry Chemical Physics, 2016, 18, 1864-1875.	2.8	60
31	Quantum Fragment Based ab Initio Molecular Dynamics for Proteins. Journal of Chemical Theory and Computation, 2015, 11, 5897-5905.	5.3	59
32	Intra-protein hydrogen bonding is dynamically stabilized by electronic polarization. Journal of Chemical Physics, 2009, 130, 115102.	3.0	58
33	Simulation of NMR Data Reveals That Proteinsâ€™ Local Structures Are Stabilized by Electronic Polarization. Journal of the American Chemical Society, 2009, 131, 8636-8641.	13.7	57
34	Fragment Quantum Mechanical Method for Large-Sized Ionâ€“Water Clusters. Journal of Chemical Theory and Computation, 2017, 13, 2021-2034.	5.3	54
35	ReacNetGenerator: an automatic reaction network generator for reactive molecular dynamics simulations. Physical Chemistry Chemical Physics, 2020, 22, 683-691.	2.8	54
36	Proteinâ€“Ligand Empirical Interaction Components for Virtual Screening. Journal of Chemical Information and Modeling, 2017, 57, 1793-1806.	5.4	51

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37	Interaction entropy for computational alanine scanning in protein-protein binding. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1342.	14.6	51
38	Structure of liquid water â€“ a dynamical mixture of tetrahedral and â€˜ring-and-chainâ€™ like structures. Physical Chemistry Chemical Physics, 2017, 19, 11931-11936.	2.8	50
39	Calculation of proteinâ€“ligand binding affinities based on a fragment quantum mechanical method. RSC Advances, 2015, 5, 107020-107030.	3.6	47
40	DenseCPD: Improving the Accuracy of Neural-Network-Based Computational Protein Sequence Design with DenseNet. Journal of Chemical Information and Modeling, 2020, 60, 1245-1252.	5.4	47
41	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.	2.5	45
42	A New Quantum Calibrated Force Field for Zincâ€“Protein Complex. Journal of Chemical Theory and Computation, 2013, 9, 1788-1798.	5.3	44
43	The impact of interior dielectric constant and entropic change on HIV-1 complex binding free energy prediction. Structural Dynamics, 2018, 5, 064101.	2.3	44
44	DeepBSPâ€”a Machine Learning Method for Accurate Prediction of Proteinâ€“Ligand Docking Structures. Journal of Chemical Information and Modeling, 2021, 61, 2231-2240.	5.4	44
45	Quantum and Molecular Dynamics Study for Binding of Macrocyclic Inhibitors to Human Î±-Thrombin. Biophysical Journal, 2007, 92, 4244-4253.	0.5	43
46	BAR-based optimum adaptive sampling regime for variance minimization in alchemical transformation. Physical Chemistry Chemical Physics, 2017, 19, 15005-15020.	2.8	41
47	Polarization of Intraprotein Hydrogen Bond Is Critical to Thermal Stability of Short Helix. Journal of Physical Chemistry B, 2012, 116, 549-554.	2.6	39
48	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.	5.4	37
49	An improved fragment-based quantum mechanical method for calculation of electrostatic solvation energy of proteins. Journal of Chemical Physics, 2013, 139, 214104.	3.0	34
50	HobPre: accurate prediction of human oral bioavailability for small molecules. Journal of Cheminformatics, 2022, 14, 1.	6.1	32
51	BAR-based optimum adaptive sampling regime for variance minimization in alchemical transformation: the nonequilibrium stratification. Physical Chemistry Chemical Physics, 2018, 20, 2009-2021.	2.8	31
52	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.	2.5	29
53	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.	3.5	29
54	The origin of the cooperativity in the streptavidin-biotin system: A computational investigation through molecular dynamics simulations. Scientific Reports, 2016, 6, 27190.	3.3	28

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55	Protonation-dependent base flipping in the catalytic triad of a small RNA. Chemical Physics Letters, 2017, 684, 239-244.	2.6	28
56	Folding of a Helix Is Critically Stabilized by Polarization of Backbone Hydrogen Bonds: Study in Explicit Water. Journal of Physical Chemistry B, 2012, 116, 3430-3435.	2.6	27
57	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.	5.4	26
58	HergSPred: Accurate Classification of hERG Blockers/Nonblockers with Machine-Learning Models. Journal of Chemical Information and Modeling, 2022, 62, 1830-1839.	5.4	26
59	Structure and Dynamics of a Dizinc Metalloprotein: Effect of Charge Transfer and Polarization. Journal of Physical Chemistry B, 2011, 115, 10154-10162.	2.6	24
60	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.	2.5	24
61	Predicting Mutation-Induced Stark Shifts in the Active Site of a Protein with a Polarized Force Field. Journal of Physical Chemistry A, 2013, 117, 6015-6023.	2.5	23
62	Computational analysis of hot spots and binding mechanism in the PD-1/PD-L1 interaction. RSC Advances, 2019, 9, 14944-14956.	3.6	23
63	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.	13.7	22
64	BARâ€based optimum adaptive steered MD for configurational sampling. Journal of Computational Chemistry, 2019, 40, 1270-1289.	3.3	22
65	Calculation of hot spots for proteinâ€“protein interaction in p53/PMIâ€MDM2/MDMX complexes. Journal of Computational Chemistry, 2019, 40, 1045-1056.	3.3	22
66	Exploring the Chemical Space of Linear Alkane Pyrolysis via Deep Potential GENerator. Energy & Fuels, 2021, 35, 762-769.	5.1	22
67	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.	5.3	21
68	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.	2.5	21
69	Study of SHMT2 Inhibitors and Their Binding Mechanism by Computational Alanine Scanning. Journal of Chemical Information and Modeling, 2019, 59, 3871-3878.	5.4	21
70	Sulfur-substitution-induced base flipping in the DNA duplex. Physical Chemistry Chemical Physics, 2019, 21, 14923-14940.	2.8	21
71	Entropic effect and residue specific entropic contribution to the cooperativity in streptavidinâ€“biotin binding. Nanoscale, 2020, 12, 7134-7145.	5.6	21
72	Effect of polarization on HIV-1protease and fluoro-substituted inhibitors binding energies by large scale molecular dynamics simulations. Scientific Reports, 2017, 7, 42223.	3.3	20

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73	An efficient method for computing excess free energy of liquid. Science China Chemistry, 2018, 61, 135-140.	8.2	20
74	Mechanistic Studies of CO2 Cycloaddition Reaction Catalyzed by Amine-Functionalized Ionic Liquids. Frontiers in Chemistry, 2019, 7, 615.	3.6	20
75	Double-Well Ultra-Coarse-Grained Model to Describe Protein Conformational Transitions. Journal of Chemical Theory and Computation, 2020, 16, 6678-6689.	5.3	20
76	Effect of interprotein polarization on proteinâ€“protein binding energy. Journal of Computational Chemistry, 2012, 33, 1416-1420.	3.3	19
77	Development of an Effective Polarizable Bond Method for Biomolecular Simulation. Journal of Physical Chemistry B, 2013, 117, 14885-14893.	2.6	19
78	Constructing Optimal Coarse-Grained Sites of Huge Biomolecules by Fluctuation Maximization. Journal of Chemical Theory and Computation, 2016, 12, 2091-2100.	5.3	19
79	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.	2.6	19
80	A new algorithm for construction of coarse-grained sites of large biomolecules. Journal of Computational Chemistry, 2016, 37, 795-804.	3.3	18
81	Optimization of convergence criteria for fragmentation methods. Chemical Physics Letters, 2017, 687, 163-170.	2.6	18
82	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.	3.5	18
83	A Fragment Quantum Mechanical Method for Metalloproteins. Journal of Chemical Theory and Computation, 2019, 15, 1430-1439.	5.3	17
84	The F130L mutation in streptavidin reduces its binding affinity to biotin through electronic polarization effect. Journal of Computational Chemistry, 2013, 34, 2677-2686.	3.3	16
85	Computational search for aflatoxin binding proteins. Chemical Physics Letters, 2017, 685, 1-8.	2.6	16
86	Residue-specific free energy analysis in ligand bindings to JAK2. Molecular Physics, 2018, 116, 2633-2641.	1.7	16
87	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.	3.5	16
88	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.	3.6	14
89	Developing an effective polarizable bond method for small molecules with application to optimized molecular docking. RSC Advances, 2020, 10, 15530-15540.	3.6	14
90	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.	4.6	14

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91	Glycosylation Modulates Human CD2-CD58 Adhesion via Conformational Adjustment. Journal of Physical Chemistry B, 2015, 119, 6493-6501.	2.6	13
92	Direct folding simulation of helical proteins using an effective polarizable bond force field. Physical Chemistry Chemical Physics, 2017, 19, 15273-15284.	2.8	13
93	Theoretical understanding of the thermodynamics and interactions in transcriptional regulator TtgRâ€“ligand binding. Physical Chemistry Chemical Physics, 2020, 22, 1511-1524.	2.8	13
94	Molecular Mechanism of Selective Binding of NMS-P118 to PARP-1 and PARP-2: A Computational Perspective. Frontiers in Molecular Biosciences, 2020, 7, 50.	3.5	13
95	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.	2.8	13
96	PBSA_E: A PBSA-Based Free Energy Estimator for Proteinâ€“Ligand Binding Affinity. Journal of Chemical Information and Modeling, 2016, 56, 854-861.	5.4	12
97	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.	5.3	12
98	A method for efficient calculation of thermal stability of proteins upon point mutations. Physical Chemistry Chemical Physics, 2020, 22, 8461-8466.	2.8	12
99	Benchmark Force Fields for the Molecular Dynamic Simulation of G-Quadruplexes. Molecules, 2021, 26, 5379.	3.8	12
100	Direct folding simulation of a long helix in explicit water. Applied Physics Letters, 2013, 102, .	3.3	11
101	Quantum mechanical calculation of electric fields and vibrational Stark shifts at active site of human aldose reductase. Journal of Chemical Physics, 2015, 143, 184111.	3.0	11
102	A theoretical study of the substituent effect on reactions of amines, carbon dioxide and ethylene oxide catalyzed by binary ionic liquids. RSC Advances, 2017, 7, 51521-51527.	3.6	11
103	Determination of binding affinities of 3-Hydroxy-3-Methylglutaryl Coenzyme A reductase inhibitors from free energy calculation. Chemical Physics Letters, 2019, 723, 1-10.	2.6	11
104	Binding Modes of Smallâ€Molecule Inhibitors to the EED Pocket of PRC2. ChemPhysChem, 2020, 21, 263-271.	2.1	11
105	Development of a New Scoring Function for Virtual Screening: APBScore. Journal of Chemical Information and Modeling, 2020, 60, 6355-6365.	5.4	11
106	Computational approaches to studying methylated H4K20 recognition by DNA repair factor 53BP1. Physical Chemistry Chemical Physics, 2020, 22, 6136-6144.	2.8	11
107	Quantitative analysis of ACE2 binding to coronavirus spike proteins: SARS-CoV-2 vs. SARS-CoV and RaTG13. Physical Chemistry Chemical Physics, 2021, 23, 13926-13933.	2.8	11
108	AA-Score: a New Scoring Function Based on Amino Acid-Specific Interaction for Molecular Docking. Journal of Chemical Information and Modeling, 2022, 62, 2499-2509.	5.4	11

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109	Brownian Dynamics Simulations of Polyalanine in Salt Solutions. The Journal of Physical Chemistry, 1996, 100, 15280-15289.	2.9	10
110	A quantum mechanical computational method for modeling electrostatic and solvation effects of protein. Scientific Reports, 2018, 8, 5475.	3.3	10
111	ES2 enhances the efficacy of chemotherapeutic agents in ABCB1-overexpressing cancer cells in vitro and in vivo. Pharmacological Research, 2018, 129, 388-399.	7.1	10
112	Computational analysis for residue-specific CDK2-inhibitor bindings. Chinese Journal of Chemical Physics, 2019, 32, 134-142.	1.3	10
113	Understanding Aldose Reductase-Inhibitors interactions with free energy simulation. Journal of Molecular Graphics and Modelling, 2019, 91, 10-21.	2.4	10
114	Automatically Constructed Neural Network Potentials for Molecular Dynamics Simulation of Zinc Proteins. Frontiers in Chemistry, 2021, 9, 692200.	3.6	10
115	Electronic polarization stabilizes tertiary structure prediction of HP-36. Journal of Molecular Modeling, 2014, 20, 2195.	1.8	9
116	Two-bead polarizable water models combined with a two-bead multipole force field (TMFF) for coarse-grained simulation of proteins. Physical Chemistry Chemical Physics, 2017, 19, 7410-7419.	2.8	9
117	Drug-resistance mechanisms of three mutations in anaplastic lymphoma kinase against two inhibitors based on MM/PBSA combined with interaction entropy. Physical Chemistry Chemical Physics, 2019, 21, 20951-20964.	2.8	9
118	Determining Optimal Coarseâ€Grained Representation for Biomolecules Using Internal Cluster Validation Indexes. Journal of Computational Chemistry, 2020, 41, 14-20.	3.3	9
119	Cyclopentadienyl radical formation from the reaction of excited nitrogen atoms with benzene: a theoretical study. Physical Chemistry Chemical Physics, 2021, 23, 12408-12420.	2.8	9
120	The intrinsic helical propensities of the helical fragments in prion protein under neutral and low pH conditions: a replica exchange molecular dynamics study. Journal of Molecular Modeling, 2013, 19, 4897-4908.	1.8	8
121	Origins of Protons in Câ€“H Bond Insertion Products of Phenols: Proton-Self-Sufficient Function via Water Molecules. Journal of Physical Chemistry A, 2017, 121, 6523-6529.	2.5	8
122	An Energy Optimization Strategy Based on the Perfect Conformation of Prolyl Endopeptidase for Improving Catalytic Efficiency. Journal of Agricultural and Food Chemistry, 2020, 68, 5129-5137.	5.2	8
123	Inhibition mechanism and hot-spot prediction of nine potential drugs for SARS-CoV-2 M^{pro} by large-scale molecular dynamic simulations combined with accurate binding free energy calculations. Nanoscale, 2021, 13, 8313-8332.	5.6	8
124	Mutational Effect of Some Major COVID-19 Variants on Binding of the S Protein to ACE2. Biomolecules, 2022, 12, 572.	4.0	8
125	Interaction specific binding hotspots in Endonuclease colicin-immunity protein complex from MD simulations. Science China Chemistry, 2013, 56, 1143-1151.	8.2	7
126	Combined effect of confinement and affinity of crowded environment on conformation switching of adenylate kinase. Journal of Molecular Modeling, 2014, 20, 2530.	1.8	7

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127	Molecular basis of SMAC-XIAP binding and the effect of electrostatic polarization. Journal of Biomolecular Structure and Dynamics, 2021, 39, 743-752.	3.5	7
128	Structure, mechanism, and enantioselectivity shifting of lipase LipK107 with a simple way. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2014, 1844, 1183-1192.	2.3	6
129	Performance Comparison of Systematic Methods for Rigorous Definition of Coarse-Grained Sites of Large Biomolecules. Journal of Chemical Information and Modeling, 2017, 57, 214-222.	5.4	6
130	Identification of three new compounds that directly target human serine hydroxymethyltransferase 2. Chemical Biology and Drug Design, 2021, 97, 221-230.	3.2	6
131	Molecular mechanism related to the binding of fluorophores to Mango-II revealed by multiple-replica molecular dynamics simulations. Physical Chemistry Chemical Physics, 2021, 23, 10636-10649.	2.8	6
132	Computational analysis of binding free energies, hotspots and the binding mechanism of Bcl-xL/Bcl-2 binding to Bad/Bax. Physical Chemistry Chemical Physics, 2021, 23, 2025-2037.	2.8	6
133	Automated Construction of Neural Network Potential Energy Surface: The Enhanced Self-Organizing Incremental Neural Network Deep Potential Method. Journal of Chemical Information and Modeling, 2021, 61, 5425-5437.	5.4	6
134	Toxic Effect of Fullerene and Its Derivatives upon the Transmembrane Î²2-Adrenergic Receptors. Molecules, 2022, 27, 4562.	3.8	6
135	Ab initio Quantum Mechanics/Molecular Mechanics Molecular Dynamics Simulation of CO in the Heme Distal Pocket of Myoglobin. Chinese Journal of Chemical Physics, 2017, 30, 705-716.	1.3	5
136	Comparison of the unfolding and oligomerization of human prion protein under acidic and neutral environments by molecular dynamics simulations. Chemical Physics Letters, 2018, 706, 594-600.	2.6	5
137	Formation mechanism and spectroscopy of C₆H radicals in extreme environments: a theoretical study. Physical Chemistry Chemical Physics, 2019, 21, 23044-23055.	2.8	5
138	How CuCl and CuCl₂ Insert into Câ€“N Bonds of Diazo Compounds: An Electronic Structure and Mechanistic Study. Journal of Physical Chemistry A, 2020, 124, 2029-2035.	2.5	5
139	Alanine scanning combined with interaction entropy studying the differences of binding mechanism on HIV-1 and HIV-2 proteases with inhibitor. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1588-1599.	3.5	5
140	Computational Analysis of Residue-Specific Binding Free Energies of Androgen Receptor to Ligands. Frontiers in Molecular Biosciences, 2021, 8, 646524.	3.5	5
141	An electrostatic energy-based charge model for molecular dynamics simulation. Journal of Chemical Physics, 2021, 154, 134107.	3.0	5
142	Rational Design of Pepsin for Enhanced Thermostability via Exploiting the Guide of Structural Weakness on Stability. Frontiers in Physics, 2021, 9, .	2.1	5
143	An ab initio/RRKM study of the reaction mechanism and product branching ratios of CH3OH+ and CH3OH++ dissociation. Journal of Molecular Structure, 2020, 1217, 128410.	3.6	4
144	Engineering the biomimetic cofactors of NMNH for cytochrome P450 BM3 based on binding conformation refinement. RSC Advances, 2021, 11, 12036-12042.	3.6	4

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145	Discovery of novel inhibitors of CDK2 using docking and physicsâ€based binding free energy calculation. Chemical Biology and Drug Design, 2022, 99, 662-673.	3.2	4
146	Protein simulation using coarse-grained two-bead multipole force field with polarizable water models. Journal of Chemical Physics, 2017, 146, 065101.	3.0	3
147	Computational Study of PCSK9-EGFA Complex with Effective Polarizable Bond Force Field. Frontiers in Molecular Biosciences, 2017, 4, 101.	3.5	3
148	A force consistent method for electrostatic energy calculation in fluctuating charge model. Journal of Chemical Physics, 2019, 151, 094105.	3.0	3
149	An Approach to Computing Solvent Reorganization Energy. Journal of Chemical Theory and Computation, 2020, 16, 6513-6519.	5.3	3
150	Ultra-coarse-graining modeling of liquid water. Journal of Chemical Physics, 2021, 154, 224506.	3.0	3
151	A Non-derivative MFCC Optimization Study of Cyclohexapeptide Monohydrate. Chinese Journal of Chemical Physics, 2007, 20, 431-437.	1.3	2
152	Discovery of novel inhibitors of SARS-CoV-2 main protease. Journal of Biomolecular Structure and Dynamics, 2022, 40, 12526-12534.	3.5	2
153	Targeting mechanism for SARS-CoV-2 in silico: interaction and key groups of TMPRSS2 toward four potential drugs. Nanoscale, 2021, 13, 19218-19237.	5.6	2
154	SeBPPI: A Sequence-Based Proteinâ€“Protein Binding Predictor. Journal of Computational Biophysics and Chemistry, 2022, 21, 729-737.	1.7	2
155	Reaction mechanism and product branching ratios of OH+C2H3F reaction: A theoretical study. Chinese Journal of Chemical Physics, 2020, 33, 203-209.	1.3	1
156	Efficient calculation of excess free energy of pure and mixed alcohol solutions. Chemical Physics Letters, 2020, 749, 137397.	2.6	1
157	A fixed multi-site interaction charge model for an accurate prediction of the QM/MM interactions. Physical Chemistry Chemical Physics, 2021, 23, 21001-21012.	2.8	1
158	Fragment-Based Ab Initio Molecular Dynamics Simulation for Combustion. Molecules, 2021, 26, 3120.	3.8	1
159	Analysis of the binding modes of the firstâ€and secondâ€generation antiandrogens with respect to F876L mutation. Chemical Biology and Drug Design, 2021, 98, 60-72.	3.2	1
160	Investigating effects of bridging water on the binding of neuraminidaseâ^'ligands using computational alanine scanning combined with interaction entropy method. Journal of Molecular Liquids, 2021, 336, 116214.	4.9	1
161	Insights into small molecule inhibitor bindings to PD-L1 with residue-specific binding free energy calculation. Journal of Biomolecular Structure and Dynamics, 2022, 40, 12277-12285.	3.5	1
162	Computational Insights into the Binding Mechanism of OxyS sRNA with Chaperone Protein Hfq. Biomolecules, 2021, 11, 1653.	4.0	1

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163	Molecular mechanism of ligand bindings to Zika virus at SAM site. Chemical Physics Letters, 2019, 735, 136771.	2.6	0
164	Residue-specific binding mechanisms of PD-L1 to its monoclonal antibodies by computational alanine scanning. Physical Chemistry Chemical Physics, 2021, 23, 15591-15600.	2.8	0
165	Introducing the effective polarizable bond (EPB) model in DNA simulations. Chemical Physics Letters, 2021, 785, 139160.	2.6	0
166	Computational Alanine Scanning Reveals Common Features of TCR/pMHC Recognition in HLA-DQ8-Associated Celiac Disease. Methods in Molecular Biology, 2022, 2385, 293-312.	0.9	0