Yifei Qi

List of Publications by Year
in descending order

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254	15,318	36303 51	23533 111
papers	citations	h-index	g-index

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

#	Article	IF	Citations
1	Discovery of novel inhibitors of SARS-CoV-2 main protease. Journal of Biomolecular Structure and Dynamics, 2022, 40, 12526-12534.	3.5	2
2	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
3	HobPre: accurate prediction of human oral bioavailability for small molecules. Journal of Cheminformatics, 2022, 14, 1.	6.1	32
4	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
5	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
6	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
7	Mutational Effect of Some Major COVID-19 Variants on Binding of the S Protein to ACE2. Biomolecules, 2022, 12, 572.	4.0	8
8	HergSPred: Accurate Classification of hERG Blockers/Nonblockers with Machine-Learning Models. Journal of Chemical Information and Modeling, 2022, 62, 1830-1839.	5.4	26
9	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
10	SeBPPI: A Sequence-Based Proteinâ€“Protein Binding Predictor. Journal of Computational Biophysics and Chemistry, 2022, 21, 729-737.	1.7	2
11	Rational Design of P450 aMOx for Improving Anti-Markovnikov Selectivity Based on the â€œButterflyâ€• Model. Frontiers in Molecular Biosciences, 2022, 9, .	3.5	2
12	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
13	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
14	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
15	Identification of three new compounds that directly target human serine hydroxymethyltransferase 2. Chemical Biology and Drug Design, 2021, 97, 221-230.	3.2	6
16	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
17	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
18	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

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19	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
20	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
21	Multiscale polarizable coarse-graining water models on cluster-level electrostatic dipoles. Physical Chemistry Chemical Physics, 2021, 23, 8926-8935.	2.8	3
22	Engineering the biomimetic cofactors of NMNH for cytochrome P450 BM3 based on binding conformation refinement. RSC Advances, 2021, 11, 12036-12042.	3.6	4
23	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
24	Thermodynamic Insights of Base Flipping in TNA Duplex: Force Fields, Salt Concentrations, and Free-Energy Simulation Methods. CCS Chemistry, 2021, 3, 1026-1039.	7.8	23
25	Computational Analysis of Residue-Specific Binding Free Energies of Androgen Receptor to Ligands. Frontiers in Molecular Biosciences, 2021, 8, 646524.	3.5	5
26	An electrostatic energy-based charge model for molecular dynamics simulation. Journal of Chemical Physics, 2021, 154, 134107.	3.0	5
27	Fragment-Based Ab Initio Molecular Dynamics Simulation for Combustion. Molecules, 2021, 26, 3120.	3.8	1
28	Investigation on the characteristics and mechanisms of ACE inhibitory peptides by a thorough analysis of all 8000 tripeptides via binding free energy calculation. Food Science and Nutrition, 2021, 9, 2943-2953.	3.4	11
29	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
30	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
31	Automatically Constructed Neural Network Potentials for Molecular Dynamics Simulation of Zinc Proteins. Frontiers in Chemistry, 2021, 9, 692200.	3.6	10
32	Ultra-coarse-graining modeling of liquid water. Journal of Chemical Physics, 2021, 154, 224506.	3.0	3
33	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
34	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
35	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
36	Rational Design of Pepsin for Enhanced Thermostability via Exploiting the Guide of Structural Weakness on Stability. Frontiers in Physics, 2021, 9, .	2.1	5

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37	CHARMM-GUI Supports Hydrogen Mass Repartitioning and Different Protonation States of Phosphates in Lipopolysaccharides. Journal of Chemical Information and Modeling, 2021, 61, 831-839.	5.4	59
38	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
39	Introducing the effective polarizable bond (EPB) model in DNA simulations. Chemical Physics Letters, 2021, 785, 139160.	2.6	0
40	Computational Insights into the Binding Mechanism of OxyS sRNA with Chaperone Protein Hfq. Biomolecules, 2021, 11, 1653.	4.0	1
41	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
42	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
43	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
44	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
45	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.	3.3	19
46	LLPSDB: a database of proteins undergoing liquidâ€“liquid phase separation in vitro. Nucleic Acids Research, 2020, 48, D320-D327.	14.5	130
47	Determining Optimal Coarseâ€Grained Representation for Biomolecules Using Internal Cluster Validation Indexes. Journal of Computational Chemistry, 2020, 41, 14-20.	3.3	9
48	Theoretical understanding of the thermodynamics and interactions in transcriptional regulator TtgRâ€“ligand binding. Physical Chemistry Chemical Physics, 2020, 22, 1511-1524.	2.8	13
49	Binding Modes of Smallâ€Molecule Inhibitors to the EED Pocket of PRC2. ChemPhysChem, 2020, 21, 263-271.	2.1	11
50	Development of a New Scoring Function for Virtual Screening: APBScore. Journal of Chemical Information and Modeling, 2020, 60, 6355-6365.	5.4	11
51	Complex reaction processes in combustion unraveled by neural network-based molecular dynamics simulation. Nature Communications, 2020, 11, 5713.	12.8	111
52	A three-point coarse-grained model of five-water cluster with permanent dipoles and quadrupoles. Physical Chemistry Chemical Physics, 2020, 22, 26289-26298.	2.8	2
53	Double-Well Ultra-Coarse-Grained Model to Describe Protein Conformational Transitions. Journal of Chemical Theory and Computation, 2020, 16, 6678-6689.	5.3	20
54	An Approach to Computing Solvent Reorganization Energy. Journal of Chemical Theory and Computation, 2020, 16, 6513-6519.	5.3	3

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55	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
56	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
57	Computational approaches to studying methylated H4K20 recognition by DNA repair factor 53BP1. Physical Chemistry Chemical Physics, 2020, 22, 6136-6144.	2.8	11
58	Entropic effect and residue specific entropic contribution to the cooperativity in streptavidinâ€“biotin binding. Nanoscale, 2020, 12, 7134-7145.	5.6	21
59	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
60	Atomic-level reconstruction of biomolecules by a rigid-fragment- and local-frame-based (RF-LF) strategy. Journal of Molecular Modeling, 2020, 26, 31.	1.8	3
61	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
62	Developing an effective polarizable bond method for small molecules with application to optimized molecular docking. RSC Advances, 2020, 10, 15530-15540.	3.6	14
63	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
64	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
65	A method for efficient calculation of thermal stability of proteins upon point mutations. Physical Chemistry Chemical Physics, 2020, 22, 8461-8466.	2.8	12
66	Accelerated Molecular Dynamics Simulation for Helical Proteins Folding in Explicit Water. Frontiers in Chemistry, 2019, 7, 540.	3.6	56
67	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
68	A Fragment Quantum Mechanical Method for Metalloproteins. Journal of Chemical Theory and Computation, 2019, 15, 1430-1439.	5.3	17
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	Computational analysis for residue-specific CDK2-inhibitor bindings. Chinese Journal of Chemical Physics, 2019, 32, 134-142.	1.3	10
71	Mechanistic Studies of CO2 Cycloaddition Reaction Catalyzed by Amine-Functionalized Ionic Liquids. Frontiers in Chemistry, 2019, 7, 615.	3.6	20
72	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

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73	A force consistent method for electrostatic energy calculation in fluctuating charge model. Journal of Chemical Physics, 2019, 151, 094105.	3.0	3
74	CHARMM-GUIGlycan Modelerfor modeling and simulation of carbohydrates and glycoconjugates. Glycobiology, 2019, 29, 320-331.	2.5	222
75	CHARMMâ€GUI Nanodisc Builder for modeling and simulation of various nanodisc systems. Journal of Computational Chemistry, 2019, 40, 893-899.	3.3	42
76	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
77	Sulfur-substitution-induced base flipping in the DNA duplex. Physical Chemistry Chemical Physics, 2019, 21, 14923-14940.	2.8	21
78	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
79	Computational analysis of hot spots and binding mechanism in the PD-1/PD-L1 interaction. RSC Advances, 2019, 9, 14944-14956.	3.6	23
80	BARâ€based optimum adaptive steered MD for configurational sampling. Journal of Computational Chemistry, 2019, 40, 1270-1289.	3.3	22
81	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
82	Understanding the selectivity of inhibitors toward PI4KIIIÎ± and PI4KIIIÎ² based molecular modeling. Physical Chemistry Chemical Physics, 2019, 21, 22103-22112.	2.8	22
83	Formation mechanism and spectroscopy of C₆H radicals in extreme environments: a theoretical study. Physical Chemistry Chemical Physics, 2019, 21, 23044-23055.	2.8	5
84	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
85	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
86	CHARMM-GUI Membrane Builder for Complex Biological Membrane Simulations with Glycolipids and Lipoglycans. Journal of Chemical Theory and Computation, 2019, 15, 775-786.	5.3	388
87	An efficient method for computing excess free energy of liquid. Science China Chemistry, 2018, 61, 135-140.	8.2	20
88	Computational Protein Design with Deep Learning Neural Networks. Scientific Reports, 2018, 8, 6349.	3.3	112
89	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
90	Multiple Conformational States Contribute to the 3D Structure of a Glucan Decasaccharide: A Combined SAXS and MD Simulation Study. Journal of Physical Chemistry B, 2018, 122, 1169-1175.	2.6	9

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91	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
92	Crius: A novel fragmentâ€based algorithm of de novo substrate prediction for enzymes. Protein Science, 2018, 27, 1526-1534.	7.6	0
93	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
94	Unfolding of a ClC chloride transporter retains memory of its evolutionary history. Nature Chemical Biology, 2018, 14, 489-496.	8.0	39
95	Interaction entropy for computational alanine scanning in protein-protein binding. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1342.	14.6	51
96	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
97	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
98	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
99	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
100	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
101	Functional loop dynamics of the S-component of ECF transporter FolT. Molecular Physics, 2018, 116, 2613-2621.	1.7	0
102	Electrostatic Polarization Effect on Cooperative Aggregation of Full Length Human Islet Amyloid. Journal of Chemical Information and Modeling, 2018, 58, 1587-1595.	5.4	2
103	Automated Fragmentation QM/MM Calculation of NMR Chemical Shifts for Protein-Ligand Complexes. Frontiers in Chemistry, 2018, 6, 150.	3.6	14
104	A Force Balanced Fragmentation Method for ab Initio Molecular Dynamic Simulation of Protein. Frontiers in Chemistry, 2018, 6, 189.	3.6	5
105	Residue-specific free energy analysis in ligand bindings to JAK2. Molecular Physics, 2018, 116, 2633-2641.	1.7	16
106	Evaluation of the Coupled Two-Dimensional Main Chain Torsional Potential in Modeling Intrinsically Disordered Proteins. Journal of Chemical Information and Modeling, 2017, 57, 267-274.	5.4	6
107	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
108	Protein simulation using coarse-grained two-bead multipole force field with polarizable water models. Journal of Chemical Physics, 2017, 146, 065101.	3.0	3

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109	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
110	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
111	Modeling and simulation of bacterial outer membranes and interactions with membrane proteins. Current Opinion in Structural Biology, 2017, 43, 131-140.	5.7	42
112	Interaction Entropy for Computational Alanine Scanning. Journal of Chemical Information and Modeling, 2017, 57, 1112-1122.	5.4	80
113	Fragment Quantum Mechanical Method for Large-Sized Ionâ€“Water Clusters. Journal of Chemical Theory and Computation, 2017, 13, 2021-2034.	5.3	54
114	Direct folding simulation of helical proteins using an effective polarizable bond force field. Physical Chemistry Chemical Physics, 2017, 19, 15273-15284.	2.8	13
115	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.	13.8	84
116	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.	6.5	45
117	Interaction entropy for protein-protein binding. Journal of Chemical Physics, 2017, 146, 124124.	3.0	92
118	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
119	CHARMM-GUI MDFF/xMDFF Utilizer for Molecular Dynamics Flexible Fitting Simulations in Various Environments. Journal of Physical Chemistry B, 2017, 121, 3718-3723.	2.6	24
120	CHARMMâ€GUI Martini Maker for modeling and simulation of complex bacterial membranes with lipopolysaccharides. Journal of Computational Chemistry, 2017, 38, 2354-2363.	3.3	150
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	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
123	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.	2.0	19
124	Proteinâ€“Ligand Empirical Interaction Components for Virtual Screening. Journal of Chemical Information and Modeling, 2017, 57, 1793-1806.	5.4	51
125	CHARMMâ€GUI 10 years for biomolecular modeling and simulation. Journal of Computational Chemistry, 2017, 38, 1114-1124.	3.3	224
126	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

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127	Asymmetric Cryo-EM Structure of Anthrax Toxin Protective Antigen Pore with Lethal Factor N-Terminal Domain. Toxins, 2017, 9, 298.	3.4	12
128	Computational Study of PCSK9-EGFA Complex with Effective Polarizable Bond Force Field. Frontiers in Molecular Biosciences, 2017, 4, 101.	3.5	3
129	Preferred conformations ofN-glycan core pentasaccharide in solution and in glycoproteins. Glycobiology, 2016, 26, cwv083.	2.5	34
130	A new algorithm for construction of coarse-grained sites of large biomolecules. Journal of Computational Chemistry, 2016, 37, 795-804.	3.3	18
131	A systematic study on RNA NMR chemical shift calculation based on the automated fragmentation QM/MM approach. RSC Advances, 2016, 6, 108590-108602.	3.6	14
132	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.	3.3	20
133	Constructing Optimal Coarse-Grained Sites of Huge Biomolecules by Fluctuation Maximization. Journal of Chemical Theory and Computation, 2016, 12, 2091-2100.	5.3	19
134	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
135	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.	2.5	12
136	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
137	Effects of Spin-Labels on Membrane Burial Depth of MARCKS-ED Residues. Biophysical Journal, 2016, 111, 1600-1603.	0.5	0
138	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
139	A Semiautomated Structure-Based Method To Predict Substrates of Enzymes via Molecular Docking: A Case Study with Candida antarctica Lipase B. Journal of Chemical Information and Modeling, 2016, 56, 1979-1994.	5.4	5
140	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
141	Examination of the quality of various force fields and solvation models for the equilibrium simulations of GA88 and GB88. Journal of Molecular Modeling, 2016, 22, 177.	1.8	5
142	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
143	BamA POTRA Domain Interacts with a Native Lipid Membrane Surface. Biophysical Journal, 2016, 110, 2698-2709.	0.5	65
144	The effect of POPC acyl chains packing by aromatic amino acid methyl esters investigated by ATR-FTIR combined with QM calculations. RSC Advances, 2016, 6, 45569-45577.	3.6	7

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145	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
146	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.	5.3	2,567
147	Dynamics and Interactions of OmpF and LPS: Influence on Pore Accessibility and Ion Permeability. Biophysical Journal, 2016, 110, 930-938.	0.5	64
148	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
149	Hybrid QM/MM study of FMO complex with polarized protein-specific charge. Scientific Reports, 2015, 5, 17096.	3.3	30
150	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
151	Roles of glycans in interactions between gp120 and HIV broadly neutralizing antibodies. Glycobiology, 2015, 26, cwv101.	2.5	15
152	Calculation of proteinâ€“ligand binding affinities based on a fragment quantum mechanical method. RSC Advances, 2015, 5, 107020-107030.	3.6	47
153	Glycosylation Modulates Human CD2-CD58 Adhesion via Conformational Adjustment. Journal of Physical Chemistry B, 2015, 119, 6493-6501.	2.6	13
154	Functional Loop Dynamics of the Streptavidin-Biotin Complex. Scientific Reports, 2015, 5, 7906.	3.3	15
155	Correct folding of an Î±-helix and a Î²-hairpin using a polarized 2D torsional potential. Scientific Reports, 2015, 5, 10359.	3.3	15
156	Solid-State NMR-Restrained Ensemble Dynamics of a Membrane Protein in Explicit Membranes. Biophysical Journal, 2015, 108, 1954-1962.	0.5	11
157	Effects of N-glycosylation on protein conformation and dynamics: Protein Data Bank analysis and molecular dynamics simulation study. Scientific Reports, 2015, 5, 8926.	3.3	187
158	Quantum Fragment Based ab Initio Molecular Dynamics for Proteins. Journal of Chemical Theory and Computation, 2015, 11, 5897-5905.	5.3	59
159	CHARMM-GUI Martini Maker for Coarse-Grained Simulations with the Martini Force Field. Journal of Chemical Theory and Computation, 2015, 11, 4486-4494.	5.3	340
160	CHARMM-GUI HMMM Builder for Membrane Simulations with the Highly Mobile Membrane-Mimetic Model. Biophysical Journal, 2015, 109, 2012-2022.	0.5	89
161	Insight into Early-Stage Unfolding of GPI-Anchored Human Prion Protein. Biophysical Journal, 2015, 109, 2090-2100.	0.5	18
162	Allosteric sites can be identified based on the residue-residue interaction energy difference. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1375-1384.	2.6	17

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163	Energetics of protein backbone hydrogen bonds and their local electrostatic environment. Science China Chemistry, 2014, 57, 1708-1715.	8.2	7
164	STâ€analyzer: A webâ€based user interface for simulation trajectory analysis. Journal of Computational Chemistry, 2014, 35, 957-963.	3.3	12
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