

List of Publications by Year in  
Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

242 papers	9,657 citations	46 h-index	92 g-index
258 ext. papers	12,573 ext. citations	4.8 avg, IF	6.57 L-index

#	Paper	IF	Citations
242	HobPre: accurate prediction of human oral bioavailability for small molecules.. <i>Journal of Cheminformatics</i> , <b>2022</b> , 14, 1	8.6	2
241	Computational Alanine Scanning Reveals Common Features of TCR/pMHC Recognition in HLA-DQ8-Associated Celiac Disease. <i>Methods in Molecular Biology</i> , <b>2022</b> , 2385, 293-312	1.4	
240	neural network MD simulation of thermal decomposition of a high energy material CL-20/TNT.. <i>Physical Chemistry Chemical Physics</i> , <b>2022</b> , 24, 11801-11811	3.6	0
239	Automated Construction of Neural Network Potential Energy Surface: The Enhanced Self-Organizing Incremental Neural Network Deep Potential Method. <i>Journal of Chemical Information and Modeling</i> , <b>2021</b> , 61, 5425-5437	6.1	2
238	Targeting mechanism for SARS-CoV-2 : interaction and key groups of TMPRSS2 toward four potential drugs. <i>Nanoscale</i> , <b>2021</b> , 13, 19218-19237	7.7	0
237	Introducing the effective polarizable bond (EPB) model in DNA simulations. <i>Chemical Physics Letters</i> , <b>2021</b> , 785, 139160	2.5	
236	An electrostatic energy-based charge model for molecular dynamics simulation. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 134107	3.9	3
235	Investigation on the characteristics and mechanisms of ACE inhibitory peptides by a thorough analysis of all 8000 tripeptides via binding free energy calculation. <i>Food Science and Nutrition</i> , <b>2021</b> , 9, 2943-2953	3.2	3
234	Analysis of the binding modes of the first- and second-generation antiandrogens with respect to F876L mutation. <i>Chemical Biology and Drug Design</i> , <b>2021</b> , 98, 60-72	2.9	
233	DeepBSP-a Machine Learning Method for Accurate Prediction of Protein-Ligand Docking Structures. <i>Journal of Chemical Information and Modeling</i> , <b>2021</b> , 61, 2231-2240	6.1	10
232	Automatically Constructed Neural Network Potentials for Molecular Dynamics Simulation of Zinc Proteins. <i>Frontiers in Chemistry</i> , <b>2021</b> , 9, 692200	5	1
231	Ultra-coarse-graining modeling of liquid water. <i>Journal of Chemical Physics</i> , <b>2021</b> , 154, 224506	3.9	2
230	Anchor-Locker Binding Mechanism of the Coronavirus Spike Protein to Human ACE2: Insights from Computational Analysis. <i>Journal of Chemical Information and Modeling</i> , <b>2021</b> , 61, 3529-3542	6.1	7
229	MolGpka: A Web Server for Small Molecule p Prediction Using a Graph-Convolutional Neural Network. <i>Journal of Chemical Information and Modeling</i> , <b>2021</b> , 61, 3159-3165	6.1	9
228	Molecular basis of SMAC-XIAP binding and the effect of electrostatic polarization. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2021</b> , 39, 743-752	3.6	5
227	Alanine scanning combined with interaction entropy studying the differences of binding mechanism on HIV-1 and HIV-2 proteases with inhibitor. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2021</b> , 39, 1588-1599	3.6	4
226	Identification of three new compounds that directly target human serine hydroxymethyltransferase 2. <i>Chemical Biology and Drug Design</i> , <b>2021</b> , 97, 221-230	2.9	2

225	Inhibition mechanism and hot-spot prediction of nine potential drugs for SARS-CoV-2 M by large-scale molecular dynamic simulations combined with accurate binding free energy calculations. <i>Nanoscale</i> , <b>2021</b> , 13, 8313-8332	7.7	4
224	A fixed multi-site interaction charge model for an accurate prediction of the QM/MM interactions. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 21001-21012	3.6	
223	Molecular mechanism related to the binding of fluorophores to Mango-II revealed by multiple-replica molecular dynamics simulations. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 10636-10649	3.6	5
222	Cyclopentadienyl radical formation from the reaction of excited nitrogen atoms with benzene: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 12408-12420	3.6	2
221	Residue-specific binding mechanisms of PD-L1 to its monoclonal antibodies by computational alanine scanning. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 15591-15600	3.6	
220	Multiscale polarizable coarse-graining water models on cluster-level electrostatic dipoles. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 8926-8935	3.6	2
219	Engineering the biomimetic cofactors of NMNH for cytochrome P450 BM3 based on binding conformation refinement.. <i>RSC Advances</i> , <b>2021</b> , 11, 12036-12042	3.7	0
218	Quantitative analysis of ACE2 binding to coronavirus spike proteins: SARS-CoV-2 SARS-CoV and RaTG13. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 13926-13933	3.6	2
217	Thermodynamic Insights of Base Flipping in TNA Duplex: Force Fields, Salt Concentrations, and Free-Energy Simulation Methods. <i>CCS Chemistry</i> , <b>2021</b> , 3, 1026-1039	7.2	11
216	Computational Analysis of Residue-Specific Binding Free Energies of Androgen Receptor to Ligands. <i>Frontiers in Molecular Biosciences</i> , <b>2021</b> , 8, 646524	5.6	1
215	Investigating effects of bridging water on the binding of neuraminidase ligands using computational alanine scanning combined with interaction entropy method. <i>Journal of Molecular Liquids</i> , <b>2021</b> , 336, 116214	6	
214	Discovery of novel inhibitors of SARS-CoV-2 main protease. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2021</b> , 1-9	3.6	1
213	Insights into small molecule inhibitor bindings to PD-L1 with residue-specific binding free energy calculation. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2021</b> , 1-9	3.6	
212	CHARMM-GUI Supports Hydrogen Mass Repartitioning and Different Protonation States of Phosphates in Lipopolysaccharides. <i>Journal of Chemical Information and Modeling</i> , <b>2021</b> , 61, 831-839	6.1	10
211	Computational analysis of binding free energies, hotspots and the binding mechanism of Bcl-xL/Bcl-2 binding to Bad/Bax. <i>Physical Chemistry Chemical Physics</i> , <b>2021</b> , 23, 2025-2037	3.6	1
210	An ab initio/RRKM study of the reaction mechanism and product branching ratios of CH <sub>3</sub> OH <sup>+</sup> and CH <sub>3</sub> OH <sup>++</sup> dissociation. <i>Journal of Molecular Structure</i> , <b>2020</b> , 1217, 128410	3.4	3
209	DenseCPD: Improving the Accuracy of Neural-Network-Based Computational Protein Sequence Design with DenseNet. <i>Journal of Chemical Information and Modeling</i> , <b>2020</b> , 60, 1245-1252	6.1	10
208	Computational approaches to studying methylated H4K20 recognition by DNA repair factor 53BP1. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 6136-6144	3.6	8

207	Entropic effect and residue specific entropic contribution to the cooperativity in streptavidin-biotin binding. <i>Nanoscale</i> , <b>2020</b> , 12, 7134-7145	7.7	16
206	How CuCl and CuCl Insert into C-N Bonds of Diazo Compounds: An Electronic Structure and Mechanistic Study. <i>Journal of Physical Chemistry A</i> , <b>2020</b> , 124, 2029-2035	2.8	2
205	Atomic-level reconstruction of biomolecules by a rigid-fragment- and local-frame-based (RF-LF) strategy. <i>Journal of Molecular Modeling</i> , <b>2020</b> , 26, 31	2	1
204	Molecular Mechanism of Selective Binding of NMS-P118 to PARP-1 and PARP-2: A Computational Perspective. <i>Frontiers in Molecular Biosciences</i> , <b>2020</b> , 7, 50	5.6	8
203	Developing an effective polarizable bond method for small molecules with application to optimized molecular docking.. <i>RSC Advances</i> , <b>2020</b> , 10, 15530-15540	3.7	7
202	LLPSDB: a database of proteins undergoing liquid-liquid phase separation in vitro. <i>Nucleic Acids Research</i> , <b>2020</b> , 48, D320-D327	20.1	63
201	Determining Optimal Coarse-Grained Representation for Biomolecules Using Internal Cluster Validation Indexes. <i>Journal of Computational Chemistry</i> , <b>2020</b> , 41, 14-20	3.5	4
200	Theoretical understanding of the thermodynamics and interactions in transcriptional regulator TtgR-ligand binding. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 1511-1524	3.6	8
199	Binding Modes of Small-Molecule Inhibitors to the EED Pocket of PRC2. <i>ChemPhysChem</i> , <b>2020</b> , 21, 263-271	3.1	8
198	Development of a New Scoring Function for Virtual Screening: APBScore. <i>Journal of Chemical Information and Modeling</i> , <b>2020</b> , 60, 6355-6365	6.1	2
197	Complex reaction processes in combustion unraveled by neural network-based molecular dynamics simulation. <i>Nature Communications</i> , <b>2020</b> , 11, 5713	17.4	43
196	A three-point coarse-grained model of five-water cluster with permanent dipoles and quadrupoles. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 26289-26298	3.6	1
195	Double-Well Ultra-Coarse-Grained Model to Describe Protein Conformational Transitions. <i>Journal of Chemical Theory and Computation</i> , <b>2020</b> , 16, 6678-6689	6.4	11
194	An Approach to Computing Solvent Reorganization Energy. <i>Journal of Chemical Theory and Computation</i> , <b>2020</b> , 16, 6513-6519	6.4	2
193	Binding modes and conformational changes of FK506-binding protein 51 induced by inhibitor bindings: insight into molecular mechanisms based on multiple simulation technologies. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2020</b> , 38, 2141-2155	3.6	11
192	Decoding molecular mechanism of inhibitor bindings to CDK2 using molecular dynamics simulations and binding free energy calculations. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2020</b> , 38, 985-996	3.6	20
191	CHARMM-GUI DEER facilitator for spin-pair distance distribution calculations and preparation of restrained-ensemble molecular dynamics simulations. <i>Journal of Computational Chemistry</i> , <b>2020</b> , 41, 415-420	3.5	5
190	An Energy Optimization Strategy Based on the Perfect Conformation of Prolyl Endopeptidase for Improving Catalytic Efficiency. <i>Journal of Agricultural and Food Chemistry</i> , <b>2020</b> , 68, 5129-5137	5.7	3

189	An accurate free energy estimator: based on MM/PBSA combined with interaction entropy for protein-ligand binding affinity. <i>Nanoscale</i> , <b>2020</b> , 12, 10737-10750	7.7	49
188	A method for efficient calculation of thermal stability of proteins upon point mutations. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 8461-8466	3.6	9
187	Study of SHMT2 Inhibitors and Their Binding Mechanism by Computational Alanine Scanning. <i>Journal of Chemical Information and Modeling</i> , <b>2019</b> , 59, 3871-3878	6.1	12
186	Computational analysis for residue-specific CDK2-inhibitor bindings. <i>Chinese Journal of Chemical Physics</i> , <b>2019</b> , 32, 134-142	0.9	8
185	Mechanistic Studies of CO Cycloaddition Reaction Catalyzed by Amine-Functionalized Ionic Liquids. <i>Frontiers in Chemistry</i> , <b>2019</b> , 7, 615	5	10
184	Drug-resistance mechanisms of three mutations in anaplastic lymphoma kinase against two inhibitors based on MM/PBSA combined with interaction entropy. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 20951-20964	3.6	6
183	A force consistent method for electrostatic energy calculation in fluctuating charge model. <i>Journal of Chemical Physics</i> , <b>2019</b> , 151, 094105	3.9	1
182	CHARMM-GUI Glycan Modeler for modeling and simulation of carbohydrates and glycoconjugates. <i>Glycobiology</i> , <b>2019</b> , 29, 320-331	5.8	101
181	CHARMM-GUI Nanodisc Builder for modeling and simulation of various nanodisc systems. <i>Journal of Computational Chemistry</i> , <b>2019</b> , 40, 893-899	3.5	27
180	End-Point Binding Free Energy Calculation with MM/PBSA and MM/GBSA: Strategies and Applications in Drug Design. <i>Chemical Reviews</i> , <b>2019</b> , 119, 9478-9508	68.1	449
179	Sulfur-substitution-induced base flipping in the DNA duplex. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 14923-14940	3.6	15
178	Effect of mutations on binding of ligands to guanine riboswitch probed by free energy perturbation and molecular dynamics simulations. <i>Nucleic Acids Research</i> , <b>2019</b> , 47, 6618-6631	20.1	77
177	Computational analysis of hot spots and binding mechanism in the PD-1/PD-L1 interaction.. <i>RSC Advances</i> , <b>2019</b> , 9, 14944-14956	3.7	16
176	BAR-based optimum adaptive steered MD for configurational sampling. <i>Journal of Computational Chemistry</i> , <b>2019</b> , 40, 1270-1289	3.5	14
175	Accelerated Molecular Dynamics Simulation for Helical Proteins Folding in Explicit Water. <i>Frontiers in Chemistry</i> , <b>2019</b> , 7, 540	5	33
174	Molecular Dynamics Simulation of Zinc Ion in Water with an ab Initio Based Neural Network Potential. <i>Journal of Physical Chemistry A</i> , <b>2019</b> , 123, 6587-6595	2.8	16
173	A Fragment Quantum Mechanical Method for Metalloproteins. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 1430-1439	6.4	9
172	DeepDDG: Predicting the Stability Change of Protein Point Mutations Using Neural Networks. <i>Journal of Chemical Information and Modeling</i> , <b>2019</b> , 59, 1508-1514	6.1	62

171	Understanding the selectivity of inhibitors toward PI4KIII $\alpha$ and PI4KIII $\beta$ based molecular modeling. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 22103-22112	3.6	19
170	Formation mechanism and spectroscopy of CH radicals in extreme environments: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 23044-23055	3.6	4
169	Accurate and Efficient Calculation of Protein-Protein Binding Free Energy-Interaction Entropy with Residue Type-Specific Dielectric Constants. <i>Journal of Chemical Information and Modeling</i> , <b>2019</b> , 59, 272-281	6.1	18
168	Calculation of hot spots for protein-protein interaction in p53/PMI-MDM2/MDMX complexes. <i>Journal of Computational Chemistry</i> , <b>2019</b> , 40, 1045-1056	3.5	17
167	CHARMM-GUI Membrane Builder for Complex Biological Membrane Simulations with Glycolipids and Lipoglycans. <i>Journal of Chemical Theory and Computation</i> , <b>2019</b> , 15, 775-786	6.4	152
166	An efficient method for computing excess free energy of liquid. <i>Science China Chemistry</i> , <b>2018</b> , 61, 135-140	4.0	13
165	Computational Protein Design with Deep Learning Neural Networks. <i>Scientific Reports</i> , <b>2018</b> , 8, 6349	4.9	72
164	Computational Alanine Scanning with Interaction Entropy for Protein-Ligand Binding Free Energies. <i>Journal of Chemical Theory and Computation</i> , <b>2018</b> , 14, 1772-1780	6.4	44
163	Multiple Conformational States Contribute to the 3D Structure of a Glucan Decasaccharide: A Combined SAXS and MD Simulation Study. <i>Journal of Physical Chemistry B</i> , <b>2018</b> , 122, 1169-1175	3.4	8
162	A Coupled Ionization-Conformational Equilibrium Is Required To Understand the Properties of Ionizable Residues in the Hydrophobic Interior of Staphylococcal Nuclease. <i>Journal of the American Chemical Society</i> , <b>2018</b> , 140, 1639-1648	16.4	16
161	Crius: A novel fragment-based algorithm of de novo substrate prediction for enzymes. <i>Protein Science</i> , <b>2018</b> , 27, 1526-1534	6.3	
160	Assessing the performance of MM/PBSA and MM/GBSA methods. 7. Entropy effects on the performance of end-point binding free energy calculation approaches. <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 14450-14460	3.6	149
159	Unfolding of a ClC chloride transporter retains memory of its evolutionary history. <i>Nature Chemical Biology</i> , <b>2018</b> , 14, 489-496	11.7	22
158	Interaction entropy for computational alanine scanning in protein-protein binding. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , <b>2018</b> , 8, e1342	7.9	34
157	Electrostatic Polarization Effect on Cooperative Aggregation of Full Length Human Islet Amyloid. <i>Journal of Chemical Information and Modeling</i> , <b>2018</b> , 58, 1587-1595	6.1	1
156	Automated Fragmentation QM/MM Calculation of NMR Chemical Shifts for Protein-Ligand Complexes. <i>Frontiers in Chemistry</i> , <b>2018</b> , 6, 150	5	7
155	A Force Balanced Fragmentation Method for Molecular Dynamic Simulation of Protein. <i>Frontiers in Chemistry</i> , <b>2018</b> , 6, 189	5	5
154	Residue-specific free energy analysis in ligand bindings to JAK2. <i>Molecular Physics</i> , <b>2018</b> , 116, 2633-2641	11.7	11



153	Hydrogen-bond structure dynamics in bulk water: insights from simulations with coupled cluster theory. <i>Chemical Science</i> , <b>2018</b> , 9, 2065-2073	9.4	68
152	The impact of interior dielectric constant and entropic change on HIV-1 complex binding free energy prediction. <i>Structural Dynamics</i> , <b>2018</b> , 5, 064101	3.2	29
151	Effect of Substituents in Different Positions of Aminothiazole Hinge-Binding Scaffolds on Inhibitor-CDK2 Association Probed by Interaction Entropy Method. <i>ACS Omega</i> , <b>2018</b> , 3, 18052-18064	3.9	12
150	Probing the Ion-Specific Effects at the Water/Air Interface and Water-Mediated Ion Pairing in Sodium Halide Solution with Ab Initio Molecular Dynamics. <i>Journal of Physical Chemistry B</i> , <b>2018</b> , 122, 10202-10209	3.4	13
149	Exploring the Reasons for Decrease in Binding Affinity of HIV-2 Against HIV-1 Protease Complex Using Interaction Entropy Under Polarized Force Field. <i>Frontiers in Chemistry</i> , <b>2018</b> , 6, 380	5	10
148	Functional loop dynamics of the S-component of ECF transporter Folt. <i>Molecular Physics</i> , <b>2018</b> , 116, 2613-2621	3.2	2
147	Evaluation of the Coupled Two-Dimensional Main Chain Torsional Potential in Modeling Intrinsically Disordered Proteins. <i>Journal of Chemical Information and Modeling</i> , <b>2017</b> , 57, 267-274	6.1	5
146	Performance Comparison of Systematic Methods for Rigorous Definition of Coarse-Grained Sites of Large Biomolecules. <i>Journal of Chemical Information and Modeling</i> , <b>2017</b> , 57, 214-222	6.1	5
145	Protein simulation using coarse-grained two-bead multipole force field with polarizable water models. <i>Journal of Chemical Physics</i> , <b>2017</b> , 146, 065101	3.9	2
144	Effect of polarization on HIV-1protease and fluoro-substituted inhibitors binding energies by large scale molecular dynamics simulations. <i>Scientific Reports</i> , <b>2017</b> , 7, 42223	4.9	17
143	Two-bead polarizable water models combined with a two-bead multipole force field (TMFF) for coarse-grained simulation of proteins. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 7410-7419	3.6	7
142	Modeling and simulation of bacterial outer membranes and interactions with membrane proteins. <i>Current Opinion in Structural Biology</i> , <b>2017</b> , 43, 131-140	8.1	30
141	Interaction Entropy for Computational Alanine Scanning. <i>Journal of Chemical Information and Modeling</i> , <b>2017</b> , 57, 1112-1122	6.1	55
140	Fragment Quantum Mechanical Method for Large-Sized Ion-Water Clusters. <i>Journal of Chemical Theory and Computation</i> , <b>2017</b> , 13, 2021-2034	6.4	39
139	Direct folding simulation of helical proteins using an effective polarizable bond force field. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 15273-15284	3.6	11
138	An Electrochemical Biosensor with Dual Signal Outputs: Toward Simultaneous Quantification of pH and O in the Brain upon Ischemia and in a Tumor during Cancer Starvation Therapy. <i>Angewandte Chemie - International Edition</i> , <b>2017</b> , 56, 10471-10475	16.4	60
137	Single Biosensor for Simultaneous Quantification of Glucose and pH in a Rat Brain of Diabetic Model Using Both Current and Potential Outputs. <i>Analytical Chemistry</i> , <b>2017</b> , 89, 6656-6662	7.8	30
136	Interaction entropy for protein-protein binding. <i>Journal of Chemical Physics</i> , <b>2017</b> , 146, 124124	3.9	65

135	Full QM Calculation of RNA Energy Using Electrostatically Embedded Generalized Molecular Fractionation with Conjugate Caps Method. <i>Journal of Physical Chemistry A</i> , <b>2017</b> , 121, 2503-2514	2.8	16
134	CHARMM-GUI MDFF/xMDFF Utilizer for Molecular Dynamics Flexible Fitting Simulations in Various Environments. <i>Journal of Physical Chemistry B</i> , <b>2017</b> , 121, 3718-3723	3.4	13
133	Computational Study of PCSK9-EGFA Complex with Effective Polarizable Bond Force Field. <i>Frontiers in Molecular Biosciences</i> , <b>2017</b> , 4, 101	5.6	3
132	Origins of Protons in C-H Bond Insertion Products of Phenols: Proton-Self-Sufficient Function via Water Molecules. <i>Journal of Physical Chemistry A</i> , <b>2017</b> , 121, 6523-6529	2.8	7
131	MFCC-Based Fragmentation Methods for Biomolecules <b>2017</b> , 323-348		3
130	A theoretical study of the substituent effect on reactions of amines, carbon dioxide and ethylene oxide catalyzed by binary ionic liquids. <i>RSC Advances</i> , <b>2017</b> , 7, 51521-51527	3.7	9
129	An Electrochemical Biosensor with Dual Signal Outputs: Toward Simultaneous Quantification of pH and O <sub>2</sub> in the Brain upon Ischemia and in a Tumor during Cancer Starvation Therapy. <i>Angewandte Chemie</i> , <b>2017</b> , 129, 10607-10611	3.6	17
128	Protein-Ligand Empirical Interaction Components for Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , <b>2017</b> , 57, 1793-1806	6.1	35
127	CHARMM-GUI 10 years for biomolecular modeling and simulation. <i>Journal of Computational Chemistry</i> , <b>2017</b> , 38, 1114-1124	3.5	119
126	Ab initio Quantum Mechanics/Molecular Mechanics Molecular Dynamics Simulation of CO in the Heme Distal Pocket of Myoglobin. <i>Chinese Journal of Chemical Physics</i> , <b>2017</b> , 30, 705-716	0.9	5
125	Asymmetric Cryo-EM Structure of Anthrax Toxin Protective Antigen Pore with Lethal Factor N-Terminal Domain. <i>Toxins</i> , <b>2017</b> , 9,	4.9	9
124	Preferred conformations of N-glycan core pentasaccharide in solution and in glycoproteins. <i>Glycobiology</i> , <b>2016</b> , 26, 19-29	5.8	26
123	A Semiautomated Structure-Based Method To Predict Substrates of Enzymes via Molecular Docking: A Case Study with Candida antarctica Lipase B. <i>Journal of Chemical Information and Modeling</i> , <b>2016</b> , 56, 1979-1994	6.1	4
122	The origin of the cooperativity in the streptavidin-biotin system: A computational investigation through molecular dynamics simulations. <i>Scientific Reports</i> , <b>2016</b> , 6, 27190	4.9	20
121	Examination of the quality of various force fields and solvation models for the equilibrium simulations of GA88 and GB88. <i>Journal of Molecular Modeling</i> , <b>2016</b> , 22, 177	2	3
120	TMFF-A Two-Bead Multipole Force Field for Coarse-Grained Molecular Dynamics Simulation of Protein. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 6147-6156	6.4	11
119	BamA POTRA Domain Interacts with a Native Lipid Membrane Surface. <i>Biophysical Journal</i> , <b>2016</b> , 110, 2698-2709	2.9	52
118	The effect of POPC acyl chains packing by aromatic amino acid methyl esters investigated by ATR-FTIR combined with QM calculations. <i>RSC Advances</i> , <b>2016</b> , 6, 45569-45577	3.7	6



117	Calculations of Solvation Free Energy through Energy Reweighting from Molecular Mechanics to Quantum Mechanics. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 499-511	6.4	70
116	CHARMM-GUI Input Generator for NAMD, GROMACS, AMBER, OpenMM, and CHARMM/OpenMM Simulations Using the CHARMM36 Additive Force Field. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 405-13	6.4	1303
115	Dynamics and Interactions of OmpF and LPS: Influence on Pore Accessibility and Ion Permeability. <i>Biophysical Journal</i> , <b>2016</b> , 110, 930-8	2.9	54
114	Mechanistic Investigation of Aromatic C(sp <sup>2</sup> )-H and Alkyl C(sp <sup>3</sup> )-H Bond Insertion by Gold Carbenes. <i>Journal of Physical Chemistry A</i> , <b>2016</b> , 120, 1925-32	2.8	23
113	Roles of glycans in interactions between gp120 and HIV broadly neutralizing antibodies. <i>Glycobiology</i> , <b>2016</b> , 26, 251-60	5.8	13
112	A new algorithm for construction of coarse-grained sites of large biomolecules. <i>Journal of Computational Chemistry</i> , <b>2016</b> , 37, 795-804	3.5	12
111	A systematic study on RNA NMR chemical shift calculation based on the automated fragmentation QM/MM approach. <i>RSC Advances</i> , <b>2016</b> , 6, 108590-108602	3.7	10
110	Conformational Flexibility of a Short Loop near the Active Site of the SARS-3CLpro is Essential to Maintain Catalytic Activity. <i>Scientific Reports</i> , <b>2016</b> , 6, 20918	4.9	13
109	Constructing Optimal Coarse-Grained Sites of Huge Biomolecules by Fluctuation Maximization. <i>Journal of Chemical Theory and Computation</i> , <b>2016</b> , 12, 2091-100	6.4	15
108	Interaction Entropy: A New Paradigm for Highly Efficient and Reliable Computation of Protein-Ligand Binding Free Energy. <i>Journal of the American Chemical Society</i> , <b>2016</b> , 138, 5722-8	16.4	178
107	Replacing Arginine 33 for Alanine in the Hemophore HasA from <i>Pseudomonas aeruginosa</i> Causes Closure of the H32 Loop in the Apo-Protein. <i>Biochemistry</i> , <b>2016</b> , 55, 2622-31	3.2	12
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