Jeremy C Smith

List of Publications by Year
in descending order

483	54,735	10351 72	1456 220
papers	citations	h-index	g-index

521	521	521	50213
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A Model for the Signal Initiation Complex Between Arrestin-3 and the Src Family Kinase Fgr. Journal of Molecular Biology, 2022, 434, 167400.	2.0	6
2	Novel Small Molecule Fibroblast Growth Factor 23 Inhibitors Increase Serum Phosphate and Improve Skeletal Abnormalities in Hyp Mice. Molecular Pharmacology, 2022, 101, 408-421.	1.0	8
3	Hit Expansion of a Noncovalent SARS-CoV-2 Main Protease Inhibitor. ACS Pharmacology and Translational Science, 2022, 5, 255-265.	2.5	17
4	Structural patterns in class 1 major histocompatibility complexâ€restricted nonamer peptide binding to Tâ€cell receptors. Proteins: Structure, Function and Bioinformatics, 2022, 90, 1645-1654.	1.5	5
5	Origins of glycan selectivity in streptococcal Siglec-like adhesins suggest mechanisms of receptor adaptation. Nature Communications, 2022, 13, 2753.	5.8	4
6	Chemical and Morphological Structure of Transgenic Switchgrass Organosolv Lignin Extracted by Ethanol, Tetrahydrofuran, and Î³-Valerolactone Pretreatments. ACS Sustainable Chemistry and Engineering, 2022, 10, 9041-9052.	3.2	10
7	Supercomputing Pipelines Search for Therapeutics Against COVID-19. Computing in Science and Engineering, 2021, 23, 7-16.	1.2	19
8	The carboxylation status of osteocalcin has important consequences for its structure and dynamics. Biochimica Et Biophysica Acta - General Subjects, 2021, 1865, 129809.	1.1	5
9	Molecular dynamics analysis of the binding of human interleukinâ€6 with interleukinâ€6 <scp>Î±â€receptor</scp>. Proteins: Structure, Function and Bioinformatics, 2021, 89, 163-173.	1.5	4
10	Antitumor T-cell Immunity Contributes to Pancreatic Cancer Immune Resistance. Cancer Immunology Research, 2021, 9, 386-400.	1.6	9
11	Full structural ensembles of intrinsically disordered proteins from unbiased molecular dynamics simulations. Communications Biology, 2021, 4, 243.	2.0	52
12	Peptide nucleic acid Hoogsteen strand linker design for major groove recognition of DNA thymine bases. Journal of Computer-Aided Molecular Design, 2021, 35, 355-369.	1.3	4
13	Spontaneous rearrangement of acetylated xylan on hydrophilic cellulose surfaces. Cellulose, 2021, 28, 3327-3345.	2.4	14
14	Cross-reactive immunogenicity of group A streptococcal vaccines designed using a recurrent neural network to identify conserved M protein linear epitopes. Vaccine, 2021, 39, 1773-1779.	1.7	4
15	Tuning Proton Transfer Thermodynamics in SARS-CoV-2 Main Protease: Implications for Catalysis and Inhibitor Design. Journal of Physical Chemistry Letters, 2021, 12, 4195-4202.	2.1	19
16	Reply to: Insufficient evidence for ageing in protein dynamics. Nature Physics, 2021, 17, 775-776.	6.5	3
17	Correlated Response of Protein Side-Chain Fluctuations and Conformational Entropy to Ligand Binding. Journal of Physical Chemistry B, 2021, 125, 9641-9651.	1.2	7
18	Design of Broadly Cross-Reactive M Proteinâ€“Based Group A Streptococcal Vaccines. Journal of Immunology, 2021, 207, 1138-1149.	0.4	9

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19	Lpp positions peptidoglycan at the AcrA-TolC interface in the AcrAB-TolC multidrug efflux pump. Biophysical Journal, 2021, 120, 3973-3982.	0.2	13
20	Locking out water at 100Â°C. Biophysical Journal, 2021, 120, 3541.	0.2	0
21	Inhibitor binding influences the protonation states of histidines in SARS-CoV-2 main protease. Chemical Science, 2021, 12, 1513-1527.	3.7	47
22	The AQUAâ€MER databases and aqueous speciation server: A web resource for multiscale modeling of mercury speciation. Journal of Computational Chemistry, 2020, 41, 147-155.	1.5	3
23	A Minimal Membrane Metal Transport System: Dynamics and Energetics of mer Proteins. Journal of Computational Chemistry, 2020, 41, 528-537.	1.5	5
24	Molecular Dynamics Simulation of the Structures, Dynamics, and Aggregation of Dissolved Organic Matter. Environmental Science & Technology, 2020, 54, 13527-13537.	4.6	36
25	Deconstruction of biomass enabled by local demixing of cosolvents at cellulose and lignin surfaces. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 16776-16781.	3.3	29
26	Mesophilic Pyrophosphatase Function at High Temperature: A Molecular Dynamics Simulation Study. Biophysical Journal, 2020, 119, 142-150.	0.2	3
27	Effects of sodium and calcium chloride ionic stresses on model yeast membranes revealed by molecular dynamics simulation. Chemistry and Physics of Lipids, 2020, 233, 104980.	1.5	4
28	Combining Three-Dimensional Modeling with Artificial Intelligence to Increase Specificity and Precision in Peptideâ€“MHC Binding Predictions. Journal of Immunology, 2020, 205, 1962-1977.	0.4	7
29	Insight into the Catalytic Mechanism of GH11 Xylanase: Computational Analysis of Substrate Distortion Based on a Neutron Structure. Journal of the American Chemical Society, 2020, 142, 17966-17980.	6.6	13
30	Role of Capping Agents in the Synthesis of Salicylate-Capped Zinc Oxide Nanoparticles. ACS Applied Nano Materials, 2020, 3, 9951-9960.	2.4	7
31	Solvent-induced membrane stress in biofuel production: molecular insights from small-angle scattering and all-atom molecular dynamics simulations. Green Chemistry, 2020, 22, 8278-8288.	4.6	9
32	Supercomputer-Based Ensemble Docking Drug Discovery Pipeline with Application to Covid-19. Journal of Chemical Information and Modeling, 2020, 60, 5832-5852.	2.5	134
33	Carotenoids promote lateral packing and condensation of lipid membranes. Physical Chemistry Chemical Physics, 2020, 22, 12281-12293.	1.3	24
34	How to Discover Antiviral Drugs Quickly. New England Journal of Medicine, 2020, 382, 2261-2264.	13.9	76
35	Polymer principles behind solubilizing lignin with organic cosolvents for bioenergy. Green Chemistry, 2020, 22, 4331-4340.	4.6	13
36	Capturing Deuteration Effects in a Molecular Mechanics Force Field: Deuterated THF and the THFâ€“Water Miscibility Gap. Journal of Chemical Theory and Computation, 2020, 16, 2529-2540.	2.3	9

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37	Discovery of multidrug efflux pump inhibitors with a novel chemical scaffold. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129546.	1.1	33
38	Prediction of peptide binding to MHC using machine learning with sequence and structure-based feature sets. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129535.	1.1	15
39	Four countries for science. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129518.	1.1	1
40	Structure-based group A streptococcal vaccine design: Helical wheel homology predicts antibody cross-reactivity among streptococcal M proteinâ€“derived peptides. Journal of Biological Chemistry, 2020, 295, 3826-3836.	1.6	8
41	Structure based virtual screening identifies small molecule effectors for the sialoglycan binding protein Hsa. Biochemical Journal, 2020, 477, 3695-3707.	1.7	7
42	GPU-Accelerated Drug Discovery with Docking on the Summit Supercomputer. , 2020, , .		36
43	A Multifunctional Cosolvent Pair Reveals Molecular Principles of Biomass Deconstruction. Journal of the American Chemical Society, 2019, 141, 12545-12557.	6.6	73
44	Using Small-Angle Scattering Data and Parametric Machine Learning to Optimize Force Field Parameters for Intrinsically Disordered Proteins. Frontiers in Molecular Biosciences, 2019, 6, 64.	1.6	22
45	Horizontal transfer of a pathway for coumarate catabolism unexpectedly inhibits purine nucleotide biosynthesis. Molecular Microbiology, 2019, 112, 1784-1797.	1.2	5
46	Ligand-Dependent Sodium Ion Dynamics within the A_{2A} Adenosine Receptor: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2019, 123, 7947-7954.	1.2	4
47	Conformational Dynamics of AcrA Govern Multidrug Efflux Pump Assembly. ACS Infectious Diseases, 2019, 5, 1926-1935.	1.8	21
48	A probabilistic perspective on thermodynamic parameter uncertainties: Understanding aqueous speciation of mercury. Geochimica Et Cosmochimica Acta, 2019, 263, 108-121.	1.6	4
49	Generation of the configurational ensemble of an intrinsically disordered protein from unbiased molecular dynamics simulation. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 20446-20452.	3.3	88
50	Identification of Binding Sites for Efflux Pump Inhibitors of the AcrAB-TolC Component AcrA. Biophysical Journal, 2019, 116, 648-658.	0.2	27
51	Environmental Mercury Chemistry â€“ In Silico. Accounts of Chemical Research, 2019, 52, 379-388.	7.6	40
52	Ensemble Docking in Drug Discovery: How Many Protein Configurations from Molecular Dynamics Simulations are Needed To Reproduce Known Ligand Binding?. Journal of Physical Chemistry B, 2019, 123, 5189-5195.	1.2	69
53	Hydration-mediated stiffening of collective membrane dynamics by cholesterol. Physical Chemistry Chemical Physics, 2019, 21, 10370-10376.	1.3	9
54	Biological Membrane Organization and Cellular Signaling. Chemical Reviews, 2019, 119, 5849-5880.	23.0	112

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55	Structural Modeling of the Reflectin Protein. Biophysical Journal, 2019, 116, 46a.	0.2	0
56	Porting Adaptive Ensemble Molecular Dynamics Workflows to the Summit Supercomputer. Lecture Notes in Computer Science, 2019, , 397-417.	1.0	5
57	Highly Interactive, Steered Scientific Workflows on HPC Systems: Optimizing Design Solutions. Lecture Notes in Computer Science, 2019, , 514-527.	1.0	2
58	Temperature-dependent phase behaviour of tetrahydrofuranâ€“water alters solubilization of xylan to improve co-production of furfurals from lignocellulosic biomass. Green Chemistry, 2018, 20, 1612-1620.	4.6	39
59	GPCR6A Is a Molecular Target for the Natural Products Gallate and EGCG in Green Tea. Molecular Nutrition and Food Research, 2018, 62, e1700770.	1.5	21
60	Catalysis of Ground State cis $$ightarrow$$ â†' trans Isomerization of Bacteriorhodopsinâ€™s Retinal Chromophore by a Hydrogen-Bond Network. Journal of Membrane Biology, 2018, 251, 315-327.	1.0	5
61	Quantum Chemical Calculation of pK_as of Environmentally Relevant Functional Groups: Carboxylic Acids, Amines, and Thiols in Aqueous Solution. Journal of Physical Chemistry A, 2018, 122, 4366-4374.	1.1	62
62	"To Be or Not to Be" Protonated: Atomic Details of Human Carbonic Anhydrase-Clinical Drug Complexes by Neutron Crystallography and Simulation. Structure, 2018, 26, 383-390.e3.	1.6	40
63	Celluloseâ€“hemicellulose interactions at elevated temperatures increase cellulose recalcitrance to biological conversion. Green Chemistry, 2018, 20, 921-934.	4.6	49
64	Effects of carotenoids on lipid bilayers. Physical Chemistry Chemical Physics, 2018, 20, 3795-3804.	1.3	19
65	Relationship between lignocellulosic biomass dissolution and physicochemical properties of ionic liquids composed of 3-methylimidazolium cations and carboxylate anions. Physical Chemistry Chemical Physics, 2018, 20, 2508-2516.	1.3	51
66	Ensemble Docking in Drug Discovery. Biophysical Journal, 2018, 114, 2271-2278.	0.2	318
67	Dynamic Neutron Scattering by Biological Systems. Annual Review of Biophysics, 2018, 47, 335-354.	4.5	27
68	Determination of Dynamical Heterogeneity from Dynamic Neutron Scattering of Proteins. Biophysical Journal, 2018, 114, 2397-2407.	0.2	5
69	Impact of hydration and temperature history on the structure and dynamics of lignin. Green Chemistry, 2018, 20, 1602-1611.	4.6	30
70	Ensemble docking to difficult targets in earlyâ€stage drug discovery: Methodology and application to fibroblast growth factor 23. Chemical Biology and Drug Design, 2018, 91, 491-504.	1.5	25
71	High-Performance Molecular Dynamics Simulation for Biological and Materials Sciences: Challenges of Performance Portability. , 2018, , .		15
72	JÃ¶rg Langowski: his scientific legacy and the future it promises. BMC Biophysics, 2018, 11, 5.	4.4	0

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73	Neutron scattering in the biological sciences: progress and prospects. Acta Crystallographica Section D: Structural Biology, 2018, 74, 1129-1168.	1.1	47
74	Quantum Mechanical/Molecular Mechanical Analysis of the Catalytic Mechanism of Phosphoserine Phosphatase. Molecules, 2018, 23, 3342.	1.7	8
75	The importance of the membrane interface as the reference state for membrane protein stability. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 2539-2548.	1.4	13
76	Molecular-level driving forces in lignocellulosic biomass deconstruction for bioenergy. Nature Reviews Chemistry, 2018, 2, 382-389.	13.8	114
77	Quantum Chemical Approach for Calculating Stability Constants of Mercury Complexes. ACS Earth and Space Chemistry, 2018, 2, 1168-1178.	1.2	14
78	Computationally identified novel agonists for GPRC6A. PLoS ONE, 2018, 13, e0195980.	1.1	19
79	Dynamics of the lignin glass transition. Physical Chemistry Chemical Physics, 2018, 20, 20504-20512.	1.3	28
80	Quasielastic neutron scattering in biology: Theory and applications. Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 3638-3650.	1.1	15
81	The tilt-dependent potential of mean force of a pair of DNA oligomers from all-atom molecular dynamics simulations. Journal of Physics Condensed Matter, 2017, 29, 084002.	0.7	8
82	Protonationâ€“stateâ€Coupled Conformational Dynamics in Reaction Mechanisms of Channel and Pump Rhodopsins. Photochemistry and Photobiology, 2017, 93, 1336-1344.	1.3	28
83	Pickinâ€™ Up Good Vibrations. Biophysical Journal, 2017, 112, 829-830.	0.2	0
84	Structure-based design of broadly protective group a streptococcal M protein-based vaccines. Vaccine, 2017, 35, 19-26.	1.7	41
85	Dynamics at a Peptideâ€“TiO₂ Anatase (101) Interface. Journal of Physical Chemistry B, 2017, 121, 8869-8877.	1.2	8
86	Dynamics of water bound to crystalline cellulose. Scientific Reports, 2017, 7, 11840.	1.6	82
87	Dynamical Transition of Collective Motions in Dry Proteins. Physical Review Letters, 2017, 119, 048101.	2.9	27
88	Modeling of the Passive Permeation of Mercury and Methylmercury Complexes Through a Bacterial Cytoplasmic Membrane. Environmental Science & Technology, 2017, 51, 10595-10604.	4.6	15
89	Organosolv-Water Cosolvent Phase Separation on Cellulose and its Influence on the Physical Deconstruction of Cellulose: A Molecular Dynamics Analysis. Scientific Reports, 2017, 7, 14494.	1.6	29
90	Identification and Structureâ€“Activity Relationships of Novel Compounds that Potentiate the Activities of Antibiotics in Escherichia coli. Journal of Medicinal Chemistry, 2017, 60, 6205-6219.	2.9	45

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91	Reviving Antibiotics: Efflux Pump Inhibitors That Interact with AcrA, a Membrane Fusion Protein of the AcrAB-TolC Multidrug Efflux Pump. ACS Infectious Diseases, 2017, 3, 89-98.	1.8	88
92	A Distal Disulfide Bridge in OXA-1 Î²-Lactamase Stabilizes the Catalytic Center and Alters the Dynamics of the Specificity Determining Î© Loop. Journal of Physical Chemistry B, 2017, 121, 3285-3296.	1.2	6
93	Polycystin-1 interacts with TAZ to stimulate osteoblastogenesis and inhibit adipogenesis. Journal of Clinical Investigation, 2017, 128, 157-174.	3.9	49
94	Community detection in sequence similarity networks based on attribute clustering. PLoS ONE, 2017, 12, e0178650.	1.1	2
95	General trends of dihedral conformational transitions in a globular protein. Proteins: Structure, Function and Bioinformatics, 2016, 84, 501-514.	1.5	8
96	Conformations of Lowâ€Molecularâ€Weight Lignin Polymers in Water. ChemSusChem, 2016, 9, 289-295.	3.6	45
97	Longâ€Range Electrostaticsâ€Induced Twoâ€Proton Transfer Captured by Neutron Crystallography in an Enzyme Catalytic Site. Angewandte Chemie, 2016, 128, 5008-5011.	1.6	6
98	Longâ€Range Electrostaticsâ€Induced Twoâ€Proton Transfer Captured by Neutron Crystallography in an Enzyme Catalytic Site. Angewandte Chemie - International Edition, 2016, 55, 4924-4927.	7.2	42
99	Homolytic Cleavage of Both Heme-Bound Hydrogen Peroxide and Hydrogen Sulfide Leads to the Formation of Sulfheme. Journal of Physical Chemistry B, 2016, 120, 7319-7331.	1.2	12
100	Evidence for Osteocalcin Binding and Activation of GPRC6A in Î²-Cells. Endocrinology, 2016, 157, 1866-1880.	1.4	101
101	Neutron structure of human carbonic anhydrase II in complex with methazolamide: mapping the solvent and hydrogen-bonding patterns of an effective clinical drug. IUCrJ, 2016, 3, 319-325.	1.0	27
102	Ensemble-based docking: From hit discovery to metabolism and toxicity predictions. Bioorganic and Medicinal Chemistry, 2016, 24, 4928-4935.	1.4	41
103	Local Phase Separation of Co-solvents Enhances Pretreatment of Biomass for Bioenergy Applications. Journal of the American Chemical Society, 2016, 138, 10869-10878.	6.6	89
104	A computationally identified compound antagonizes excess FGF-23 signaling in renal tubules and a mouse model of hypophosphatemia. Science Signaling, 2016, 9, ra113.	1.6	27
105	Modeling Mercury in Proteins. Methods in Enzymology, 2016, 578, 103-122.	0.4	9
106	Toward Quantitatively Accurate Calculation of the Redox-Associated Acidâ€“Base and Ligand Binding Equilibria of Aquacobalamin. Journal of Physical Chemistry B, 2016, 120, 7307-7318.	1.2	3
107	Relative Binding Affinities of Monolignols to Horseradish Peroxidase. Journal of Physical Chemistry B, 2016, 120, 7635-7640.	1.2	6
108	Determination of functional collective motions in a protein at atomic resolution using coherent neutron scattering. Science Advances, 2016, 2, e1600886.	4.7	30

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109	Enhanced sampling simulation analysis of the structure of lignin in the THFâ€“water miscibility gap. Physical Chemistry Chemical Physics, 2016, 18, 6394-6398.	1.3	24
110	Molecular Driving Forces behind the Tetrahydrofuranâ€“Water Miscibility Gap. Journal of Physical Chemistry B, 2016, 120, 740-747.	1.2	30
111	A Structural Study of CESA1 Catalytic Domain of Arabidopsis Cellulose Synthesis Complex: Evidence for CESA Trimers. Plant Physiology, 2016, 170, 123-135.	2.3	104
112	The dynamics of single protein molecules is non-equilibrium and self-similar over thirteen decades in time. Nature Physics, 2016, 12, 171-174.	6.5	140
113	Cosolvent pretreatment in cellulosic biofuel production: effect of tetrahydrofuran-water on lignin structure and dynamics. Green Chemistry, 2016, 18, 1268-1277.	4.6	122
114	Motional displacements in proteins: The origin of wave-vector-dependent values. Physical Review E, 2015, 91, 052705.	0.8	12
115	Mechanism of lignin inhibition of enzymatic biomass deconstruction. Biotechnology for Biofuels, 2015, 8, 217.	6.2	195
116	Structural and Functional Evidence for Testosterone Activation of GPRC6A in Peripheral Tissues. Molecular Endocrinology, 2015, 29, 1759-1773.	3.7	52
117	Tri-peptide reference structures for the calculation of relative solvent accessible surface area in protein amino acid residues. Computational Biology and Chemistry, 2015, 54, 33-43.	1.1	7
118	Membrane Protein Structure, Function, and Dynamics: a Perspective from Experiments and Theory. Journal of Membrane Biology, 2015, 248, 611-640.	1.0	157
119	Lateral organization, bilayer asymmetry, and inter-leaflet coupling of biological membranes. Chemistry and Physics of Lipids, 2015, 192, 87-99.	1.5	104
120	GROMACS: High performance molecular simulations through multi-level parallelism from laptops to supercomputers. SoftwareX, 2015, 1-2, 19-25.	1.2	14,414
121	Monitoring the Folding Kinetics of a Î²-Hairpin by Time-Resolved IR Spectroscopy in Silico. Journal of Physical Chemistry B, 2015, 119, 4849-4856.	1.2	11
122	HackaMol: An Object-Oriented Modern Perl Library for Molecular Hacking on Multiple Scales. Journal of Chemical Information and Modeling, 2015, 55, 721-726.	2.5	6
123	Mechanical Properties of Nanoscopic Lipid Domains. Journal of the American Chemical Society, 2015, 137, 15772-15780.	6.6	108
124	Why genetic modification of lignin leads to low-recalcitrance biomass. Physical Chemistry Chemical Physics, 2015, 17, 358-364.	1.3	38
125	Multi-Conformer Ensemble Docking to Difficult Protein Targets. Journal of Physical Chemistry B, 2015, 119, 1026-1034.	1.2	59
126	Determination of cellulose crystallinity from powder diffraction diagrams. Biopolymers, 2015, 103, 67-73.	1.2	15

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127	Mechanism by which Untwisting of Retinal Leads to Productive Bacteriorhodopsin Photocycle States. Journal of Physical Chemistry B, 2015, 119, 2229-2240.	1.2	12
128	Polypharmacology and supercomputer-based docking: opportunities and challenges. Molecular Simulation, 2014, 40, 848-854.	0.9	16
129	The Role of Histone Tails in the Nucleosome: A Computational Study. Biophysical Journal, 2014, 107, 2911-2922.	0.2	70
130	X-ray Structure of a Hg²⁺ Complex of Mercuric Reductase (MerA) and Quantum Mechanical/Molecular Mechanical Study of Hg²⁺ Transfer between the C-Terminal and Buried Catalytic Site Cysteine Pairs. Biochemistry, 2014, 53, 7211-7222.	1.2	46
131	de Gennes Narrowing Describes the Relative Motion of Protein Domains. Physical Review Letters, 2014, 112, 158102.	2.9	30
132	Biomolecular Structure and Dynamics with Neutrons: The View from Simulation. Israel Journal of Chemistry, 2014, 54, 1264-1273.	1.0	2
133	Accelerating virtual highâ€throughput ligand docking: current technology and case study on a petascale supercomputer. Concurrency Computation Practice and Experience, 2014, 26, 1268-1277.	1.4	7
134	Catalytic mechanism and origin of high activity of cellulase TmCel12A at high temperature: a quantum mechanical/molecular mechanical study. Cellulose, 2014, 21, 937-949.	2.4	9
135	Simulation of a cellulose fiber in ionic liquid suggests a synergistic approach to dissolution. Cellulose, 2014, 21, 983-997.	2.4	58
136	Common processes drive the thermochemical pretreatment of lignocellulosic biomass. Green Chemistry, 2014, 16, 63-68.	4.6	198
137	Hydration Control of the Mechanical and Dynamical Properties of Cellulose. Biomacromolecules, 2014, 15, 4152-4159.	2.6	44
138	Coarse-Grain Model for Natural Cellulose Fibrils in Explicit Water. Journal of Physical Chemistry B, 2014, 118, 3026-3034.	1.2	22
139	Chemical Factors that Control Lignin Polymerization. Journal of Physical Chemistry B, 2014, 118, 164-170.	1.2	46
140	Solvent Friction Effects Propagate over the Entire Protein Molecule through Low-Frequency Collective Modes. Journal of Physical Chemistry B, 2014, 118, 8559-8565.	1.2	6
141	Structure and Dynamics of a Compact State of a Multidomain Protein, the Mercuric Ion Reductase. Biophysical Journal, 2014, 107, 393-400.	0.2	19
142	L-Arabinose Binding, Isomerization, and Epimerization by D-Xylose Isomerase: X-Ray/Neutron Crystallographic and Molecular Simulation Study. Structure, 2014, 22, 1287-1300.	1.6	22
143	Replica-Exchange Molecular Dynamics Simulations of Cellulose Solvated in Water and in the Ionic Liquid 1-Butyl-3-Methylimidazolium Chloride. Journal of Physical Chemistry B, 2014, 118, 11037-11049.	1.2	29
144	Simulation analysis of the cellulase Cel7A carbohydrate binding module on the surface of the cellulose Iβ. Cellulose, 2014, 21, 951-971.	2.4	19

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145	Mercury Methylation by HgcA: Theory Supports Carbanion Transfer to Hg(II). Inorganic Chemistry, 2014, 53, 772-777.	1.9	34
146	Hydrolysis of DFP and the Nerve Agent (S)-Sarin by DFPase Proceeds along Two Different Reaction Pathways: Implications for Engineering Bioscavengers. Journal of Physical Chemistry B, 2014, 118, 4479-4489.	1.2	42
147	Hidden Regularity and Universal Classification of Fast Side Chain Motions in Proteins. Journal of the American Chemical Society, 2014, 136, 8590-8605.	6.6	12
148	A Closed-Loop Model of the Respiratory System: Focus on Hypercapnia and Active Expiration. PLoS ONE, 2014, 9, e109894.	1.1	62
149	Why Mercury Prefers Soft Ligands. Journal of Physical Chemistry Letters, 2013, 4, 2317-2322.	2.1	54
150	Ab Initio Study of Molecular Interactions in Cellulose Iβ. Journal of Physical Chemistry B, 2013, 117, 10430-10443.	1.2	22
151	Zaccai neutron resilience and site-specific hydration dynamics in a globular protein. European Physical Journal E, 2013, 36, 72.	0.7	7
152	Soft Collective Fluctuations Governing Hydrophobic Association. Physical Review Letters, 2013, 111, 127801.	2.9	8
153	Cluster-Continuum Calculations of Hydration Free Energies of Anions and Group 12 Divalent Cations. Journal of Chemical Theory and Computation, 2013, 9, 555-569.	2.3	44
154	Eppur Si Muove! The 2013 Nobel Prize in Chemistry. Structure, 2013, 21, 2102-2105.	1.6	26
155	Elastic and Conformational Softness of a Globular Protein. Biophysical Journal, 2013, 104, 59a.	0.2	0
156	Dynamics of Nucleosome Tails Studied by All-Atom and Coarse-Grained MD Simulations. Biophysical Journal, 2013, 104, 6a.	0.2	0
157	Nucleosome Dynamics Studied by Single-Pair FRET and Computer Simulations. Biophysical Journal, 2013, 104, 38a.	0.2	0
158	GROMACS 4.5: a high-throughput and highly parallel open source molecular simulation toolkit. Bioinformatics, 2013, 29, 845-854.	1.8	6,072
159	Elastic and Conformational Softness of a Globular Protein. Physical Review Letters, 2013, 110, 028104.	2.9	47
160	The Genetic Basis for Bacterial Mercury Methylation. Science, 2013, 339, 1332-1335.	6.0	778
161	Three Entropic Classes of Side Chain in a Globular Protein. Journal of Physical Chemistry B, 2013, 117, 3127-3134.	1.2	9
162	Solvent-Driven Preferential Association of Lignin with Regions of Crystalline Cellulose in Molecular Dynamics Simulation. Biomacromolecules, 2013, 14, 3390-3398.	2.6	68

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163	Impact of Resistance Mutations on Inhibitor Binding to HIV-1 Integrase. Journal of Chemical Information and Modeling, 2013, 53, 3297-3307.	2.5	14
164	Publisherâ€™s Note: Elastic and Conformational Softness of a Globular Protein [Phys. Rev. Lett.110, 028104 (2013)]. Physical Review Letters, 2013, 110, .	2.9	0
165	Dynamic neutron scattering from conformational dynamics. I. Theory and Markov models. Journal of Chemical Physics, 2013, 139, 175101.	1.2	22
166	Dynamic neutron scattering from conformational dynamics. II. Application using molecular dynamics simulation and Markov modeling. Journal of Chemical Physics, 2013, 139, 175102.	1.2	12
167	VinaMPI: Facilitating multiple receptor high-throughput virtual docking on high-performance computers. Journal of Computational Chemistry, 2013, 34, 2212-2221.	1.5	62
168	Long-time mean-square displacements in proteins. Physical Review E, 2013, 88, 052706.	0.8	17
169	Surface Hydration Amplifies Single-Well Protein Atom Diffusion Propagating into the Macromolecular Core. Physical Review Letters, 2012, 108, 238102.	2.9	45
170	Neutron Technologies for Bioenergy Research. Industrial Biotechnology, 2012, 8, 209-216.	0.5	17
171	DNA bending potentials for loop-mediated nucleosome repositioning. Europhysics Letters, 2012, 97, 38004.	0.7	7
172	Temperature-Dependent Dynamical Transitions of Different Classes of Amino Acid Residue in a Globular Protein. Journal of the American Chemical Society, 2012, 134, 19576-19579.	6.6	41
173	Coupled Flexibility Change in Cytochrome P450cam Substrate Binding Determined by Neutron Scattering, NMR, and Molecular Dynamics Simulation. Biophysical Journal, 2012, 103, 2167-2176.	0.2	25
174	Time-Dependent Density Functional Theory Assessment of UV Absorption of Benzoic Acid Derivatives. Journal of Physical Chemistry A, 2012, 116, 11870-11879.	1.1	55
175	Normal modes and neutrons: defining collective, functional biomolecular motions. Neutron News, 2012, 23, 26-30.	0.1	0
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