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	GROMACS: High performance molecular simulations through multi-level parallelism from laptops to supercomputers. SoftwareX, 2015, 1-2, 19-25.	1.2	14,414
2	All-Atom Empirical Potential for Molecular Modeling and Dynamics Studies of Proteinsâ€. Journal of Physical Chemistry B, 1998, 102, 3586-3616.	1.2	12,915
3	GROMACS 4.5: a high-throughput and highly parallel open source molecular simulation toolkit. Bioinformatics, 2013, 29, 845-854.	1.8	6,072
4	Analysis of any point mutation in DNA. The amplification refractory mutation system (ARMS). Nucleic Acids Research, 1989, 17, 2503-2516.	6.5	2,376
5	The Genetic Basis for Bacterial Mercury Methylation. Science, 2013, 339, 1332-1335.	6.0	778
6	Hierarchical analysis of conformational dynamics in biomolecules: Transition networks of metastable states. Journal of Chemical Physics, 2007, 126, 155102.	1.2	363
7	Is the first hydration shell of lysozyme of higher density than bulk water?. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 5378-5383.	3.3	355
8	Protein dynamics: comparison of simulations with inelastic neutron scattering experiments. Quarterly Reviews of Biophysics, 1991, 24, 227-291.	2.4	328
9	The Role of Dynamics in Enzyme Activity. Annual Review of Biophysics and Biomolecular Structure, 2003, 32, 69-92.	18.3	319
10	Ensemble Docking in Drug Discovery. Biophysical Journal, 2018, 114, 2271-2278.	0.2	318
11	Thermodynamic stability of water molecules in the bacteriorhodopsin proton channel: a molecular dynamics free energy perturbation study. Biophysical Journal, 1996, 71, 670-681.	0.2	246
12	A Model for the Photosystem II Reaction Center Core Including the Structure of the Primary Donor P680â€,â€¡. Biochemistry, 1996, 35, 14486-14502.	1.2	209
13	Determinants of Degree Performance in UK Universities: A Statistical Analysis of the 1993 Student Cohort. Oxford Bulletin of Economics and Statistics, 2001, 63, 29-60.	0.9	208
14	Common processes drive the thermochemical pretreatment of lignocellulosic biomass. Green Chemistry, 2014, 16, 63-68.	4.6	198
15	Dual Function of the Hydration Layer around an Antifreeze Protein Revealed by Atomistic Molecular Dynamics Simulations. Journal of the American Chemical Society, 2008, 130, 13066-13073.	6.6	197
16	Mechanism of lignin inhibition of enzymatic biomass deconstruction. Biotechnology for Biofuels, 2015, 8, 217.	6.2	195
17	Translational Hydration Water Dynamics Drives the Protein Glass Transition. Biophysical Journal, 2003, 85, 1871-1875.	0.2	191
18	Principal Components of the Protein Dynamical Transition. Physical Review Letters, 2003, 91, 208106.	2.9	169

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19	Structural mechanism of the recovery stroke in the Myosin molecular motor. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 6873-6878.	3.3	166
20	Mutant alcohol dehydrogenase leads to improved ethanol tolerance in Clostridium thermocellum. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 13752-13757.	3.3	159
21	Membrane Protein Structure, Function, and Dynamics: a Perspective from Experiments and Theory. Journal of Membrane Biology, 2015, 248, 611-640.	1.0	157
22	Dynamics of myoglobin: comparison of simulation results with neutron scattering spectra.. Proceedings of the National Academy of Sciences of the United States of America, 1990, 87, 1601-1605.	3.3	154
23	Fluorescence Quenching of Dyes by Tryptophan:Â Interactions at Atomic Detail from Combination of Experiment and Computer Simulation. Journal of the American Chemical Society, 2003, 125, 14564-14572.	6.6	151
24	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
25	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
26	Enzyme Activity below the Dynamical Transition at 220 K. Biophysical Journal, 1998, 75, 2504-2507.	0.2	131
27	Differential Effects of Cholesterol, Ergosterol and Lanosterol on a Dipalmitoyl Phosphatidylcholine Membrane:Â A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2007, 111, 1786-1801.	1.2	129
28	Simulation Analysis of the Temperature Dependence of Lignin Structure and Dynamics. Journal of the American Chemical Society, 2011, 133, 20277-20287.	6.6	126
29	Empirical force field study of geometries and conformational transitions of some organic molecules. Journal of the American Chemical Society, 1992, 114, 801-812.	6.6	124
30	Cosolvent pretreatment in cellulosic biofuel production: effect of tetrahydrofuran-water on lignin structure and dynamics. Green Chemistry, 2016, 18, 1268-1277.	4.6	122
31	Solvent dependence of dynamic transitions in protein solutions. Proceedings of the National Academy of Sciences of the United States of America, 2000, 97, 9961-9966.	3.3	121
32	Dynamics of Protein and its Hydration Water: Neutron Scattering Studies on Fully Deuterated GFP. Biophysical Journal, 2012, 103, 1566-1575.	0.2	121
33	Paradigm for industrial strain improvement identifies sodium acetate tolerance loci in Zymomonas mobilis and Saccharomyces cerevisiae. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 10395-10400.	3.3	116
34	Molecular-level driving forces in lignocellulosic biomass deconstruction for bioenergy. Nature Reviews Chemistry, 2018, 2, 382-389.	13.8	114
35	Direct Determination of Vibrational Density of States Change on Ligand Binding to a Protein. Physical Review Letters, 2004, 93, 028103.	2.9	113
36	Biological Membrane Organization and Cellular Signaling. Chemical Reviews, 2019, 119, 5849-5880.	23.0	112

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37	Mechanical Properties of Nanoscopic Lipid Domains. Journal of the American Chemical Society, 2015, 137, 15772-15780.	6.6	108
38	Mechanism of Primary Proton Transfer in Bacteriorhodopsin. Structure, 2004, 12, 1281-1288.	1.6	105
39	Dynamical fingerprints for probing individual relaxation processes in biomolecular dynamics with simulations and kinetic experiments. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 4822-4827.	3.3	105
40	Role of Histone Tails in Structural Stability of the Nucleosome. PLoS Computational Biology, 2011, 7, e1002279.	1.5	104
41	Lateral organization, bilayer asymmetry, and inter-leaflet coupling of biological membranes. Chemistry and Physics of Lipids, 2015, 192, 87-99.	1.5	104
42	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
43	Radical Coupling Reactions in Lignin Synthesis: A Density Functional Theory Study. Journal of Physical Chemistry B, 2012, 116, 4760-4768.	1.2	101
44	Evidence for Osteocalcin Binding and Activation of GPRC6A in Î²-Cells. Endocrinology, 2016, 157, 1866-1880.	1.4	101
45	Liquid-like Side-chain Dynamics in Myoglobin. Journal of Molecular Biology, 1994, 242, 181-185.	2.0	97
46	Protein/Ligand Binding Free Energies Calculated with Quantum Mechanics/Molecular Mechanics. Journal of Physical Chemistry B, 2005, 109, 10474-10483.	1.2	97
47	Neutron Frequency Windows and the Protein Dynamical Transition. Biophysical Journal, 2004, 87, 1436-1444.	0.2	96
48	Down-regulation of the caffeic acid O-methyltransferase gene in switchgrass reveals a novel monolignol analog. Biotechnology for Biofuels, 2012, 5, 71.	6.2	96
49	Inelastic neutron scattering analysis of picosecond internal protein dynamics. Journal of Molecular Biology, 1988, 202, 903-908.	2.0	95
50	Functional interactions in bacteriorhodopsin: a theoretical analysis of retinal hydrogen bonding with water. Biophysical Journal, 1995, 68, 25-39.	0.2	95
51	Structural Basis of Cellulosome Efficiency Explored by Small Angle X-ray Scattering. Journal of Biological Chemistry, 2005, 280, 38562-38568.	1.6	95
52	Key Role of Electrostatic Interactions in Bacteriorhodopsin Proton Transfer. Journal of the American Chemical Society, 2004, 126, 14668-14677.	6.6	94
53	Scaling of Multimillion-Atom Biological Molecular Dynamics Simulation on a Petascale Supercomputer. Journal of Chemical Theory and Computation, 2009, 5, 2798-2808.	2.3	94
54	Coarse-Grained Biomolecular Simulation with REACH: Realistic Extension Algorithm via Covariance Hessian. Biophysical Journal, 2007, 93, 3460-3469.	0.2	93

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55	In Silico Partitioning and Transmembrane Insertion of Hydrophobic Peptides under Equilibrium Conditions. Journal of the American Chemical Society, 2011, 133, 15487-15495.	6.6	92
56	How random is a highly denatured protein?. Biophysical Chemistry, 1994, 53, 105-113.	1.5	90
57	The Î± Helix Dipole: Screened Out?. Structure, 2005, 13, 849-855.	1.6	89
58	A molecular mechanics force field for lignin. Journal of Computational Chemistry, 2009, 30, 457-467.	1.5	89
59	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
60	Enzyme Dynamics and Activity: Time-Scale Dependence of Dynamical Transitions in Glutamate Dehydrogenase Solution. Biophysical Journal, 1999, 77, 2184-2190.	0.2	88
61	Temperature Dependence of Protein Dynamics: Computer Simulation Analysis of Neutron Scattering Properties. Biophysical Journal, 2002, 82, 1216-1225.	0.2	88
62	Transition Networks for the Comprehensive Characterization of Complex Conformational Change in Proteins. Journal of Chemical Theory and Computation, 2006, 2, 840-857.	2.3	88
63	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
64	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
65	Inelastic neutron scattering analysis of lowâ€frequency motions in proteins: Harmonic and damped harmonic models of bovine pancreatic tryspin inhibitor. Journal of Chemical Physics, 1990, 93, 2974-2991.	1.2	84
66	Dynamics of water bound to crystalline cellulose. Scientific Reports, 2017, 7, 11840.	1.6	82
67	Mechanism and Kinetics of Peptide Partitioning into Membranes from All-Atom Simulations of Thermostable Peptides. Journal of the American Chemical Society, 2010, 132, 3452-3460.	6.6	80
68	Dissecting the Vibrational Entropy Change on Protein/Ligand Binding:Â Burial of a Water Molecule in Bovine Pancreatic Trypsin Inhibitor. Journal of Physical Chemistry B, 2001, 105, 8050-8055.	1.2	79
69	Correlated intramolecular motions and diffuse xâ€“ray scattering in lysozyme. Nature Structural and Molecular Biology, 1994, 1, 124-128.	3.6	78
70	Subdiffusion in time-averaged, confined random walks. Physical Review E, 2009, 80, 011109.	0.8	78
71	Fluctuations and Correlations in Crystalline Protein Dynamics: A Simulation Analysis of Staphylococcal Nuclease. Biophysical Journal, 2005, 88, 2554-2563.	0.2	77
72	Coarseâ€grained force field for the nucleosome from selfâ€consistent multiscaling. Journal of Computational Chemistry, 2008, 29, 1429-1439.	1.5	77

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73	Three Classes of Motion in the Dynamic Neutron-Scattering Susceptibility of a Globular Protein. Physical Review Letters, 2011, 107, 148102.	2.9	76
74	How to Discover Antiviral Drugs Quickly. New England Journal of Medicine, 2020, 382, 2261-2264.	13.9	76
75	Cloning and characterization of a senescence inducing and class II tumor suppressor gene in ovarian carcinoma at chromosome region 6q27. Oncogene, 2001, 20, 980-988.	2.6	73
76	A Multifunctional Cosolvent Pair Reveals Molecular Principles of Biomass Deconstruction. Journal of the American Chemical Society, 2019, 141, 12545-12557.	6.6	73
77	Radially Softening Diffusive Motions in a Globular Protein. Biophysical Journal, 2001, 81, 1666-1676.	0.2	72
78	Energy resolution and dynamical heterogeneity effects on elastic incoherent neutron scattering from molecular systems. Physical Review E, 2003, 67, 021904.	0.8	72
79	Dehydration-driven solvent exposure of hydrophobic surfaces as a driving force in peptide folding. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 15230-15235.	3.3	72
80	The Structural Coupling between ATPase Activation and Recovery Stroke in the Myosin II Motor. Structure, 2007, 15, 825-837.	1.6	72
81	Self-similar multiscale structure of lignin revealed by neutron scattering and molecular dynamics simulation. Physical Review E, 2011, 83, 061911.	0.8	72
82	Picosecond fluctuating protein energy landscape mapped by pressure temperature molecular dynamics simulation. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 17261-17265.	3.3	71
83	Mechanism of Hgâ˜C Protonolysis in the Organomercurial Lyase MerB. Journal of the American Chemical Society, 2009, 131, 13278-13285.	6.6	70
84	The Role of Histone Tails in the Nucleosome: A Computational Study. Biophysical Journal, 2014, 107, 2911-2922.	0.2	70
85	The Serotonin Binding Site of Human and Murine 5-HT2BReceptors. Journal of Biological Chemistry, 2002, 277, 17170-17178.	1.6	69
86	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
87	Solvent-Driven Preferential Association of Lignin with Regions of Crystalline Cellulose in Molecular Dynamics Simulation. Biomacromolecules, 2013, 14, 3390-3398.	2.6	68
88	Key Role of Active-Site Water Molecules in Bacteriorhodopsin Proton-Transfer Reactions. Journal of Physical Chemistry B, 2008, 112, 14729-14741.	1.2	66
89	Unwrapping of Nucleosomal DNA Ends: A Multiscale Molecular Dynamics Study. Biophysical Journal, 2012, 102, 849-858.	0.2	65
90	Can the calculation of ligand binding free energies be improved with continuum solvent electrostatics and an ideal-gas entropy correction?. Journal of Computational Chemistry, 2002, 23, 1143-1149.	1.5	64

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91	Subdiffusion in Peptides Originates from the Fractal-Like Structure of Configuration Space. Physical Review Letters, 2008, 100, 188103.	2.9	63
92	VinaMPI: Facilitating multiple receptor high-throughput virtual docking on high-performance computers. Journal of Computational Chemistry, 2013, 34, 2212-2221.	1.5	62
93	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
94	Inelastic neutron scattering analysis of low frequency motion in proteins: A normal mode study of the bovine pancreatic trypsin inhibitor. Journal of Chemical Physics, 1986, 85, 3636-3654.	1.2	62
95	A Closed-Loop Model of the Respiratory System: Focus on Hypercapnia and Active Expiration. PLoS ONE, 2014, 9, e109894.	1.1	62
96	Detection of Individual p53-Autoantibodies by Using Quenched Peptide-Based Molecular Probes. Angewandte Chemie - International Edition, 2002, 41, 4769-4773.	7.2	59
97	Enzyme Activity and Flexibility at Very Low Hydration. Biophysical Journal, 2005, 89, 1282-1287.	0.2	59
98	Multi-Conformer Ensemble Docking to Difficult Protein Targets. Journal of Physical Chemistry B, 2015, 119, 1026-1034.	1.2	59
99	Picosecond dynamical changes on denaturation of yeast phosphoglycerate kinase revealed by quasielastic neutron scattering. Proteins: Structure, Function and Bioinformatics, 1997, 28, 380-387.	1.5	58
100	Simulation of a cellulose fiber in ionic liquid suggests a synergistic approach to dissolution. Cellulose, 2014, 21, 983-997.	2.4	58
101	Structure, dynamics and reactions of protein hydration water. Philosophical Transactions of the Royal Society B: Biological Sciences, 2004, 359, 1181-1190.	1.8	57
102	Molecular Dynamics Simulations of Proteins:â€‰ Can the Explicit Water Model Be Varied?. Journal of Chemical Theory and Computation, 2007, 3, 1550-1560.	2.3	56
103	Molecular simulation as a tool for studying lignin. Environmental Progress and Sustainable Energy, 2012, 31, 47-54.	1.3	56
104	Insights into the Chemomechanical Coupling of the Myosin Motor from Simulation of Its ATP Hydrolysis Mechanism. Biochemistry, 2006, 45, 5830-5847.	1.2	55
105	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
106	SASSIM: a method for calculating small-angle X-ray and neutron scattering and the associated molecular envelope from explicit-atom models of solvated proteins. Acta Crystallographica Section D: Biological Crystallography, 2002, 58, 242-249.	2.5	54
107	Protein Dynamics and Stability: The Distribution of Atomic Fluctuations in Thermophilic and Mesophilic Dihydrofolate Reductase Derived Using Elastic Incoherent Neutron Scattering. Biophysical Journal, 2008, 94, 4812-4818.	0.2	54
108	Why Mercury Prefers Soft Ligands. Journal of Physical Chemistry Letters, 2013, 4, 2317-2322.	2.1	54

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109	Sassena â€" X-ray and neutron scattering calculated from molecular dynamics trajectories using massively parallel computers. Computer Physics Communications, 2012, 183, 1491-1501.	3.0	53
110	A Solvent-Free Coarse Grain Model for Crystalline and Amorphous Cellulose Fibrils. Journal of Chemical Theory and Computation, 2011, 7, 2539-2548.	2.3	52
111	Structural and Functional Evidence for Testosterone Activation of GPRC6A in Peripheral Tissues. Molecular Endocrinology, 2015, 29, 1759-1773.	3.7	52
112	Full structural ensembles of intrinsically disordered proteins from unbiased molecular dynamics simulations. Communications Biology, 2021, 4, 243.	2.0	52
113	Methyl group dynamics in the crystalline alanine dipeptide: A combined computer simulation and inelastic neutron scattering analysis. Journal of Chemical Physics, 1992, 97, 8864-8879.	1.2	51
114	Reorientation and Dimerization of the Membrane-Bound Antimicrobial Peptide PGLa from Microsecond All-Atom MD Simulations. Biophysical Journal, 2012, 103, 472-482.	0.2	51
115	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
116	X-ray diffuse scattering and rigid-body motion in crystalline lysozyme probed by molecular dynamics simulation 1 1Edited by R. Huber. Journal of Molecular Biology, 1998, 279, 303-319.	2.0	50
117	High-Resolution Vibrational Inelastic Neutron Scattering:Â A New Spectroscopic Tool for Globular ProteinsâŠ¥. Journal of the American Chemical Society, 1997, 119, 9268-9273.	6.6	49
118	Celluloseâ€"hemicellulose interactions at elevated temperatures increase cellulose recalcitrance to biological conversion. Green Chemistry, 2018, 20, 921-934.	4.6	49
119	Polycystin-1 interacts with TAZ to stimulate osteoblastogenesis and inhibit adipogenesis. Journal of Clinical Investigation, 2017, 128, 157-174.	3.9	49
120	Picosecond timescale rigid-helix and side-chain motions in deoxymyoglobin. Proteins: Structure, Function and Bioinformatics, 1993, 16, 141-154.	1.5	48
121	Methyl Group Dynamics and the Onset of Anharmonicity in Myoglobin. Journal of Physical Chemistry B, 2008, 112, 5522-5533.	1.2	48
122	Derivation of Mean-Square Displacements for Protein Dynamics from Elastic Incoherent Neutron Scattering. Journal of Physical Chemistry B, 2012, 116, 5028-5036.	1.2	48
123	The Principal Motions Involved in the Coupling Mechanism of the Recovery Stroke of the Myosin Motor. Journal of Molecular Biology, 2007, 367, 591-602.	2.0	47
124	Elastic and Conformational Softness of a Globular Protein. Physical Review Letters, 2013, 110, 028104.	2.9	47
125	Neutron scattering in the biological sciences: progress and prospects. Acta Crystallographica Section D: Structural Biology, 2018, 74, 1129-1168.	1.1	47
126	Inhibitor binding influences the protonation states of histidines in SARS-CoV-2 main protease. Chemical Science, 2021, 12, 1513-1527.	3.7	47

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127	Optimal use of data in parallel tempering simulations for the construction of discrete-state Markov models of biomolecular dynamics. Journal of Chemical Physics, 2011, 134, 244108.	1.2	46
128	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
129	Chemical Factors that Control Lignin Polymerization. Journal of Physical Chemistry B, 2014, 118, 164-170.	1.2	46
130	A molecular mechanics force field for biologically important sterols. Journal of Computational Chemistry, 2005, 26, 1383-1399.	1.5	45
131	Lattice Dynamics of a Protein Crystal. Physical Review Letters, 2007, 99, 138101.	2.9	45
132	Surface Hydration Amplifies Single-Well Protein Atom Diffusion Propagating into the Macromolecular Core. Physical Review Letters, 2012, 108, 238102.	2.9	45
133	Conformations of Lowâ€Molecularâ€Weight Lignin Polymers in Water. ChemSusChem, 2016, 9, 289-295.	3.6	45
134	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
135	Hydrogen-Bond Driven Loop-Closure Kinetics in Unfolded Polypeptide Chains. PLoS Computational Biology, 2010, 6, e1000645.	1.5	44
136	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
137	Hydration Control of the Mechanical and Dynamical Properties of Cellulose. Biomacromolecules, 2014, 15, 4152-4159.	2.6	44
138	Enzyme activity and dynamics: xylanase activity in the absence of fast anharmonic dynamics. Biochemical Journal, 2000, 346, 355-358.	1.7	43
139	Protein dynamics from X-ray crystallography: Anisotropic, global motion in diffuse scattering patterns. Proteins: Structure, Function and Bioinformatics, 2006, 66, 941-953.	1.5	42
140	Suppression of the back proton-transfer from Asp85 to the retinal Schiff base in bacteriorhodopsin: A theoretical analysis of structural elements. Journal of Structural Biology, 2007, 157, 454-469.	1.3	42
141	Temperature Dependence of Protein Dynamics Simulated with Three Different Water Models. Journal of Chemical Theory and Computation, 2010, 6, 1390-1400.	2.3	42
142	Functional Domain Motions in Proteins on the â^¼1â€“100Âns Timescale: Comparison of Neutron Spin-Echo Spectroscopy of Phosphoglycerate Kinase with Molecular-Dynamics Simulation. Biophysical Journal, 2012, 102, 1108-1117.	0.2	42
143	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
144	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

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145	Low-Temperature Protein Dynamics:Â A Simulation Analysis of Interprotein Vibrations and the Boson Peak at 150 K. Journal of the American Chemical Society, 2006, 128, 2356-2364.	6.6	41
146	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
147	Ensemble-based docking: From hit discovery to metabolism and toxicity predictions. Bioorganic and Medicinal Chemistry, 2016, 24, 4928-4935.	1.4	41
148	Structure-based design of broadly protective group a streptococcal M protein-based vaccines. Vaccine, 2017, 35, 19-26.	1.7	41
149	Structural modeling and molecular dynamics simulation of the actin filament. Proteins: Structure, Function and Bioinformatics, 2011, 79, 2033-2043.	1.5	40
150	"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
151	Environmental Mercury Chemistry â€“ In Silico. Accounts of Chemical Research, 2019, 52, 379-388.	7.6	40
152	Chargeâ€Based Interactions between Peptides Observed as the Dominant Force for Association in Aqueous Solution. Angewandte Chemie - International Edition, 2008, 47, 9059-9062.	7.2	39
153	Vibrational Softening of a Protein on Ligand Binding. Journal of Physical Chemistry B, 2011, 115, 6811-6817.	1.2	39
154	Taskâ€parallel message passing interface implementation of Autodock4 for docking of very large databases of compounds using highâ€performance superâ€computers. Journal of Computational Chemistry, 2011, 32, 1202-1209.	1.5	39
155	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
156	Catalytic Mechanism of Cellulose Degradation by a Cellobiohydrolase, CelS. PLoS ONE, 2010, 5, e12947.	1.1	39
157	AFMM: A molecular mechanics force field vibrational parametrization program. Computer Physics Communications, 2005, 167, 34-42.	3.0	38
158	Correlated Dynamics Determining X-Ray Diffuse Scattering from a Crystalline Protein Revealed by Molecular Dynamics Simulation. Physical Review Letters, 2005, 95, 218103.	2.9	38
159	Why genetic modification of lignin leads to low-recalcitrance biomass. Physical Chemistry Chemical Physics, 2015, 17, 358-364.	1.3	38
160	Conformational distribution of heptaalanine: Analysis using a new Monte Carlo chain growth method. Journal of Computational Chemistry, 1992, 13, 1216-1233.	1.5	37
161	Collective Vibrations in Crystalline L-Alanine. The Journal of Physical Chemistry, 1995, 99, 5645-5657.	2.9	37
162	Understanding the energetics of helical peptide orientation in membranes. Proteins: Structure, Function and Bioinformatics, 2005, 58, 913-922.	1.5	37

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163	Configurational Distribution of Denatured Phosphoglycerate Kinase. Journal of Molecular Biology, 1993, 231, 840-848.	2.0	36
164	Mechanism of a Molecular Valve in the Halorhodopsin Chloride Pump. Structure, 2005, 13, 617-627.	1.6	36
165	Simulations of the Myosin II Motor Reveal a Nucleotide-state Sensing Element that Controls the Recovery Stroke. Journal of Molecular Biology, 2006, 361, 604-616.	2.0	36
166	Analyzing largeâ€scale structural change in proteins: Comparison of principal component projection and sammon mapping. Proteins: Structure, Function and Bioinformatics, 2006, 64, 210-218.	1.5	36
167	Common Folding Mechanism of a Î²-Hairpin Peptide via Non-native Turn Formation Revealed by Unbiased Molecular Dynamics Simulations. Journal of the American Chemical Society, 2009, 131, 18147-18152.	6.6	36
168	Increase of both Order and Disorder in the First Hydration Shell with Increasing Solute Polarity. Physical Review Letters, 2011, 107, 267801.	2.9	36
169	Molecular Dynamics Simulation of the Structures, Dynamics, and Aggregation of Dissolved Organic Matter. Environmental Science & Technology, 2020, 54, 13527-13537.	4.6	36
170	GPU-Accelerated Drug Discovery with Docking on the Summit Supercomputer. , 2020, , .		36
171	Protein hydration water: Structure and thermodynamics. Journal of Molecular Liquids, 2002, 101, 27-33.	2.3	35
172	Direct Measurement of Hydration-Related Dynamic Changes in Lysozyme using Inelastic Neutron Scattering Spectroscopy. Journal of Biomolecular Structure and Dynamics, 1987, 4, 583-588.	2.0	34
173	Molecular mechanics force field parameterization of the fluorescent probe rhodamine 6G using automated frequency matching. Journal of Computational Chemistry, 2003, 24, 632-639.	1.5	34
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