Jeremy C Smith

List of Publications by Year
in descending order

483 papers	54,735 citations	11908 72 h-index	1680 220 g-index
521 all docs	521 docs citations	521 times ranked	56267 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
176	How does Water Boost the Protein Dynamics?. Biophysical Journal, 2012, 102, 451a.	0.2	0
177	Reconstruction of Protein Side-Chain Conformational Free Energy Surfaces From NMR-Derived Methyl Axis Order Parameters. Journal of Physical Chemistry B, 2012, 116, 4124-4133.	1.2	15
178	Radical Coupling Reactions in Lignin Synthesis: A Density Functional Theory Study. Journal of Physical Chemistry B, 2012, 116, 4760-4768.	1.2	101
179	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
180	REACH Coarse-Grained Simulation of a Cellulose Fiber. Biomacromolecules, 2012, 13, 2634-2644.	2.6	33

#	Article	IF	Citations
181	Unwrapping of Nucleosomal DNA Ends: A Multiscale Molecular Dynamics Study. Biophysical Journal, 2012, 102, 849-858.	0.2	65
182	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
183	Structural Alterations in the Nucleosome upon H3 Tail-Truncation Reveals a Crucial Role for the H2A C Terminal Docking Domain in Nucleosome Destabilization. Biophysical Journal, 2012, 102, 73a.	0.2	0
184	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
185	Alteration of Water Structure by Peptide Clusters Revealed by Neutron Scattering in the Small-Angle Region (below 1ÂÃ…â^'1). Biophysical Journal, 2012, 103, 1518-1524.	0.2	5
186	Dynamics of Protein and its Hydration Water: Neutron Scattering Studies on Fully Deuterated GFP. Biophysical Journal, 2012, 103, 1566-1575.	0.2	121
187	Molecular Simulation in the Energy Biosciences. RSC Biomolecular Sciences, 2012, , 87-114.	0.4	0
188	Stereoselection in the dielsâ€“alderase ribozyme: A molecular dynamics study. Journal of Computational Chemistry, 2012, 33, 1603-1614.	1.5	6
189	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
190	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
191	Enabling grandâ€canonical Monte Carlo: Extending the flexibility of GROMACS through the GromPy python interface module. Journal of Computational Chemistry, 2012, 33, 1207-1214.	1.5	4
192	Molecular simulation as a tool for studying lignin. Environmental Progress and Sustainable Energy, 2012, 31, 47-54.	1.3	56
193	Structure and Dynamics of Biological Systems: Integration of Neutron Scattering with Computer Simulation. Neutron Scattering Applications and Techniques, 2012, , 189-204.	0.2	4
194	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
195	Configurational subdiffusion of peptides: A network study. Physical Review E, 2011, 83, 021902.	0.8	12
196	Simulation Analysis of the Temperature Dependence of Lignin Structure and Dynamics. Journal of the American Chemical Society, 2011, 133, 20277-20287.	6.6	126
197	Molecular Origin of Gerstmann-StrÃussler-Scheinker Syndrome: Insight from Computer Simulation of an Amyloidogenic Prion Peptide. Biophysical Journal, 2011, 100, 3000-3007.	0.2	11
198	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

#	Article	IF	Citations
199	Mercury Detoxification by Bacteria: Simulations of Transcription Activation and Mercuryï£¿Carbon Bond Cleavage. , 2011, , 311-324.		0
200	Structural Characterization of Intramolecular Hg2+ Transfer between Flexibly Linked Domains of Mercuric Ion Reductase. Journal of Molecular Biology, 2011, 413, 639-656.	2.0	24
201	Vibrational Softening of a Protein on Ligand Binding. Journal of Physical Chemistry B, 2011, 115, 6811-6817.	1.2	39
202	Increase of both Order and Disorder in the First Hydration Shell with Increasing Solute Polarity. Physical Review Letters, 2011, 107, 267801.	2.9	36
203	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
204	Role of magnesium ions in DNA recognition by the EcoRV restriction endonuclease. FEBS Letters, 2011, 585, 2739-2743.	1.3	11
205	The solvation structures of cellulose microfibrils in ionic liquids. Interdisciplinary Sciences, Computational Life Sciences, 2011, 3, 308-320.	2.2	17
206	Ground-state properties of the retinal molecule: from quantum mechanical to classical mechanical computations of retinal proteins. Theoretical Chemistry Accounts, 2011, 130, 1169-1183.	0.5	15
207	Water Pathways in the Bacteriorhodopsin Proton Pump. Journal of Membrane Biology, 2011, 239, 73-84.	1.0	11
208	Structural modeling and molecular dynamics simulation of the actin filament. Proteins: Structure, Function and Bioinformatics, 2011, 79, 2033-2043.	1.5	40
209	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
210	Efficient Computation, Sensitivity, and Error Analysis of Committor Probabilities for Complex Dynamical Processes. Multiscale Modeling and Simulation, 2011, 9, 545-567.	0.6	26
211	Three Classes of Motion in the Dynamic Neutron-Scattering Susceptibility of a Globular Protein. Physical Review Letters, 2011, 107, 148102.	2.9	76
212	Transfer matrix approach to the hydrogen-bonding in cellulose Iβ fibrils describes the recalcitrance to thermal deconstruction. Journal of Chemical Physics, 2011, 135, 085106.	1.2	4
213	Publisherâ€™s Note: Self-similar multiscale structure of lignin revealed by neutron scattering and molecular dynamics simulation [Phys. Rev. E83, 061911 (2011)]. Physical Review E, 2011, 84, .	0.8	2
214	Self-similar multiscale structure of lignin revealed by neutron scattering and molecular dynamics simulation. Physical Review E, 2011, 83, 061911.	0.8	72
215	Small Angle Neutron Scattering Reveals pH-dependent Conformational Changes in Trichoderma reesei Cellobiohydrolase I. Journal of Biological Chemistry, 2011, 286, 32801-32809.	1.6	29
216	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

#	Article	IF	Citations
217	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
218	Response of water to electric fields at temperatures below the glass transition: A molecular dynamics analysis. Journal of Chemical Physics, 2011, 135, 134507.	1.2	14
219	Role of Histone Tails in Structural Stability of the Nucleosome. PLoS Computational Biology, 2011, 7, e1002279.	1.5	104
220	Structured Pathway across the Transition State for Peptide Folding Revealed by Molecular Dynamics Simulations. PLoS Computational Biology, 2011, 7, e1002137.	1.5	7
221	QM/MM Analysis of Cellulase Active Sites and Actions of the Enzymes on Substrates. ACS Symposium Series, 2010, , 135-154.	0.5	3
222	Mechanism of a proton pump analyzed with computer simulations. Theoretical Chemistry Accounts, 2010, 125, 353-363.	0.5	15
223	Atomistic Simulation of Lignocellulosic Biomass and Associated Cellulosomal Protein Complexes. ACS Symposium Series, 2010, , 55-73.	0.5	4
224	Probing the mechanism of cellulosome attachment to the Clostridium thermocellum cell surface: computer simulation of the Type II cohesin-dockerin complex and its variants. Protein Engineering, Design and Selection, 2010, 23, 759-768.	1.0	3
225	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
226	Hydrogen-Bond Driven Loop-Closure Kinetics in Unfolded Polypeptide Chains. PLoS Computational Biology, 2010, 6, e1000645.	1.5	44
227	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
228	Magnesium-Dependent Active-Site Conformational Selection in the Dielsâ^'Alderase Ribozyme. Journal of the American Chemical Society, 2010, 132, 12587-12596.	6.6	17
229	Peptide Partitioning Properties from Direct Insertion Studies. Biophysical Journal, 2010, 98, L60-L62.	0.2	26
230	Activity and Dynamics of an Enzyme, Pig Liver Esterase, in Near-Anhydrous Conditions. Biophysical Journal, 2010, 99, L62-L64.	0.2	16
231	Theory and Normal-Mode Analysis of Change in Protein Vibrational Dynamics on Ligand Binding. Journal of Physical Chemistry B, 2010, 114, 1479-1485.	1.2	20
232	Temperature Dependence of Protein Dynamics Simulated with Three Different Water Models. Journal of Chemical Theory and Computation, 2010, 6, 1390-1400.	2.3	42
233	Structure and Conformational Dynamics of the Metalloregulator MerR upon Binding of Hg(II). Journal of Molecular Biology, 2010, 398, 555-568.	2.0	32
234	Mechanism of DNA Recognition by the Restriction Enzyme EcoRV. Journal of Molecular Biology, 2010, 401, 415-432.	2.0	24

#	Article	IF	Citations
235	Common Folding Mechanism of a Peptide Revealed by Multiple MD Simulations. Biophysical Journal, 2010, 98, 199a-200a.	0.2	0
236	Catalytic Mechanism of Cellulose Degradation by a Cellobiohydrolase, CelS. PLoS ONE, 2010, 5, e12947.	1.1	39
237	Enzyme activity and dynamics in near-anhydrous conditions. Nature Precedings, 2009, , .	0.1	0
238	Protein Dynamical Transition: Role of Methyl Dynamics and Local Diffusion. , 2009, , .		3
239	Energy Triplets for Writing Epigenetic Marks: Insights from QM/MM Freeâ€Energy Simulations of Protein Lysine Methyltransferases. Chemistry - A European Journal, 2009, 15, 12596-12599.	1.7	22
240	A molecular mechanics force field for lignin. Journal of Computational Chemistry, 2009, 30, 457-467.	1.5	89
241	REACH: A program for coarse-grained biomolecular simulation. Computer Physics Communications, 2009, 180, 1188-1195.	3.0	6
242	Nucleotideâ€dependence of Gâ€actin conformation from multiple molecular dynamics simulations and observation of a putatively polymerizationâ€competent superclosed state. Proteins: Structure, Function and Bioinformatics, 2009, 76, 353-364.	1.5	20
243	Building a foundation for structureâ€based cellulosome design for cellulosic ethanol: Insight into cohesinâ€dockerin complexation from computer simulation. Protein Science, 2009, 18, 949-959.	3.1	17
244	Subdiffusion in time-averaged, confined random walks. Physical Review E, 2009, 80, 011109.	0.8	78
245	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
246	Long-Distance Proton Transfer with a Break in the Bacteriorhodopsin Active Site. Journal of the American Chemical Society, 2009, 131, 7064-7078.	6.6	31
247	Response of Small-Scale, Methyl Rotors to Proteinâ^'Ligand Association: A Simulation Analysis of Calmodulinâ^'Peptide Binding. Journal of the American Chemical Society, 2009, 131, 10083-10091.	6.6	15
248	Peptide Partitioning and Folding into Lipid Bilayers. Journal of Chemical Theory and Computation, 2009, 5, 2202-2205.	2.3	17
249	Instantaneous Normal Modes and the Protein Glass Transition. Biophysical Journal, 2009, 96, 476-484.	0.2	12
250	REACH Coarse-Grained Normal Mode Analysis of Protein Dimer Interaction Dynamics. Biophysical Journal, 2009, 97, 1158-1167.	0.2	18
251	Catalytic Mechanism of DNA Backbone Cleavage by the Restriction Enzyme EcoRV: A Quantum Mechanical/Molecular Mechanical Analysis. Biochemistry, 2009, 48, 9061-9075.	1.2	31
252	Water Molecules in Shortâ€and Longâ€Distance Proton Transfer Steps of Bacteriorhodopsin Proton Pumping. Israel Journal of Chemistry, 2009, 49, 155-161.	1.0	7

#	Article	IF	Citations
253	Mechanism of Hgâ˜C Protonolysis in the Organomercurial Lyase MerB. Journal of the American Chemical Society, 2009, 131, 13278-13285.	6.6	70
254	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
255	Coarse Graining Methodology for the Multiscale Simulation of Complex Biological Systems. Biophysical Journal, 2009, 96, 404a.	0.2	1
256	Coarseâ€grained force field for the nucleosome from selfâ€consistent multiscaling. Journal of Computational Chemistry, 2008, 29, 1429-1439.	1.5	77
257	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
258	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
259	REACH Coarse-Grained Biomolecular Simulation: Transferability between Different Protein Structural Classes. Biophysical Journal, 2008, 95, 1639-1648.	0.2	28
260	Subdiffusion in Peptides Originates from the Fractal-Like Structure of Configuration Space. Physical Review Letters, 2008, 100, 188103.	2.9	63
261	Solvent Electrostriction-Driven Peptide Folding Revealed by Quasi-Gaussian Entropy Theory and Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2008, 112, 11155-11163.	1.2	9
262	Packing Density of the Erythropoietin Receptor Transmembrane Domain Correlates with Amplification of Biological Responses. Biochemistry, 2008, 47, 11771-11782.	1.2	15
263	Partitioning of amino-acid analogues in a five-slab membrane model. Biochimica Et Biophysica Acta - Biomembranes, 2008, 1778, 2234-2243.	1.4	26
264	Methyl Group Dynamics and the Onset of Anharmonicity in Myoglobin. Journal of Physical Chemistry B, 2008, 112, 5522-5533.	1.2	48
265	Key Role of Active-Site Water Molecules in Bacteriorhodopsin Proton-Transfer Reactions. Journal of Physical Chemistry B, 2008, 112, 14729-14741.	1.2	66
266	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
267	Hydration-Dependent Dynamical Transition in Protein: Protein Interactions at<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mo>â‰ˆ</mml:mo><mml:mn>240</mml:mn><mml:mtext>â€‰</mml:mtext><mml:mtext>â€‰</mml:mtext><mml:mi mathvariant="normal">K</mml:mi></mml:math>. Physical Review Letters, 2008, 100, 138102.	2.9	17
268	Cellulosic ethanol: progress towards a simulation model of lignocellulosic biomass. Journal of Physics: Conference Series, 2008, 125, 012055.	0.3	4
269	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
270	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

#	Article	IF	Citations
271	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
272	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
273	Hierarchical analysis of conformational dynamics in biomolecules: Transition networks of metastable states. Journal of Chemical Physics, 2007, 126, 155102.	1.2	363
274	Lattice Dynamics of a Protein Crystal. Physical Review Letters, 2007, 99, 138101.	2.9	45
275	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
276	Orientation Preferences of Backbone Secondary Amide Functional Groups in Peptide Nucleic Acid Complexes: Quantum Chemical Calculations Reveal an Intrinsic Preference of Cationic D-Amino Acid-Based Chiral PNA Analogues for the P-form. Biophysical Journal, 2007, 92, 769-786.	0.2	18
277	Coarse-Grained Biomolecular Simulation with REACH: Realistic Extension Algorithm via Covariance Hessian. Biophysical Journal, 2007, 93, 3460-3469.	0.2	93
278	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
279	Forceâ€Field Development and Molecular Dynamics Simulations of Ferroceneâ€“Peptide Conjugates as a Scaffold for Hydrogenase Mimics. Chemistry - A European Journal, 2007, 13, 8139-8152.	1.7	30
280	The Structural Coupling between ATPase Activation and Recovery Stroke in the Myosin II Motor. Structure, 2007, 15, 825-837.	1.6	72
281	AM1/d Parameters for Magnesium in Metalloenzymes. Journal of Chemical Theory and Computation, 2006, 2, 1050-1056.	2.3	23
282	Structural and energetic determinants of primary proton transfer in bacteriorhodopsin. Photochemical and Photobiological Sciences, 2006, 5, 547-552.	1.6	25
283	Conformational heterogeneity and low-frequency vibrational modes of proteins. Physical Chemistry Chemical Physics, 2006, 8, 5543.	1.3	26
284	Computing Best Transition Pathways in High-Dimensional Dynamical Systems: Application to the AlphaL leftrightharpoons Beta leftrightharpoons AlphaR Transitions in Octaalanine. Multiscale Modeling and Simulation, 2006, 5, 393-419.	0.6	17
285	Dynamics of Immobilized and Native Escherichia coli Dihydrofolate Reductase by Quasielastic Neutron Scattering. Biophysical Journal, 2006, 90, 1090-1097.	0.2	22
286	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
287	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
288	Temperature-Dependent Protein Dynamics:Â A Simulation-Based Probabilistic Diffusion-Vibration Langevin Description. Journal of Physical Chemistry B, 2006, 110, 5807-5816.	1.2	21

#	Article	IF	Citations
289	Insights into the Chemomechanical Coupling of the Myosin Motor from Simulation of Its ATP Hydrolysis Mechanism. Biochemistry, 2006, 45, 5830-5847.	1.2	55
290	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
291	Enzyme hydration, activity and flexibility: A neutron scattering approach. Journal of Non-Crystalline Solids, 2006, 352, 4387-4393.	1.5	5
292	SCC-DFTB energy barriers for single and double proton transfer processes in the model molecular systems malonaldehyde and porphycene. International Journal of Quantum Chemistry, 2006, 106, 636-640.	1.0	17
293	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
294	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
295	Tight in Titin. Structure, 2006, 14, 389-390.	1.6	1
296	Structural Basis of Cellulosome Efficiency Explored by Small Angle X-ray Scattering. Journal of Biological Chemistry, 2005, 280, 38562-38568.	1.6	95
297	Density functional theory analysis of dimethylphosphate hydrolysis: effect of solvation and nucleophile variation. Computational and Theoretical Chemistry, 2005, 713, 1-5.	1.5	14
298	Low frequency enzyme dynamics as a function of temperature and hydration: A neutron scattering study. Chemical Physics, 2005, 317, 267-273.	0.9	23
299	AFMM: A molecular mechanics force field vibrational parametrization program. Computer Physics Communications, 2005, 167, 34-42.	3.0	38
300	Mechanism of a Molecular Valve in the Halorhodopsin Chloride Pump. Structure, 2005, 13, 617-627.	1.6	36
301	The Î± Helix Dipole: Screened Out?. Structure, 2005, 13, 849-855.	1.6	89
302	Nonuniform charge scaling (NUCS): A practical approximation of solvent electrostatic screening in proteins. Journal of Computational Chemistry, 2005, 26, 1359-1371.	1.5	17
303	A molecular mechanics force field for biologically important sterols. Journal of Computational Chemistry, 2005, 26, 1383-1399.	1.5	45
304	Understanding the energetics of helical peptide orientation in membranes. Proteins: Structure, Function and Bioinformatics, 2005, 58, 913-922.	1.5	37
305	Automated computation of low-energy pathways for complex rearrangements in proteins: Application to the conformational switch of Ras p21. Proteins: Structure, Function and Bioinformatics, 2005, 59, 534-544.	1.5	34
306	Direct proton transfer in a putative L-state intermediate of the bacteriorhodopsin photocycle. Phase Transitions, 2005, 78, 5-9.	0.6	7

#	Article	IF	Citations
307	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
308	QM/MM investigation of the hydrogen-bonding interactions in putative K and early-M intermediates of the bacteriorhodopsin photocycle. Phase Transitions, 2005, 78, 671-675.	0.6	4
309	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
310	Pressure-dependent transition in protein dynamics at about4kbarrevealed by molecular dynamics simulation. Physical Review E, 2005, 72, 061908.	0.8	19
311	Temperature and timescale dependence of protein dynamics in methanol : water mixtures. Physical Chemistry Chemical Physics, 2005, 7, 1388-1393.	1.3	14
312	Tuning of Retinal Twisting in Bacteriorhodopsin Controls the Directionality of the Early Photocycle Steps. Journal of Physical Chemistry B, 2005, 109, 14786-14788.	1.2	26
313	Can Proteins and Crystals Self-Catalyze Methyl Rotations?. Journal of Physical Chemistry B, 2005, 109, 20572-20578.	1.2	12
314	Langevin Model of the Temperature and Hydration Dependence of Protein Vibrational Dynamics. Journal of Physical Chemistry B, 2005, 109, 12182-12194.	1.2	31
315	Fluctuations and Correlations in Crystalline Protein Dynamics: A Simulation Analysis of Staphylococcal Nuclease. Biophysical Journal, 2005, 88, 2554-2563.	0.2	77
316	Enzyme Activity and Flexibility at Very Low Hydration. Biophysical Journal, 2005, 89, 1282-1287.	0.2	59
317	Catalytic Transesterification of Dialkyl Phosphates by a Bioinspired Dicopper(II) Macrocyclic Complex. Journal of the American Chemical Society, 2005, 127, 15061-15070.	6.6	34
318	Protein/Ligand Binding Free Energies Calculated with Quantum Mechanics/Molecular Mechanics. Journal of Physical Chemistry B, 2005, 109, 10474-10483.	1.2	97
319	High-Density Hydration Layer of Lysozymes:Â Molecular Dynamics Decomposition of Solution Scattering Data. Journal of Chemical Information and Modeling, 2005, 45, 1593-1599.	2.5	23
320	Molecular modeling of O6-methylguanine-DNA methyltransferase mutant proteins encoded by single nucleotide polymorphisms. International Journal of Molecular Medicine, 2005, 16, 553-7.	1.8	12
321	Computer Simulation of Energy-Transducing Proteins and Peptide:Membrane Interactions. ACS Symposium Series, 2004, , 175-186.	0.5	0
322	Derivation of a molecular mechanics force field for cholesterol. Pure and Applied Chemistry, 2004, 76, 189-196.	0.9	27
323	Direct Determination of Vibrational Density of States Change on Ligand Binding to a Protein. Physical Review Letters, 2004, 93, 028103.	2.9	113
324	Structure, dynamics and reactions of protein hydration water. Philosophical Transactions of the Royal Society B: Biological Sciences, 2004, 359, 1181-1190.	1.8	57

#	Article	IF	Citations
325	Mechanism of Primary Proton Transfer in Bacteriorhodopsin. Structure, 2004, 12, 1281-1288.	1.6	105
326	Convergence properties of X-ray scattering calculated from protein crystal molecular dynamics simulations. Physica B: Condensed Matter, 2004, 350, 127-131.	1.3	0
327	Kinetics of breaking a salt-bridge critical in protein unfolding. Chemical Physics Letters, 2004, 385, 337-340.	1.2	16
328	Key Role of Electrostatic Interactions in Bacteriorhodopsin Proton Transfer. Journal of the American Chemical Society, 2004, 126, 14668-14677.	6.6	94
329	Can coordinate driving describe proton transfer coupled to complex protein motions?. Phase Transitions, 2004, 77, 47-52.	0.6	14
330	A Common Pharmacophoric Footprint for AIDS Vaccine Design. Journal of Medicinal Chemistry, 2004, 47, 3723-3729.	2.9	3
331	Neutron Frequency Windows and the Protein Dynamical Transition. Biophysical Journal, 2004, 87, 1436-1444.	0.2	96
332	Glucose-6-phosphate dehydrogenase (G6PD) deficiencyâ€“type Zurich: a splice site mutation as an uncommon mechanism producing enzyme deficiency. Blood, 2004, 104, 2608-2608.	0.6	16
333	Conformational Transitions in Proteins and Membranes. , 2004, , 485-502.		0
334	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
335	Convergence in peptide folding simulation: Multiple trajectories of a potential AIDS pharmacophore. Biopolymers, 2003, 70, 121-133.	1.2	2
336	Use of computer simulation in the interpretation of elastic neutron scattering in complex molecular systems: a small protein in various environments. Chemical Physics, 2003, 292, 389-396.	0.9	7
337	Molecular dynamics simulation reveals a surface salt bridge forming a kinetic trap in unfolding of truncated Staphylococcal nuclease. Proteins: Structure, Function and Bioinformatics, 2003, 50, 507-515.	1.5	26
338	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
339	The Role of Dynamics in Enzyme Activity. Annual Review of Biophysics and Biomolecular Structure, 2003, 32, 69-92.	18.3	319
340	Molecular Dynamics Decomposition of Temperature-Dependent Elastic Neutron Scattering by a Protein Solution. Biophysical Journal, 2003, 85, 679-685.	0.2	29
341	Translational Hydration Water Dynamics Drives the Protein Glass Transition. Biophysical Journal, 2003, 85, 1871-1875.	0.2	191
342	The Position of QB in the Photosynthetic Reaction Center Depends on pH: A Theoretical Analysis of the Proton Uptake upon QB Reduction. Biophysical Journal, 2003, 84, 2090-2098.	0.2	30

#	Article	IF	Citations
343	The dynamic transition in proteins may have a simple explanation. Faraday Discussions, 2003, 122, 163-169.	1.6	26
344	Time-resolved computational protein biochemistry: Solvent effects on interactions, conformational transitions and equilibrium fluctuations. Faraday Discussions, 2003, 122, 243-251.	1.6	3
345	Solvent caging of internal motions in myoglobin at low temperaturesThis paper was originally presented as a poster at the Faraday Discussion 122 meeting.. PhysChemComm, 2003, 6, 6-8.	0.8	3
346	Energy resolution and dynamical heterogeneity effects on elastic incoherent neutron scattering from molecular systems. Physical Review E, 2003, 67, 021904.	0.8	72
347	Principal Components of the Protein Dynamical Transition. Physical Review Letters, 2003, 91, 208106.	2.9	169
348	Neutron Inelastic Scattering as a High-Resolution Vibrational Spectroscopy: New Tool for the Study of Protein Dynamics. Spectroscopy, 2003, 17, 529-535.	0.8	13
349	The Glass Transition in Proteins. , 2003, , 503-511.		0
350	How well does charge reparametrisation account for solvent screening in molecular mechanics calculations? The example of myosin. In Silico Biology, 2003, 3, 187-96.	0.4	6
351	Computational tools for analysing structural changes in proteins in solution. Applied Bioinformatics, 2003, 2, S11-7.	1.7	0
352	The Serotonin Binding Site of Human and Murine 5-HT2BReceptors. Journal of Biological Chemistry, 2002, 277, 17170-17178.	1.6	69
353	Solution Structure of a Putative HIV1 Immunogenic Peptide:â€‰ Computer Simulation of the Principal CD4 Binding Domain of gp120. Journal of Medicinal Chemistry, 2002, 45, 1019-1025.	2.9	5
354	Protein Unfolding Transitions in an Intrinsically Unstable Annexin Domain: Molecular Dynamics Simulation and Comparison with Nuclear Magnetic Resonance Data. Biophysical Journal, 2002, 83, 681-698.	0.2	8
355	Temperature Dependence of Protein Dynamics: Computer Simulation Analysis of Neutron Scattering Properties. Biophysical Journal, 2002, 82, 1216-1225.	0.2	88
356	Detection of Individual p53-Autoantibodies by Using Quenched Peptide-Based Molecular Probes. Angewandte Chemie - International Edition, 2002, 41, 4769-4773.	7.2	59
357	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
358	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
359	Protein hydration water: Structure and thermodynamics. Journal of Molecular Liquids, 2002, 101, 27-33.	2.3	35
360	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

#	Article	IF	Citations
361	Computer Simulation of Protein Unfolding. , 2002, , 260-268.		0
362	From Sequence to Structure and Function. , 2002, , 141-148.		0
363	Calculation of small angle scattering intensities from molecular dynamics simulation. Cellular and Molecular Biology Letters, 2002, 7, 134-5.	2.7	0
364	Radially Softening Diffusive Motions in a Globular Protein. Biophysical Journal, 2001, 81, 1666-1676.	0.2	72
365	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
366	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
367	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
368	X-Ray and Neutron Scattering as Probes of the Dynamics ofBiological Molecules. , 2001, , .		0
369	Enzyme activity and dynamics: xylanase activity in the absence of fast anharmonic dynamics. Biochemical Journal, 2000, 346, 355.	1.7	19
370	Enzyme activity and dynamics: xylanase activity in the absence of fast anharmonic dynamics. Biochemical Journal, 2000, 346, 355-358.	1.7	43
371	Dynamic simulation of the mouse prion protein. Biopolymers, 2000, 54, 406-415.	1.2	26
372	Collective dynamics of a photosynthetic protein probed by neutron spin-echo spectroscopy and molecular dynamics simulation. Physica B: Condensed Matter, 2000, 276-278, 514-515.	1.3	10
373	Change in backbone torsion angle distribution on protein folding. Protein Science, 2000, 9, 1129-1136.	3.1	12
374	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
375	Structure of the MÎ±2-3 toxin Î± antibodyâ€“antigen complex: combination of modelling with functional mapping experimental results. Protein Engineering, Design and Selection, 2000, 13, 345-351.	1.0	1
376	Atomic Detail Peptide-Membrane Interactions: Molecular Dynamics Simulation of Gramicidin S in a DMPC Bilayer. Biophysical Journal, 2000, 79, 1718-1730.	0.2	33
377	Cryosolvents useful for protein and enzyme studies below â^'100Â°C. Journal of Proteomics, 2000, 42, 97-103.	2.4	8
378	S100 proteinâ€“annexin interactions: a model of the (Anx2-p11)2 heterotetramer complex. Biochimica Et Biophysica Acta - Molecular Cell Research, 2000, 1498, 181-191.	1.9	25

#	Article	IF	Citations
379	Pathway for Large-Scale Conformational Change in Annexin V. Biochemistry, 2000, 39, 14065-14074.	1.2	26
380	Enzyme activity and dynamics: xylanase activity in the absence of fast anharmonic dynamics. Biochemical Journal, 2000, 346 Pt 2, 355-8.	1.7	17
381	Dynamical and structural modifications of staphylococcal nuclease on C-terminal truncation. Physica B: Condensed Matter, 1999, 266, 20-26.	1.3	17
382	Molecular dynamics simulations of the isolated domain 1 of annexin I. Theoretical Chemistry Accounts, 1999, 101, 82-86.	0.5	5
383	Efficient calculation of two-dimensional adiabatic and free energy maps: Application to the isomerization of the C13?C14 and C15?N16 bonds in the retinal of bacteriorhodopsin. Journal of Computational Chemistry, 1999, 20, 1644-1658.	1.5	28
384	Modelling and simulation of light-activated membrane proteins: Dynamical transitions in bacteriorhodopsin. Faraday Discussions, 1999, 111, 95-102.	1.6	1
385	Enzyme Dynamics and Activity: Time-Scale Dependence of Dynamical Transitions in Glutamate Dehydrogenase Solution. Biophysical Journal, 1999, 77, 2184-2190.	0.2	88
386	Simulation Analysis of the Retinal Conformational Equilibrium in Dark-Adapted Bacteriorhodopsin. Biophysical Journal, 1999, 76, 1909-1917.	0.2	33
387	Molecular Dynamics Simulation of the Cyclic Decapeptide Antibiotic, Gramicidin S, in Dimethyl Sulfoxide Solution. Journal of Physical Chemistry B, 1999, 103, 1586-1594.	1.2	14
388	The influence of helix morphology on co-operative polyamide backbone conformational flexibility in peptide nucleic acid complexes 1 1Edited by I. Tinoco. Journal of Molecular Biology, 1999, 292, 1017-1038.	2.0	9
389	A man presenting with limb weakness and electrolyte imbalance. Postgraduate Medical Journal, 1999, 75, 691-693.	0.9	4
390	The use of dynamic BNR and two-dimensional clarifier modelling to investigate nitrogen removal at Eastern Treatment Plant, Melbourne, Australia. Water Science and Technology, 1999, 39, 89-96.	1.2	5
391	Nolan, Christopher W. Managing the Reference Collection. Chicago: ALA, 1999. 231p. $30, acid-free paper (ISBN 0-8389-0748-2). LC 98-037178.. College and Research Libraries, 1999, 60, 398-400.	0.2	0
392	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
393	Oxidation of tetrahydro-beta-carboline by cytochrome P-450cam . Determination and rationalisation of product distribution. FEBS Journal, 1998, 251, 398-404.	0.2	3
394	Simulation evidence for experimentally detectable low-temperature vibrational inhomogeneity in a globular protein. Biopolymers, 1998, 39, 471-478.	1.2	17
395	Structural modeling of the complex between an acetylcholine receptor-mimicking antibody and its snake toxin antigen. , 1998, 30, 249-263.		3
396	Excluded volume in the configurational distribution of a stronglyâ€denatured protein. Protein Science, 1998, 7, 1396-1403.	3.1	27

#	Article	IF	Citations
397	Nanosecond Protein Dynamics:Â First Detection of a Neutron Incoherent Spinâ˜Echo Signal. Journal of the American Chemical Society, 1998, 120, 7347-7348.	6.6	10
398	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
399	Enzyme Activity below the Dynamical Transition at 220 K. Biophysical Journal, 1998, 75, 2504-2507.	0.2	131
400	Structural modeling of the pro-ocytocin-neurophysin precursor. Protein Engineering, Design and Selection, 1998, 11, 909-916.	1.0	4
401	Dynamics of alkane chains included in an organic matrix: Molecular dynamics simulation and comparison with neutron scattering experiment. Journal of Chemical Physics, 1998, 109, 2883-2894.	1.2	20
402	Structural modeling of the complex between an acetylcholine receptor-mimicking antibody and its snake toxin antigen. Proteins: Structure, Function and Bioinformatics, 1998, 30, 249-63.	1.5	1
403	Simulation of Collective Dynamics ofn-Nonadecane in the Urea Inclusion Compound. Journal of Physical Chemistry B, 1997, 101, 6753-6757.	1.2	12
404	Fluctuation and Correlation in Crystalline Lysozyme. Journal of Chemical Information and Computer Sciences, 1997, 37, 1011-1017.	2.8	7
405	Quantum Chemical and Free Energy Simulation Analysis of Retinal Conformational Energetics. Journal of Chemical Information and Computer Sciences, 1997, 37, 1018-1024.	2.8	30
406	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
407	Small-angle neutron scattering by a strongly denatured protein: analysis using random polymer theory. Biophysical Journal, 1997, 72, 335-342.	0.2	33
408	Structure of human annexin I: Comparison of homology modelling and crystallographic experiment. Biochimie, 1997, 79, 691-703.	1.3	5
409	Dynamics of proteins: Correlation and diffusion. Physica B: Condensed Matter, 1997, 234-236, 175-182.	1.3	1
410	Motions in native and denatured proteins. Physica B: Condensed Matter, 1997, 241-243, 1110-1114.	1.3	2
411	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
412	Picosecond dynamical changes on denaturation of yeast phosphoglycerate kinase revealed by quasielastic neutron scattering. , 1997, 28, 380.		1
413	Dynamics of Biomolecules : Simulation Versus X-Ray and Far-Infrared Experiments. , 1997, , 35-46.		0
414	Picosecond dynamical changes on denaturation of yeast phosphoglycerate kinase revealed by quasielastic neutron scattering. Proteins: Structure, Function and Bioinformatics, 1997, 28, 380-7.	1.5	20

#	Article	IF	Citations
415	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
416	Denaturation of Truncated Staphylococcal Nuclease in Molecular Dynamics Simulation at 300 K. Journal of the American Chemical Society, 1996, 118, 7326-7328.	6.6	18
417	Molecular dynamics analysis of charge fluctuations associated with far-infrared absorption in water. Molecular Physics, 1996, 87, 1333-1347.	0.8	32
418	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
419	Force field development and conformational search strategy in the simulation of biomolecular recognition processes. Biochemical Society Transactions, 1996, 24, 268-274.	1.6	2
420	Structural model of the anti-snake-toxin antibody, MÎ±2,3. , 1996, 26, 9-31.		11
421	Molecular dynamics simulation ofnâ€nonadecane in urea inclusion compound. I. Comparison with quasielastic neutron scattering experiment. Journal of Chemical Physics, 1996, 105, 1516-1528.	1.2	28
422	Molecular dynamics simulation ofnâ€nonadecane in urea inclusion compound. II. Rotational distribution and elastic incoherent structure factor. Journal of Chemical Physics, 1996, 105, 1529-1536.	1.2	23
423	Low-frequency vibrations in ?-helices: Helicoidal analysis of polyalanine and deoxymyoglobin molecular dynamics trajectories. Biopolymers, 1995, 35, 555-571.	1.2	10
424	Conformational energetics of a partially symmetrized photosynthetic reaction centre. Chemical Physics Letters, 1995, 242, 238-243.	1.2	5
425	SERENA: a program for calculating X-ray diffuse scattering intensities from molecular dynamics trajectories. Computer Physics Communications, 1995, 91, 331-338.	3.0	16
426	Structural model of the photosynthetic reaction center ofRhodobacter capsulatus. Proteins: Structure, Function and Bioinformatics, 1995, 22, 226-244.	1.5	23
427	Dynamics of proteins: Simulations versus scattering and spectroscopy experiments. AIP Conference Proceedings, 1995, , .	0.3	0
428	Dynamics of pure and sodium-doped polyacetylene. AIP Conference Proceedings, 1995, , .	0.3	0
429	Quantum chemical analysis of retinal schiff base hydration in bacteriorhodopsin. AIP Conference Proceedings, 1995, , .	0.3	0
430	Dynamics of N-Nonadecane Chains in Urea Inclusion Compounds as seen by Incoherent Quasielastic Neutron Scattering and Computer Simulations. , 1995, , 609-624.		2
431	Collective Vibrations in Crystalline L-Alanine. The Journal of Physical Chemistry, 1995, 99, 5645-5657.	2.9	37
432	Structural Basis of Antibody Cross-Reactivity: Solution Conformation of an Immunogenic Peptide Fragment Containing both T and B Epitopes. Biochemistry, 1995, 34, 12782-12789.	1.2	13

#	Article	IF	Citations
433	Functional interactions in bacteriorhodopsin: a theoretical analysis of retinal hydrogen bonding with water. Biophysical Journal, 1995, 68, 25-39.	0.2	95
434	Dynamics of crystalline acetanilide: Analysis using neutron scattering and computer simulation. Journal of Chemical Physics, 1995, 102, 5525-5541.	1.2	30
435	Engineering of protein epitopes: a single deletion in a snake toxin generates full binding capacity to a previously unrecognized antibody. Protein Engineering, Design and Selection, 1994, 7, 917-923.	1.0	7
436	Dynamics of sodiumâ€doped polyacetylene. Journal of Chemical Physics, 1994, 101, 634-644.	1.2	13
437	How random is a highly denatured protein?. Biophysical Chemistry, 1994, 53, 105-113.	1.5	90
438	Protein interactions and dynamics probed by quantum chemistry, computer simulations and neutron experiments. Biophysical Chemistry, 1994, 53, 131-143.	1.5	0
439	Molecular mechanics analysis of peptide group hydrogen bonding cooperativity and influence on Î¦ and Î¨ rotational barriers. Computational and Theoretical Chemistry, 1994, 308, 103-113.	1.5	10
440	Correlated intramolecular motions and diffuse xâ€“ray scattering in lysozyme. Nature Structural and Molecular Biology, 1994, 1, 124-128.	3.6	78
441	Liquid-like Side-chain Dynamics in Myoglobin. Journal of Molecular Biology, 1994, 242, 181-185.	2.0	97
442	Dynamics of pristine and doped polyacetylene: a combined inelastic neutron scattering and computer simulation analysis. Journal of Non-Crystalline Solids, 1994, 172-174, 472-480.	1.5	1
443	Supramolecular Interactions and Atomic Dynamics in Proteins and Peptide Crystals. Jumps, Lattice Waves, ane Liquid-Like Diffusion. , 1994, , 457-475.		0
444	Structure, Dynamics and Function of Hydrogen-Bonded Networks in Proteins and Related Systems. , 1994, , 489-508.		0
445	On the Configurations Accessible to Folded and to Denatured Proteins. NATO ASI Series Series B: Physics, 1994, , 135-145.	0.2	0
446	Lattice vibrations in crystallineL-alanine. Biopolymers, 1993, 33, 725-733.	1.2	14
447	Computer simulations of the flexibility of a series of synthetic cyclic peptide analogues. Biopolymers, 1993, 33, 1249-1270.	1.2	10
448	Picosecond timescale rigid-helix and side-chain motions in deoxymyoglobin. Proteins: Structure, Function and Bioinformatics, 1993, 16, 141-154.	1.5	48
449	Structure and dynamics of bacteriorhodopsin. FEBS Letters, 1993, 327, 256-260.	1.3	20
450	Configurational Distribution of Denatured Phosphoglycerate Kinase. Journal of Molecular Biology, 1993, 231, 840-848.	2.0	36

#	Article	IF	Citations
451	Combination of Neutron Scattering and Molecular Dynamics to Determine Internal Motions in Biomolecules. Molecular Simulation, 1993, 10, 363-375.	0.9	19
452	The polarized density of states of crystalline polyacetylene. Molecular dynamics analysis and comparison with neutron scattering results. Journal of Chemical Physics, 1993, 99, 5586-5596.	1.2	24
453	843 ESTIMATION OF MAXIMAL SUSTAINABLE EXERTION FROM THE VELOCITY-TIME RELATIONSHIP IN HIGH-INTENSITY WHEELCHAIR EXERCISE. Medicine and Science in Sports and Exercise, 1993, 25, S151.	0.2	0
454	Structure of proteins unfolded by guanidinium chloride. European Physical Journal Special Topics, 1993, 03, C8-253-C8-256.	0.2	6
455	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
456	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
457	Hydration-dependent far-infrared absorption in lysozyme detected using synchrotron radiation. Biophysical Journal, 1992, 61, 276-280.	0.2	27
458	Conformational distribution of heptaalanine: Analysis using a new Monte Carlo chain growth method. Journal of Computational Chemistry, 1992, 13, 1216-1233.	1.5	37
459	Potential Energy Function for Photosynthetic Reaction Centre Chromophores: Energy Minimisations of a Crystalline Bacteriopheophytin a Analog. , 1992, , 43-48.		5
460	Protein dynamics: comparison of simulations with inelastic neutron scattering experiments. Quarterly Reviews of Biophysics, 1991, 24, 227-291.	2.4	328
461	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
462	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
463	Internal dynamics of globular proteins: Comparison of neutron scattering measurements and theoretical models. Physica B: Condensed Matter, 1989, 156-157, 437-443.	1.3	30
464	Analysis of any point mutation in DNA. The amplification refractory mutation system (ARMS). Nucleic Acids Research, 1989, 17, 2503-2516.	6.5	2,376
465	Inelastic neutron scattering analysis of picosecond internal protein dynamics. Journal of Molecular Biology, 1988, 202, 903-908.	2.0	95
466	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
467	Low Frequency Dynamics of BPTI Studied by Inelastic Neutron Scattering. Springer Series in Biophysics, 1987, , 93-97.	0.4	1
468	Low frequency dynamics of proteins studied by neutron time-of-flight spectroscopy. Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics, 1986, 136, 256-259.	0.9	7

#	Article	IF	Citations
469	Using Categorical Variables in Discriminant Analysis. Multivariate Behavioral Research, 1986, 21, 479-496.	1.8	14
470	Low frequency dynamics of proteins studied by neutron time-of-flight spectroscopy. Physica B: Physics of Condensed Matter & C: Atomic, Molecular and Plasma Physics, Optics, 1986, 136, 256-259.	0.9	5
471	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
472	Radial distributions of waterâ€"water distances in protein crystals. International Journal of Biological Macromolecules, 1985, 7, 223-225.	3.6	4
473	Ultrasonically induced temperature elevation in mouse ovary. Ultrasound in Medicine and Biology, 1984, 10, L488-L492.	0.7	0
474	Ultrasound Velocity in Fixed Human Liver: Empirical Anova and Regression Modelling on Histologically Assessed Abnormalities. Ultrasonic Imaging, 1983, 5, 280-294.	1.4	7
475	Trophoblastic Pulmonary Embolism. Southern Medical Journal, 1981, 74, 916-919.	0.3	6
476	Evidence for permanent population differences in the annual cycle of plasma "antifreeze" levels of winter flounder. Canadian Journal of Zoology, 1980, 58, 507-512.	0.4	21
477	Colitis cystica profounda. Case report. Missouri Medicine, 1978, 75, 560-3.	0.3	0
478	The oxoglutarate shunt and fatty acid biosynthesis in the neonatal rat brain. Journal of Neurochemistry, 1975, 24, 597-600.	2.1	6
479	Polarizations of Low Energy Snâ†•S0 Transitions in Phthalaldehyde and 10â€Methylene Anthrone. Journal of Chemical Physics, 1972, 57, 1308-1316.	1.2	3
480	Effects of pregnancy on the diameter of the uterine arteries in the rabbit. Obstetrics and Gynecology, 1968, 31, 788-94.	1.2	1
481	Chitty on Contracts (The Common Law Library No. 1). Twenty-second edition. General editor: John Morris, D.c.l., of Gray's Inn, Barrister-at-Law, Fellow of Magdalen College, Oxford. Editors: T. H. Bingham, M.a., of Gray's Inn, Barrister-at-Law; Raoul P. Colinvaux, of Gray's Inn, Barrister-at-Law; A. G. Guest, M.a., of Gray's Inn, Barrister-at-Law, Fellow of University College, Oxford; D. R. Harris, M.a., b.c.l., of the Inner Temple, Barrister-at-Law, Fellow of Balliol College, Oxford; Lever Jeremy, M.a., of. Cambridge Law Journal, 1962, 20, 262-265.	0.0	0
482	Protein Dynamics: Glass Transition and Mechanical Function. Advances in Solid State Physics, 0, , 677-694.	0.8	0
483	Molecular dynamics analysis of charge fluctuations associated with far-infrared absorption in water. , 0, .		3