J Andrew Mccammon

List of Publications by Year
in descending order

356 papers	36,638 citations	4641 85 h-index	3997 176 g-index
374 all docs	374 docs citations	374 times ranked	29075 citing authors

#	Article	IF	Citations
1	PDB2PQR: an automated pipeline for the setup of Poisson-Boltzmann electrostatics calculations. Nucleic Acids Research, 2004, 32, W665-W667.	6.5	3,014
2	Molecular dynamics simulations of biomolecules. Nature Structural Biology, 2002, 9, 646-652.	9.7	2,473
3	Dynamics of folded proteins. Nature, 1977, 267, 585-590.	13.7	1,731
4	Bio3d: an R package for the comparative analysis of protein structures. Bioinformatics, 2006, 22, 2695-2696.	1.8	1,440
5	Improvements to the <scp>APBS</scp> biomolecular solvation software suite. Protein Science, 2018, 27, 112-128.	3.1	1,399
6	Accelerated molecular dynamics: A promising and efficient simulation method for biomolecules. Journal of Chemical Physics, 2004, 120, 11919-11929.	1.2	1,313
7	Molecular Dynamics:Â Survey of Methods for Simulating the Activity of Proteins. Chemical Reviews, 2006, 106, 1589-1615.	23.0	1,007
8	Molecular dynamics simulations and drug discovery. BMC Biology, 2011, 9, 71.	1.7	881
9	Electrostatics in biomolecular structure and dynamics. Chemical Reviews, 1990, 90, 509-521.	23.0	643
10	Gaussian Accelerated Molecular Dynamics: Unconstrained Enhanced Sampling and Free Energy Calculation. Journal of Chemical Theory and Computation, 2015, 11, 3584-3595.	2.3	544
11	The Internal Dynamics of Globular Protein. Critical Reviews in Biochemistry, 1981, 9, 293-349.	7.5	488
12	The Determinants of pKas in Proteins. Biochemistry, 1996, 35, 7819-7833.	1.2	439
13	Routine Access to Millisecond Time Scale Events with Accelerated Molecular Dynamics. Journal of Chemical Theory and Computation, 2012, 8, 2997-3002.	2.3	435
14	Computational Drug Design Accommodating Receptor Flexibility:Â The Relaxed Complex Scheme. Journal of the American Chemical Society, 2002, 124, 5632-5633.	6.6	401
15	Brownian dynamics simulation of diffusionâ€influenced bimolecular reactions. Journal of Chemical Physics, 1984, 80, 1517-1524.	1.2	360
16	The hinge-bending mode in lysozyme. Nature, 1976, 262, 325-326.	13.7	349
17	Improved Reweighting of Accelerated Molecular Dynamics Simulations for Free Energy Calculation. Journal of Chemical Theory and Computation, 2014, 10, 2677-2689.	2.3	344
18	Discovery of a Novel Binding Trench in HIV Integrase. Journal of Medicinal Chemistry, 2004, 47, 1879-1881.	2.9	341

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19	Ewald artifacts in computer simulations of ionic solvation and ionâ€“ion interaction: A continuum electrostatics study. Journal of Chemical Physics, 1999, 110, 1856-1872.	1.2	325
20	Computation of electrostatic forces on solvated molecules using the Poisson-Boltzmann equation. The Journal of Physical Chemistry, 1993, 97, 3591-3600.	2.9	324
21	Ensemble Docking in Drug Discovery. Biophysical Journal, 2018, 114, 2271-2278.	0.2	318
22	Allostery in Its Many Disguises: From Theory to Applications. Structure, 2019, 27, 566-578.	1.6	285
23	An improved relaxed complex scheme for receptor flexibility in computer-aided drug design. Journal of Computer-Aided Molecular Design, 2008, 22, 693-705.	1.3	283
24	Developing a Dynamic Pharmacophore Model for HIV-1 Integrase. Journal of Medicinal Chemistry, 2000, 43, 2100-2114.	2.9	271
25	A glycan gate controls opening of the SARS-CoV-2 spike protein. Nature Chemistry, 2021, 13, 963-968.	6.6	254
26	Water in Cavityâ^'Ligand Recognition. Journal of the American Chemical Society, 2010, 132, 12091-12097.	6.6	236
27	Conformation gating as a mechanism for enzyme specificity. Proceedings of the National Academy of Sciences of the United States of America, 1998, 95, 9280-9283.	3.3	221
28	HIV-1 protease molecular dynamics of a wild-type and of the V82F/I84V mutant: Possible contributions to drug resistance and a potential new target site for drugs. Protein Science, 2004, 13, 1108-1123.	3.1	217
29	Trapping the dynamic acyl carrier protein in fatty acid biosynthesis. Nature, 2014, 505, 427-431.	13.7	216
30	Large conformational changes in proteins: signaling and other functions. Current Opinion in Structural Biology, 2010, 20, 142-147.	2.6	213
31	Activation and dynamic network of the M2 muscarinic receptor. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 10982-10987.	3.3	210
32	Stochastically gated diffusionâ€influenced reactions. Journal of Chemical Physics, 1982, 77, 4484-4493.	1.2	205
33	How Can Hydrophobic Association Be Enthalpy Driven?. Journal of Chemical Theory and Computation, 2010, 6, 2866-2871.	2.3	205
34	Ensemble-Based Virtual Screening Reveals Potential Novel Antiviral Compounds for Avian Influenza Neuraminidase. Journal of Medicinal Chemistry, 2008, 51, 3878-3894.	2.9	195
35	POVME: An algorithm for measuring binding-pocket volumes. Journal of Molecular Graphics and Modelling, 2011, 29, 773-776.	1.3	186
36	A molecular mechanics/grid method for evaluation of ligand-receptor interactions. Journal of Computational Chemistry, 1995, 16, 454-464.	1.5	175

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37	The relaxed complex method: Accommodating receptor flexibility for drug design with an improved scoring scheme. Biopolymers, 2003, 68, 47-62.	1.2	175
38	Free energy difference calculations by thermodynamic integration: Difficulties in obtaining a precise value. Journal of Computational Chemistry, 1991, 12, 271-275.	1.5	170
39	Molecular Recognition and Ligand Association. Annual Review of Physical Chemistry, 2013, 64, 151-175.	4.8	165
40	Acetylcholinesterase: electrostatic steering increases the rate of ligand binding. Biochemistry, 1993, 32, 401-403.	1.2	150
41	Gated binding of ligands to proteins. Nature, 1981, 293, 316-317.	13.7	148
42	Computing ionization states of proteins with a detailed charge model. Journal of Computational Chemistry, 1996, 17, 1633-1644.	1.5	139
43	STRUCTURE-BASED DRUG DESIGN:Computational Advances. Annual Review of Pharmacology and Toxicology, 1997, 37, 71-90.	4.2	139
44	Unconstrained enhanced sampling for free energy calculations of biomolecules: a review. Molecular Simulation, 2016, 42, 1046-1055.	0.9	139
45	Antiinfectives targeting enzymes and the proton motive force. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E7073-82.	3.3	138
46	Allosteric networks in thrombin distinguish procoagulant vs. anticoagulant activities. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 21216-21222.	3.3	137
47	Accelerated molecular dynamics simulations of protein folding. Journal of Computational Chemistry, 2015, 36, 1536-1549.	1.5	134
48	A gating mechanism proposed from a simulation of a human Â7 nicotinic acetylcholine receptor. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 6813-6818.	3.3	133
49	CRISPR-Cas9 conformational activation as elucidated from enhanced molecular simulations. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 7260-7265.	3.3	133
50	Graded activation and free energy landscapes of a muscarinic G-proteinâ€“coupled receptor. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 12162-12167.	3.3	132
51	Exploring Global Motions and Correlations in the Ribosome. Biophysical Journal, 2005, 89, 1455-1463.	0.2	131
52	Annealing Accounts for the Length of Actin Filaments Formed by Spontaneous Polymerization. Biophysical Journal, 1999, 77, 2911-2919.	0.2	129
53	Order N algorithm for computation of electrostatic interactions in biomolecular systems. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 19314-19319.	3.3	129
54	Exploring the role of receptor flexibility in structure-based drug discovery. Biophysical Chemistry, 2014, 186, 31-45.	1.5	129

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55	Discovery of drug-like inhibitors of an essential RNA-editing ligase in Trypanosoma brucei. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 17278-17283.	3.3	128
56	Accelerated molecular dynamics simulations of ligand binding to a muscarinic G-protein-coupled receptor. Quarterly Reviews of Biophysics, 2015, 48, 479-487.	2.4	127
57	Dielectric boundary smoothing in finite difference solutions of the poisson equation: An approach to improve accuracy and convergence. Journal of Computational Chemistry, 1991, 12, 909-912.	1.5	123
58	A coarse grained model for the dynamics of flap opening in HIV-1 protease. Chemical Physics Letters, 2005, 413, 123-128.	1.2	123
59	Diffusive langevin dynamics of model alkanes. Chemical Physics Letters, 1979, 65, 4-11.	1.2	119
60	Agonist-mediated Conformational Changes in Acetylcholine-binding Protein Revealed by Simulation and Intrinsic Tryptophan Fluorescence. Journal of Biological Chemistry, 2005, 280, 8443-8451.	1.6	119
61	Poissonâ€“Nernstâ€“Planck equations for simulating biomolecular diffusionâ€“reaction processes I: Finite element solutions. Journal of Computational Physics, 2010, 229, 6979-6994.	1.9	119
62	Gaussian Accelerated Molecular Dynamics in NAMD. Journal of Chemical Theory and Computation, 2017, 13, 9-19.	2.3	117
63	Targeted Molecular Dynamics Study of C-Loop Closure and Channel Gating in Nicotinic Receptors. PLoS Computational Biology, 2006, 2, e134.	1.5	113
64	Mechanism of the G-protein mimetic nanobody binding to a muscarinic G-protein-coupled receptor. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 3036-3041.	3.3	111
65	Gaussian Accelerated Molecular Dynamics: Theory, Implementation, and Applications. Annual Reports in Computational Chemistry, 2017, 13, 231-278.	0.9	107
66	Mapping the Druggable Allosteric Space of Gâ€Protein Coupled Receptors: a Fragmentâ€Based Molecular Dynamics Approach. Chemical Biology and Drug Design, 2010, 76, 201-217.	1.5	106
67	Toward a Unified Representation of Protein Structural Dynamics in Solution. Journal of the American Chemical Society, 2009, 131, 16968-16975.	6.6	105
68	Channel Opening Motion of Î±7 Nicotinic Acetylcholine Receptor as Suggested by Normal Mode Analysis. Journal of Molecular Biology, 2006, 355, 310-324.	2.0	104
69	Protospacer Adjacent Motif-Induced Allostery Activates CRISPR-Cas9. Journal of the American Chemical Society, 2017, 139, 16028-16031.	6.6	104
70	Method for Including the Dynamic Fluctuations of a Protein in Computer-Aided Drug Design. Journal of Physical Chemistry A, 1999, 103, 10213-10219.	1.1	103
71	Striking Plasticity of CRISPR-Cas9 and Key Role of Non-target DNA, as Revealed by Molecular Simulations. ACS Central Science, 2016, 2, 756-763.	5.3	103
72	Accessing a Hidden Conformation of the Maltose Binding Protein Using Accelerated Molecular Dynamics. PLoS Computational Biology, 2011, 7, e1002034.	1.5	102

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73	Studying Enzyme Binding Specificity in Acetylcholinesterase Using a Combined Molecular Dynamics and Multiple Docking Approach. Journal of the American Chemical Society, 2002, 124, 8260-8267.	6.6	101
74	Accounting for Receptor Flexibility and Enhanced Sampling Methods in Computerâ€Aided Drug Design. Chemical Biology and Drug Design, 2013, 81, 41-49.	1.5	100
75	Fast Peptidyl cisâ^'trans Isomerization within the Flexible Gly-Rich Flaps of HIV-1 Protease. Journal of the American Chemical Society, 2005, 127, 13778-13779.	6.6	99
76	Deciphering Off-Target Effects in CRISPR-Cas9 through Accelerated Molecular Dynamics. ACS Central Science, 2019, 5, 651-662.	5.3	99
77	Solving the finite-difference non-linear Poisson-Boltzmann equation. Journal of Computational Chemistry, 1992, 13, 1114-1118.	1.5	98
78	Novel Druggable Hot Spots in Avian Influenza Neuraminidase H5N1 Revealed by Computational Solvent Mapping of a Reduced and Representative Receptor Ensemble. Chemical Biology and Drug Design, 2008, 71, 106-116.	1.5	97
79	Molecular dynamics simulation with a continuum electrostatic model of the solvent. Journal of Computational Chemistry, 1995, 16, 1081-1095.	1.5	96
80	The Influence of Macromolecular Crowding on HIV-1 Protease Internal Dynamics. Journal of the American Chemical Society, 2006, 128, 6006-6007.	6.6	96
81	Internal mobility of ferrocytochrome c. Nature, 1980, 287, 659-660.	13.7	95
82	Computation of electrostatic forces between solvated molecules determined by the Poissonâ€“Boltzmann equation using a boundary element method. Journal of Chemical Physics, 2005, 122, 214102.	1.2	95
83	Active Site Binding Modes of HIV-1 Integrase Inhibitors. Journal of Medicinal Chemistry, 2000, 43, 4109-4117.	2.9	94
84	Population Based Reweighting of Scaled Molecular Dynamics. Journal of Physical Chemistry B, 2013, 117, 12759-12768.	1.2	94
85	Feature-preserving adaptive mesh generation for molecular shape modeling and simulation. Journal of Molecular Graphics and Modelling, 2008, 26, 1370-1380.	1.3	92
86	Predictive Power of Molecular Dynamics Receptor Structures in Virtual Screening. Journal of Chemical Information and Modeling, 2011, 51, 1439-1446.	2.5	91
87	Potentials of Mean Force for Acetylcholine Unbinding from the Alpha7 Nicotinic Acetylcholine Receptor Ligand-Binding Domain. Journal of the American Chemical Society, 2006, 128, 3019-3026.	6.6	90
88	Phosphorylation Effects on cis/trans Isomerization and the Backbone Conformation of Serineâ^'Proline Motifs:Â Accelerated Molecular Dynamics Analysis. Journal of the American Chemical Society, 2005, 127, 1969-1974.	6.6	89
89	Improving the Efficiency of Free Energy Calculations in the Amber Molecular Dynamics Package. Journal of Chemical Theory and Computation, 2013, 9, 4131-4139.	2.3	89
90	Induced Fit or Conformational Selection? The Role of the Semi-closed State in the Maltose Binding Protein. Biochemistry, 2011, 50, 10530-10539.	1.2	88

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91	Simulation methods for protein structure fluctuations. Biopolymers, 1980, 19, 1001-1016.	1.2	86
92	Solvent fluctuations in hydrophobic cavityâ€“ligand binding kinetics. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 1197-1202.	3.3	86
93	Browndye: A software package for Brownian dynamics. Computer Physics Communications, 2010, 181, 1896-1905.	3.0	85
94	Membranes serve as allosteric activators of phospholipase A ₂ , enabling it to extract, bind, and hydrolyze phospholipid substrates. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E516-25.	3.3	85
95	Electrostatic Free Energy and Its Variations in Implicit Solvent Models. Journal of Physical Chemistry B, 2008, 112, 3058-3069.	1.2	84
96	Enhanced Conformational Space Sampling Improves the Prediction of Chemical Shifts in Proteins. Journal of the American Chemical Society, 2010, 132, 1220-1221.	6.6	84
97	Accelerated structure-based design of chemically diverse allosteric modulators of a muscarinic G protein-coupled receptor. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E5675-84.	3.3	82
98	Finite Element Solution of the Steady-State Smoluchowski Equation for Rate Constant Calculations. Biophysical Journal, 2004, 86, 2017-2029.	0.2	81
99	Application of the level-set method to the implicit solvation of nonpolar molecules. Journal of Chemical Physics, 2007, 127, 084503.	1.2	81
100	Gated Binding of Ligands to HIV-1 Protease: Brownian Dynamics Simulations in a Coarse-Grained Model. Biophysical Journal, 2006, 90, 3880-3885.	0.2	80
101	Modelling cardiac calcium sparks in a threeâ€dimensional reconstruction of a calcium release unit. Journal of Physiology, 2012, 590, 4403-4422.	1.3	80
102	G-protein coupled receptors: advances in simulation and drug discovery. Current Opinion in Structural Biology, 2016, 41, 83-89.	2.6	80
103	Allosteric Effects of Sodium Ion Binding on Activation of the M3 Muscarinic G-Protein-Coupled Receptor. Biophysical Journal, 2015, 108, 1796-1806.	0.2	79
104	Key role of the REC lobe during CRISPRâ€“Cas9 activation by â€˜sensingâ€™, â€˜regulatingâ€™, and â€˜lockingâ€™ the catalytic HNH domain. Quarterly Reviews of Biophysics, 2018, 51, .	2.4	79
105	Molecular Dynamics Studies on the HIV-1 Integrase Catalytic Domain. Biophysical Journal, 1999, 76, 2999-3011.	0.2	78
106	Optimized Radii for Poissonâ€“Boltzmann Calculations with the AMBER Force Field. Journal of Chemical Theory and Computation, 2005, 1, 484-493.	2.3	78
107	Electrodiffusion: A continuum modeling framework for biomolecular systems with realistic spatiotemporal resolution. Journal of Chemical Physics, 2007, 127, 135102.	1.2	77
108	Asymmetric Structural Motions of the Homomeric Î±7 Nicotinic Receptor Ligand Binding Domain Revealed by Molecular Dynamics Simulation. Biophysical Journal, 2003, 85, 3007-3018.	0.2	76

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109	Relating kinetic rates and local energetic roughness by accelerated molecular-dynamics simulations. Journal of Chemical Physics, 2005, 122, 241103.	1.2	76
110	Distinct Glycan Topology for Avian and Human Sialopentasaccharide Receptor Analogues upon Binding Different Hemagglutinins: A Molecular Dynamics Perspective. Journal of Molecular Biology, 2009, 387, 465-491.	2.0	75
111	Absolute Configuration of Bromochlorofluoromethane from Molecular Dynamics Simulation of Its Enantioselective Complexation by Cryptophane-C. Journal of the American Chemical Society, 1997, 119, 3818-3823.	6.6	74
112	HIV-1 Protease Substrate Binding and Product Release Pathways Explored with Coarse-Grained Molecular Dynamics. Biophysical Journal, 2007, 92, 4179-4187.	0.2	74
113	Free energy landscape of G-protein coupled receptors, explored by accelerated molecular dynamics. Physical Chemistry Chemical Physics, 2014, 16, 6398.	1.3	74
114	Generalized Langevin dynamics simulations with arbitrary timeâ€dependent memory kernels. Journal of Chemical Physics, 1983, 78, 3256-3261.	1.2	71
115	Simulation of enzymeâ€“substrate encounter with gated active sites. Nature Structural and Molecular Biology, 1994, 1, 65-69.	3.6	71
116	Evidence for Electrostatic Channeling in a Fusion Protein of Malate Dehydrogenase and Citrate Synthaseâ€. Biochemistry, 1996, 35, 12652-12658.	1.2	70
117	The structure of Sky1p reveals a novel mechanism for constitutive activity. Nature Structural Biology, 2001, 8, 176-183.	9.7	70
118	Biological Applications of Electrostatic Calculations and Brownian Dynamics Simulations. Reviews in Computational Chemistry, 2007, , 229-267.	1.5	70
119	Nanosecond-Timescale Conformational Dynamics of the Human Î±7 Nicotinic Acetylcholine Receptor. Biophysical Journal, 2007, 93, 2622-2634.	0.2	70
120	A molecular dynamics study of thermodynamic and structural aspects of the hydration of cavities in proteins. Biopolymers, 1991, 31, 919-931.	1.2	69
121	Internal Dynamics of Green Fluorescent Protein. Journal of Physical Chemistry B, 1999, 103, 3263-3269.	1.2	69
122	Ordered Water and Ligand Mobility in the HIV-1 Integrase-5CITEP Complex:Â A Molecular Dynamics Study. Journal of Medicinal Chemistry, 2001, 44, 3043-3047.	2.9	69
123	Ligand-Induced Conformational Change in the Î±7 Nicotinic Receptor Ligand Binding Domain. Biophysical Journal, 2005, 88, 2564-2576.	0.2	67
124	Binding Pathways of Ligands to HIV-1 Protease: Coarse-grained and Atomistic Simulations. Chemical Biology and Drug Design, 2007, 69, 5-13.	1.5	67
125	Diffusive reaction rates from Brownian dynamics simulations: Replacing the outer cutoff surface by an analytical treatment. Journal of Chemical Physics, 1992, 97, 5682-5686.	1.2	66
126	Electrostatic Channeling of Substrates between Enzyme Active Sites:â€‰ Comparison of Simulation and Experiment. Biochemistry, 1997, 36, 16049-16058.	1.2	64

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127	A Dynamic Model of HIV Integrase Inhibition and Drug Resistance. Journal of Molecular Biology, 2010, 397, 600-615.	2.0	63
128	Fast and flexible gpu accelerated binding free energy calculations within the amber molecular dynamics package. Journal of Computational Chemistry, 2018, 39, 1354-1358.	1.5	63
129	Target flexibility in molecular recognition. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2005, 1754, 221-224.	1.1	60
130	Molecular docking of balanol to dynamics snapshots of protein kinase A. Proteins: Structure, Function and Bioinformatics, 2005, 61, 850-858.	1.5	60
131	Membrane Allostery and Unique Hydrophobic Sites Promote Enzyme Substrate Specificity. Journal of the American Chemical Society, 2018, 140, 3285-3291.	6.6	60
132	Rapid binding of a cationic active site inhibitor to wild type and mutant mouse acetylcholinesterase: Brownian dynamics simulation including diffusion in the active site gorge. Biopolymers, 1998, 46, 465-474.	1.2	58
133	Identification of SLAC1 anion channel residues required for CO ₂ /bicarbonate sensing and regulation of stomatal movements. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 11129-11137.	3.3	58
134	Electrostatic energy calculations by a Finite-difference method: Rapid calculation of charge-solvent interaction energies. Journal of Computational Chemistry, 1992, 13, 768-771.	1.5	57
135	Molecular dynamics of a ÎºB DNA element: base flipping via cross-strand intercalative stacking in a microsecond-scale simulation. Nucleic Acids Research, 2008, 36, 4941-4955.	6.5	56
136	Computer-Aided Identification ofTrypanosoma bruceiUridine Diphosphate Galactose 4â€²-Epimerase Inhibitors: Toward the Development of Novel Therapies for African Sleeping Sickness. Journal of Medicinal Chemistry, 2010, 53, 5025-5032.	2.9	56
137	Role of Secondary Sialic Acid Binding Sites in Influenza N1 Neuraminidase. Journal of the American Chemical Society, 2010, 132, 2883-2885.	6.6	55
138	Finite Element Simulations of Acetylcholine Diffusion in Neuromuscular Junctions. Biophysical Journal, 2003, 84, 2234-2241.	0.2	54
139	How To Deal with Multiple Binding Poses in Alchemical Relative Proteinâ€“Ligand Binding Free Energy Calculations. Journal of Chemical Theory and Computation, 2015, 11, 2670-2679.	2.3	54
140	The folding energy landscape and phosphorylation: modeling the conformational switch of the NFAT regulatory domain. FASEB Journal, 2005, 19, 1389-1395.	0.2	53
141	Mechanistic Insight into the Role of Transition-State Stabilization in Cyclophilin A. Journal of the American Chemical Society, 2009, 131, 147-152.	6.6	53
142	Molecular dynamics of ferrocytochrome c. Nature, 1980, 286, 304-305.	13.7	52
143	Computer Simulation and the Design of New Biological Molecules. Israel Journal of Chemistry, 1986, 27, 211-215.	1.0	52
144	Ligand Binding Pathways and Conformational Transitions of the HIV Protease. Biochemistry, 2018, 57, 1533-1541.	1.2	52

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145	Free energy from simulations. Current Opinion in Structural Biology, 1991, 1, 196-200.	2.6	51
146	Elucidation of Cryptic and Allosteric Pockets within the SARS-CoV-2 Main Protease. Journal of Chemical Information and Modeling, 2021, 61, 3495-3501.	2.5	51
147	Atomistic Brownian Dynamics Simulation of Peptide Phosphorylation. Journal of the American Chemical Society, 2001, 123, 9107-9111.	6.6	50
148	Conformational sampling with Poisson-Boltzmann forces and a stochastic dynamics/Monte Carlo method: Application to alanine dipeptide. Journal of Computational Chemistry, 1997, 18, 1750-1759.	1.5	49
149	Using Selectively Applied Accelerated Molecular Dynamics to Enhance Free Energy Calculations. Journal of Chemical Theory and Computation, 2010, 6, 3285-3292.	2.3	49
150	Structure, mechanism, and dynamics of UDP-galactopyranose mutase. Archives of Biochemistry and Biophysics, 2014, 544, 128-141.	1.4	49
151	Optimization of Brownian dynamics methods for diffusionâ€influenced rate constant calculations. Journal of Chemical Physics, 1986, 84, 2196-2203.	1.2	48
152	Computational Studies of the Effect of the S23D/S24D Troponin I Mutation on Cardiac Troponin Structural Dynamics. Biophysical Journal, 2014, 107, 1675-1685.	0.2	48
153	Molecular Recognition in the Case of Flexible Targets. Current Pharmaceutical Design, 2011, 17, 1663-1671.	0.9	47
154	The Dynamic Structure of Thrombin in Solution. Biophysical Journal, 2012, 103, 79-88.	0.2	47
155	Intramolecular flexibility in phenylalanine transfer RNA. Nature, 1981, 294, 286-287.	13.7	46
156	High-fidelity geometric modeling for biomedical applications. Finite Elements in Analysis and Design, 2008, 44, 715-723.	1.7	46
157	Dynamics and Calcium Association to the N-Terminal Regulatory Domain of Human Cardiac Troponin C: A Multiscale Computational Study. Journal of Physical Chemistry B, 2012, 116, 8449-8459.	1.2	46
158	A model study of sequential enzyme reactions and electrostatic channeling. Journal of Chemical Physics, 2014, 140, 105101.	1.2	46
159	3D mesh processing using GAMer 2 to enable reaction-diffusion simulations in realistic cellular geometries. PLoS Computational Biology, 2020, 16, e1007756.	1.5	46
160	Saddleâ€point avoidance in diffusional reactions. Journal of Chemical Physics, 1983, 78, 987-989.	1.2	45
161	The hinge-bending mode of a lysozyme-inhibitor complex. Biopolymers, 1986, 25, 1767-1802.	1.2	45
162	Dynamics, Hydration, and Motional Averaging of a Loop-Gated Artificial Protein Cavity:â€‰ The W191G Mutant of Cytochrome c Peroxidase in Water as Revealed by Molecular Dynamics Simulations. Biochemistry, 2007, 46, 10629-10642.	1.2	45

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163	Variational Implicit Solvation with Poissonâ€“Boltzmann Theory. Journal of Chemical Theory and Computation, 2014, 10, 1454-1467.	2.3	45
164	PKA Phosphorylation of Cardiac Troponin I Modulates Activation andÂRelaxation Kinetics of Ventricular Myofibrils. Biophysical Journal, 2014, 107, 1196-1204.	0.2	45
165	Simulation of the bimolecular reaction between superoxide and superoxide dismutase: synthesis of the encounter and reaction steps. Journal of the American Chemical Society, 1993, 115, 11874-11877.	6.6	44
166	A proposed signaling motif for nuclear import in mRNA processing via the formation of arginine claw. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 14947-14951.	3.3	44
167	Coupling the Level-Set Method with Molecular Mechanics for Variational Implicit Solvation of Nonpolar Molecules. Journal of Chemical Theory and Computation, 2009, 5, 257-266.	2.3	44
168	Simulations of Biased Agonists in the Î²₂ Adrenergic Receptor with Accelerated Molecular Dynamics. Biochemistry, 2013, 52, 5593-5603.	1.2	44
169	Gating mechanism of elongating Î²-ketoacyl-ACP synthases. Nature Communications, 2020, 11, 1727.	5.8	44
170	Mapping of Allosteric Druggable Sites in Activationâ€Associated Conformers of the M2 Muscarinic Receptor. Chemical Biology and Drug Design, 2014, 83, 237-246.	1.5	43
171	Effects of HCM cTnI Mutation R145G on Troponin Structure and Modulation by PKA Phosphorylation Elucidated by Molecular Dynamics Simulations. Biophysical Journal, 2015, 108, 395-407.	0.2	43
172	AFMPB: An adaptive fast multipole Poissonâ€“Boltzmann solver for calculating electrostatics in biomolecular systems. Computer Physics Communications, 2010, 181, 1150-1160.	3.0	42
173	Electrostatic steering of substrate to acetylcholinesterase: Analysis of field fluctuations. Biopolymers, 2000, 53, 265-271.	1.2	41
174	Studying the roles of W86, E202, and Y337 in binding of acetylcholine to acetylcholinesterase using a combined molecular dynamics and multiple docking approach. Protein Science, 2003, 12, 2675-2684.	3.1	41
175	Structural and dynamical rationale for fatty acid unsaturation in Escherichia coli. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 6775-6783.	3.3	41
176	Activation of atypical protein kinase C by sphingosine 1-phosphate revealed by an aPKC-specific activity reporter. Science Signaling, 2019, 12, .	1.6	41
177	Memory kernels from molecular dynamics. Journal of Chemical Physics, 1981, 75, 2462-2463.	1.2	40
178	Phosphorylation stabilizes the N-termini of ?-helices. , 1999, 49, 225-233.		40
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356	Title is missing!. , 2020, 16, e1007756.		0