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	Lipoprotein-associated phospholipase A ₂ : A paradigm for allosteric regulation by membranes. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	3.3	17
2	Coupling Monte Carlo, Variational Implicit Solvation, and Binary Level-Set for Simulations of Biomolecular Binding. Journal of Chemical Theory and Computation, 2021, 17, 2465-2478.	2.3	6
3	The myosin II coiled-coil domain atomic structure in its native environment. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	19
4	Decoding allosteric regulation by the acyl carrier protein. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	14
5	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
6	Characterizing protein kinase A (PKA) subunits as macromolecular regulators of PKA RIÎ± liquidâ€“liquid phase separation. Journal of Chemical Physics, 2021, 154, 221101.	1.2	6
7	A glycan gate controls opening of the SARS-CoV-2 spike protein. Nature Chemistry, 2021, 13, 963-968.	6.6	254
8	Data for molecular dynamics simulations of Escherichia coli cytochrome bd oxidase with the Amber force field. Data in Brief, 2021, 38, 107401.	0.5	1
9	Gaussian-Accelerated Molecular Dynamics with the Weighted Ensemble Method: A Hybrid Method Improves Thermodynamic and Kinetic Sampling. Journal of Chemical Theory and Computation, 2021, 17, 7938-7951.	2.3	15
10	Predicting the effects of dATP on cardiac contraction using multiscale modeling of the sarcomere. Archives of Biochemistry and Biophysics, 2020, 695, 108582.	1.4	5
11	Interfacial plasticity facilitates high reaction rate of E. coli FAS malonyl-CoA:ACP transacylase, FabD. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 24224-24233.	3.3	31
12	An Open-Source Mesh Generation Platform for Biophysical Modeling Using Realistic Cellular Geometries. Biophysical Journal, 2020, 118, 1003-1008.	0.2	24
13	Gating mechanism of elongating Î²-ketoacyl-ACP synthases. Nature Communications, 2020, 11, 1727.	5.8	44
14	3D mesh processing using GAMer 2 to enable reaction-diffusion simulations in realistic cellular geometries. PLoS Computational Biology, 2020, 16, e1007756.	1.5	46
15	Multiscale Simulations Examining Glycan Shield Effects on Drug Binding to Influenza Neuraminidase. Biophysical Journal, 2020, 119, 2275-2289.	0.2	13
16	Title is missing!. , 2020, 16, e1007756.		0
17	Title is missing!. , 2020, 16, e1007756.		0
18	Title is missing!. , 2020, 16, e1007756.		0

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19	Title is missing!. , 2020, 16, e1007756.		0
20	Title is missing!. , 2020, 16, e1007756.		0
21	Title is missing!. , 2020, 16, e1007756.		0
22	Shifting the Hydrolysis Equilibrium of Substrate Loaded Acyl Carrier Proteins. Biochemistry, 2019, 58, 3557-3560.	1.2	7
23	Modifying the Thioester Linkage Affects the Structure of the Acyl Carrier Protein. Angewandte Chemie, 2019, 131, 11004-11008.	1.6	3
24	Variational implicit-solvent predictions of the dryâ€“wet transition pathways for ligandâ€“receptor binding and unbinding kinetics. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 14989-14994.	3.3	12
25	A Stochastic Multiscale Model of Cardiac Thin Filament Activation Using Brownian-Langevin Dynamics. Biophysical Journal, 2019, 117, 2255-2272.	0.2	11
26	Brownian Dynamics Simulations of Biological Molecules. Trends in Chemistry, 2019, 1, 727-738.	4.4	37
27	Modifying the Thioester Linkage Affects the Structure of the Acyl Carrier Protein. Angewandte Chemie - International Edition, 2019, 58, 10888-10892.	7.2	14
28	Deciphering Off-Target Effects in CRISPR-Cas9 through Accelerated Molecular Dynamics. ACS Central Science, 2019, 5, 651-662.	5.3	99
29	Understanding the mechanistic basis of non-coding RNA through molecular dynamics simulations. Journal of Structural Biology, 2019, 206, 267-279.	1.3	37
30	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
31	The invisible dance of CRISPR-Cas9. Physics Today, 2019, 72, 30-36.	0.3	10
32	Computational Predictions of Drug-Protein Binding Kinetics with a Hybrid Molecular Dynamics, Brownian Dynamics, and Milestoning Approach. Biophysical Journal, 2019, 116, 562a.	0.2	2
33	Allostery in Its Many Disguises: From Theory to Applications. Structure, 2019, 27, 566-578.	1.6	285
34	Activation of atypical protein kinase C by sphingosine 1-phosphate revealed by an aPKC-specific activity reporter. Science Signaling, 2019, 12, .	1.6	41
35	Docking simulation and antibiotic discovery targeting the MlaC protein in Gramâ€negative bacteria. Chemical Biology and Drug Design, 2019, 93, 647-652.	1.5	5
36	Mechanisms for Benzene Dissociation through the Excited State of T4 Lysozyme L99A Mutant. Biophysical Journal, 2019, 116, 205-214.	0.2	20

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37	Mechanistic Probes for the Epimerization Domain of Nonribosomal Peptide Synthetases. ChemBioChem, 2019, 20, 147-152.	1.3	12
38	<scp>pH</scp>â€dependent conformational dynamics of betaâ€secretase 1: <scp>A</scp> molecular dynamics study. Journal of Molecular Recognition, 2019, 32, e2765.	1.1	14
39	The Implementation of the Colored Abstract Simplicial Complex and Its Application to Mesh Generation. ACM Transactions on Mathematical Software, 2019, 45, 1-20.	1.6	6
40	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
41	Replica Exchange Gaussian Accelerated Molecular Dynamics: Improved Enhanced Sampling and Free Energy Calculation. Journal of Chemical Theory and Computation, 2018, 14, 1853-1864.	2.3	29
42	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
43	Ligand Binding Pathways and Conformational Transitions of the HIV Protease. Biochemistry, 2018, 57, 1533-1541.	1.2	52
44	Membrane Allostery and Unique Hydrophobic Sites Promote Enzyme Substrate Specificity. Journal of the American Chemical Society, 2018, 140, 3285-3291.	6.6	60
45	Remarkable similarity in Plasmodium falciparum and Plasmodium vivax geranylgeranyl diphosphate synthase dynamics and its implication for antimalarial drug design. Chemical Biology and Drug Design, 2018, 91, 1068-1077.	1.5	5
46	Ensemble Docking in Drug Discovery. Biophysical Journal, 2018, 114, 2271-2278.	0.2	318
47	Improvements to the <scp>APBS</scp> biomolecular solvation software suite. Protein Science, 2018, 27, 112-128.	3.1	1,399
48	Brownian dynamic study of an enzyme metabolon in the TCA cycle: Substrate kinetics and channeling. Protein Science, 2018, 27, 463-471.	3.1	29
49	Heterogeneous Solvation in Distinctive Proteinâ€“Protein Interfaces Revealed by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2018, 122, 11695-11701.	1.2	7
50	A Computational Modeling Approach Predicts Interaction of the Antifungal Protein AFP from Aspergillus giganteus with Fungal Membranes via Its Î³-Core Motif. MSphere, 2018, 3, .	1.3	22
51	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
52	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
53	Hierarchical Orthogonal Matrix Generation and Matrix-Vector Multiplications in Rigid Body Simulations. SIAM Journal of Scientific Computing, 2018, 40, A1345-A1361.	1.3	0
54	Tailoring the Variational Implicit Solvent Method for New Challenges: Biomolecular Recognition and Assembly. Frontiers in Molecular Biosciences, 2018, 5, 13.	1.6	6

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55	Membrane Allostery and Hydrophobic Binding Sites Control Substrate Specificity of Lipolytic Enzymes. FASEB Journal, 2018, 32, 528.6.	0.2	0
56	Atypical Protein Kinase Câ€šspecific Activity Reporter Reveals Novel Activation Mechanism of Atypical Protein Kinase C by Sphingosine 1â€phosphate. FASEB Journal, 2018, 32, 662.1.	0.2	0
57	<scp>NMR</scp> structureâ€based optimization of Staphylococcus aureus sortase A pyridazinone inhibitors. Chemical Biology and Drug Design, 2017, 90, 327-344.	1.5	20
58	Spectroscopic and Computational Investigations of Ligand Binding to IspH: Discovery of Nonâ€diphosphate Inhibitors. ChemBioChem, 2017, 18, 914-920.	1.3	10
59	Effect of donor atom identity on metal-binding pharmacophore coordination. Journal of Biological Inorganic Chemistry, 2017, 22, 605-613.	1.1	8
60	<scp>A</scp>ctivation mechanisms of the first sphingosineâ€1â€phosphate receptor. Protein Science, 2017, 26, 1150-1160.	3.1	13
61	Gaussian Accelerated Molecular Dynamics in NAMD. Journal of Chemical Theory and Computation, 2017, 13, 9-19.	2.3	117
62	Manipulating Proteinâ€“Protein Interactions in Nonribosomal Peptide Synthetase Type II Peptidyl Carrier Proteins. Biochemistry, 2017, 56, 5269-5273.	1.2	16
63	Protospacer Adjacent Motif-Induced Allostery Activates CRISPR-Cas9. Journal of the American Chemical Society, 2017, 139, 16028-16031.	6.6	104
64	â€œMartinizingâ€•the Variational Implicit Solvent Method (VISM): Solvation Free Energy for Coarse-Grained Proteins. Journal of Physical Chemistry B, 2017, 121, 6538-6548.	1.2	10
65	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
66	Gaussian Accelerated Molecular Dynamics: Theory, Implementation, and Applications. Annual Reports in Computational Chemistry, 2017, 13, 231-278.	0.9	107
67	G-protein coupled receptors: advances in simulation and drug discovery. Current Opinion in Structural Biology, 2016, 41, 83-89.	2.6	80
68	General trends of dihedral conformational transitions in a globular protein. Proteins: Structure, Function and Bioinformatics, 2016, 84, 501-514.	1.5	8
69	Unconstrained enhanced sampling for free energy calculations of biomolecules: a review. Molecular Simulation, 2016, 42, 1046-1055.	0.9	139
70	Stochastic level-set variational implicit-solvent approach to solute-solvent interfacial fluctuations. Journal of Chemical Physics, 2016, 145, 054114.	1.2	10
71	Hybrid finite element and Brownian dynamics method for charged particles. Journal of Chemical Physics, 2016, 144, 164107.	1.2	1
72	Substrate channeling between the human dihydrofolate reductase and thymidylate synthase. Protein Science, 2016, 25, 79-86.	3.1	21

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73	Development of Potent and Selective Inhibitors for Group VIA Calcium-Independent Phospholipase A₂ Guided by Molecular Dynamics and Structureâ€“Activity Relationships. Journal of Medicinal Chemistry, 2016, 59, 4403-4414.	2.9	39
74	Computer-aided drug design guided by hydrogen/deuterium exchange mass spectrometry: A powerful combination for the development of potent and selective inhibitors of Group VIA calcium-independent phospholipase A2. Bioorganic and Medicinal Chemistry, 2016, 24, 4801-4811.	1.4	21
75	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
76	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
77	Computation of p<scp>H</scp>â€dependent binding free energies. Biopolymers, 2016, 105, 43-49.	1.2	22
78	Dynamic Structure and Inhibition of a Malaria Drug Target: Geranylgeranyl Diphosphate Synthase. Biochemistry, 2016, 55, 5180-5190.	1.2	8
79	Autobiography of J. Andrew McCammon. Journal of Physical Chemistry B, 2016, 120, 8057-8060.	1.2	2
80	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
81	Molecular dynamic study of MlaC protein in Gramâ€negative bacteria: conformational flexibility, solvent effect and proteinâ€phospholipid binding. Protein Science, 2016, 25, 1430-1437.	3.1	26
82	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
83	Troponin I Mutations R146G and R21C Alter Cardiac Troponin Function, Contractile Properties, and Modulation by Protein Kinase A (PKA)-mediated Phosphorylation. Journal of Biological Chemistry, 2015, 290, 27749-27766.	1.6	36
84	A self-consistent phase-field approach to implicit solvation of charged molecules with Poissonâ€“Boltzmann electrostatics. Journal of Chemical Physics, 2015, 143, 243110.	1.2	8
85	Accelerated molecular dynamics simulations of protein folding. Journal of Computational Chemistry, 2015, 36, 1536-1549.	1.5	134
86	Electrostatic steering enhances the rate of cAMP binding to phosphodiesterase: Brownian dynamics modeling. Protein Science, 2015, 24, 1884-1889.	3.1	15
87	Investigation of the conformational dynamics of the apo A_{2A} adenosine receptor. Protein Science, 2015, 24, 1004-1012.	3.1	11
88	Conformational Dynamics and Binding Free Energies of Inhibitors of BACE-1: From the Perspective of Protonation Equilibria. PLoS Computational Biology, 2015, 11, e1004341.	1.5	31
89	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
90	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

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91	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
92	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
93	Enhanced Ligand Sampling for Relative Proteinâ€“Ligand Binding Free Energy Calculations. Journal of Physical Chemistry B, 2015, 119, 6190-6197.	1.2	15
94	Gaussian Accelerated Molecular Dynamics: Unconstrained Enhanced Sampling and Free Energy Calculation. Journal of Chemical Theory and Computation, 2015, 11, 3584-3595.	2.3	544
95	LS-VISM: A software package for analysis of biomolecular solvation. Journal of Computational Chemistry, 2015, 36, 1047-1059.	1.5	18
96	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
97	Taxodione and arenarone inhibit farnesyl diphosphate synthase by binding to the isopentenyl diphosphate site. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, E2530-9.	3.3	34
98	Poissonâ€“Boltzmann versus Size-Modified Poissonâ€“Boltzmann Electrostatics Applied to Lipid Bilayers. Journal of Physical Chemistry B, 2014, 118, 14827-14832.	1.2	11
99	Allosteric Inhibition of Epac. Journal of Biological Chemistry, 2014, 289, 29148-29157.	1.6	27
100	Exploring the role of receptor flexibility in structure-based drug discovery. Biophysical Chemistry, 2014, 186, 31-45.	1.5	129
101	Free energy landscape of G-protein coupled receptors, explored by accelerated molecular dynamics. Physical Chemistry Chemical Physics, 2014, 16, 6398.	1.3	74
102	A model study of sequential enzyme reactions and electrostatic channeling. Journal of Chemical Physics, 2014, 140, 105101.	1.2	46
103	Trapping the dynamic acyl carrier protein in fatty acid biosynthesis. Nature, 2014, 505, 427-431.	13.7	216
104	Electrostatic Channeling in P.Âfalciparum DHFR-TS: Brownian Dynamics and Smoluchowski Modeling. Biophysical Journal, 2014, 107, 2394-2402.	0.2	23
105	Use of Broken-Symmetry Density Functional Theory To Characterize the IspH Oxidized State: Implications for IspH Mechanism and Inhibition. Journal of Chemical Theory and Computation, 2014, 10, 3871-3884.	2.3	21
106	Accelerated Adaptive Integration Method. Journal of Physical Chemistry B, 2014, 118, 5109-5118.	1.2	12
107	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
108	Variational Implicit Solvation with Poissonâ€“Boltzmann Theory. Journal of Chemical Theory and Computation, 2014, 10, 1454-1467.	2.3	45

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109	Trypsinogen activation as observed in accelerated molecular dynamics simulations. Protein Science, 2014, 23, 1550-1558.	3.1	3
110	Heterogeneous Hydration of p53/MDM2 Complex. Journal of Chemical Theory and Computation, 2014, 10, 1302-1313.	2.3	22
111	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
112	Improved Reweighting of Accelerated Molecular Dynamics Simulations for Free Energy Calculation. Journal of Chemical Theory and Computation, 2014, 10, 2677-2689.	2.3	344
113	Structure, mechanism, and dynamics of UDP-galactopyranose mutase. Archives of Biochemistry and Biophysics, 2014, 544, 128-141.	1.4	49
114	Dipeptide Aggregation in Aqueous Solution from Fixed Point-Charge Force Fields. Journal of Chemical Theory and Computation, 2014, 10, 1631-1637.	2.3	10
115	PKA Phosphorylation of Cardiac Troponin I Modulates Activation andÂRelaxation Kinetics of Ventricular Myofibrils. Biophysical Journal, 2014, 107, 1196-1204.	0.2	45
116	Drug screening strategy for human membrane proteins: From NMR protein backbone structure to in silica- and NMR-screened hits. Biochemical and Biophysical Research Communications, 2014, 445, 724-733.	1.0	11
117	Molecular Dynamics Simulation Study of Conformational Changes of Transcription Factor TFIIS during RNA Polymerase II Transcriptional Arrest and Reactivation. PLoS ONE, 2014, 9, e97975.	1.1	10
118	Substrateâ€dependent dynamics of UDPâ€galactopyranose mutase: Implications for drug design. Protein Science, 2013, 22, 1490-1501.	3.1	11
119	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
120	Population Based Reweighting of Scaled Molecular Dynamics. Journal of Physical Chemistry B, 2013, 117, 12759-12768.	1.2	94
121	AFMPB: An adaptive fast multipole Poissonâ€“Boltzmann solver for calculating electrostatics in biomolecular systems. Computer Physics Communications, 2013, 184, 2618-2619.	3.0	5
122	Accelerated Molecular Dynamics Simulations with the AMOEBA Polarizable Force Field on Graphics Processing Units. Journal of Chemical Theory and Computation, 2013, 9, 4684-4691.	2.3	39
123	Variational Implicit-Solvent Modeling of Hostâ€“Guest Binding: A Case Study on Cucurbit[7]uril|. Journal of Chemical Theory and Computation, 2013, 9, 4195-4204.	2.3	12
124	Simulations of Biased Agonists in the Î²₂ Adrenergic Receptor with Accelerated Molecular Dynamics. Biochemistry, 2013, 52, 5593-5603.	1.2	44
125	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
126	Structural insight into the separate roles of inositol tetraphosphate and deacetylaseâ€activating domain in activation of histone deacetylase 3. Protein Science, 2013, 22, 83-92.	3.1	26

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127	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
128	Molecular Recognition and Ligand Association. Annual Review of Physical Chemistry, 2013, 64, 151-175.	4.8	165
129	w-REXAMD: A Hamiltonian Replica Exchange Approach to Improve Free Energy Calculations for Systems with Kinetically Trapped Conformations. Journal of Chemical Theory and Computation, 2013, 9, 18-23.	2.3	40
130	Evaluation of Hydration Free Energy by Level-Set Variational Implicit-Solvent Model with Coulomb-Field Approximation. Journal of Chemical Theory and Computation, 2013, 9, 1778-1787.	2.3	27
131	Utilizing a Dynamical Description of IspH to Aid in the Development of Novel Antimicrobial Drugs. PLoS Computational Biology, 2013, 9, e1003395.	1.5	7
132	Insertion of the Ca2+-Independent Phospholipase A2 into a Phospholipid Bilayer via Coarse-Grained and Atomistic Molecular Dynamics Simulations. PLoS Computational Biology, 2013, 9, e1003156.	1.5	33
133	Inactivating mutation in histone deacetylase 3 stabilizes its active conformation. Protein Science, 2013, 22, 1306-1312.	3.1	7
134	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
135	Multi-core CPU or GPU-accelerated Multiscale Modeling for Biomolecular Complexes. Computational and Mathematical Biophysics, 2013, 1, 164-179.	0.6	20
136	Phase-field approach to implicit solvation of biomolecules with Coulomb-field approximation. Journal of Chemical Physics, 2013, 139, 024111.	1.2	15
137	Mathematical and Numerical Aspects of the Adaptive Fast Multipole Poisson-Boltzmann Solver. Communications in Computational Physics, 2013, 13, 107-128.	0.7	12
138	Modeling Effects of L-Type Ca2+ Current and Na+-Ca2+ Exchanger on Ca2+ Trigger Flux in Rabbit Myocytes with Realistic T-Tubule Geometries. Frontiers in Physiology, 2012, 3, 351.	1.3	28
139	Accelerated molecular dynamics: Theory, implementation and applications. , 2012, , .		4
140	Modelling cardiac calcium sparks in a threeâ€dimensional reconstruction of a calcium release unit. Journal of Physiology, 2012, 590, 4403-4422.	1.3	80
141	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
142	The binding mechanism, multiple binding modes, and allosteric regulation of Staphylococcus aureus Sortase A probed by molecular dynamics simulations. Protein Science, 2012, 21, 1858-1871.	3.1	36
143	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
144	Level-Set Variational Implicit-Solvent Modeling of Biomolecules with the Coulomb-Field Approximation. Journal of Chemical Theory and Computation, 2012, 8, 386-397.	2.3	33

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145	Routine Access to Millisecond Time Scale Events with Accelerated Molecular Dynamics. Journal of Chemical Theory and Computation, 2012, 8, 2997-3002.	2.3	435
146	Calcium binding and allosteric signaling mechanisms for the sarcoplasmic reticulum Ca²⁺ ATPase. Protein Science, 2012, 21, 1429-1443.	3.1	28
147	The Dynamic Structure of Thrombin in Solution. Biophysical Journal, 2012, 103, 79-88.	0.2	47
148	Computer-aided Drug Discovery: Two Antiviral Drugs for HIV/AIDS. RSC Biomolecular Sciences, 2012, , 316-319.	0.4	1
149	Inside Back Cover: Multi-Timescale Conformational Dynamics of the SH3 Domain of CD2-Associated Protein using NMR Spectroscopy and Accelerated Molecular Dynamics (Angew. Chem. Int. Ed. 25/2012). Angewandte Chemie - International Edition, 2012, 51, 6279-6279.	7.2	0
150	A Molecular Dynamics Ensemble-Based Approach for the Mapping of Druggable Binding Sites. Methods in Molecular Biology, 2012, 819, 3-12.	0.4	23
151	Predictive Power of Molecular Dynamics Receptor Structures in Virtual Screening. Journal of Chemical Information and Modeling, 2011, 51, 1439-1446.	2.5	91
152	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
153	Molecular Recognition in the Case of Flexible Targets. Current Pharmaceutical Design, 2011, 17, 1663-1671.	0.9	47
154	Novel inhibitors of Mycobacterium tuberculosis dTDP-6-deoxy-l-lyxo-4-hexulose reductase (RmlD) identified by virtual screening. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 7064-7067.	1.0	23
155	Molecular dynamics simulations and drug discovery. BMC Biology, 2011, 9, 71.	1.7	881
156	Gated Diffusion-controlled Reactions. BMC Biophysics, 2011, 4, 4.	4.4	22
157	POVME: An algorithm for measuring binding-pocket volumes. Journal of Molecular Graphics and Modelling, 2011, 29, 773-776.	1.3	186
158	Accessing a Hidden Conformation of the Maltose Binding Protein Using Accelerated Molecular Dynamics. PLoS Computational Biology, 2011, 7, e1002034.	1.5	102
159	Including receptor flexibility and induced fit effects into the design of MMPâ€2 inhibitors. Journal of Molecular Recognition, 2010, 23, 173-182.	1.1	29
160	Browndye: A software package for Brownian dynamics. Computer Physics Communications, 2010, 181, 1896-1905.	3.0	85
161	Large conformational changes in proteins: signaling and other functions. Current Opinion in Structural Biology, 2010, 20, 142-147.	2.6	213
162	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

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163	Potential drug-like inhibitors of Group 1 influenza neuraminidase identified through computer-aided drug design. Computational Biology and Chemistry, 2010, 34, 97-105.	1.1	22
164	AFMPB: An adaptive fast multipole Poissonâ€“Boltzmann solver for calculating electrostatics in biomolecular systems. Computer Physics Communications, 2010, 181, 1150-1160.	3.0	42
165	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
166	Numerical Analysis of Ca2+ Signaling in Rat Ventricular Myocytes with Realistic Transverse-Axial Tubular Geometry and Inhibited Sarcoplasmic Reticulum. PLoS Computational Biology, 2010, 6, e1000972.	1.5	35
167	How Can Hydrophobic Association Be Enthalpy Driven?. Journal of Chemical Theory and Computation, 2010, 6, 2866-2871.	2.3	205
168	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
169	Water in Cavityâ^'Ligand Recognition. Journal of the American Chemical Society, 2010, 132, 12091-12097.	6.6	236
170	A Dynamic Model of HIV Integrase Inhibition and Drug Resistance. Journal of Molecular Biology, 2010, 397, 600-615.	2.0	63
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