Benoit Roux

List of Publications by Year
in descending order

370 papers	38,830 citations	1238 110 h-index	3732 179 g-index
378 all docs	378 docs citations	378 times ranked	21853 citing authors

#	Article	IF	Citations
1	Scalable molecular dynamics on CPU and GPU architectures with NAMD. Journal of Chemical Physics, 2020, 153, 044130.	3.0	1,548
2	The calculation of the potential of mean force using computer simulations. Computer Physics Communications, 1995, 91, 275-282.	7.5	1,496
3	Finite representation of an infinite bulk system: Solvent boundary potential for computer simulations. Journal of Chemical Physics, 1994, 100, 9050-9063.	3.0	911
4	Energetics of ion conduction through the K+ channel. Nature, 2001, 414, 73-77.	27.8	745
5	Calculation of absolute protein-ligand binding free energy from computer simulations. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 6825-6830.	7.1	594
6	A polarizable model of water for molecular dynamics simulations of biomolecules. Chemical Physics Letters, 2006, 418, 245-249.	2.6	548
7	Control of ion selectivity in potassium channels by electrostatic and dynamic properties of carbonyl ligands. Nature, 2004, 431, 830-834.	27.8	528
8	Continuum solvation model: Computation of electrostatic forces from numerical solutions to the Poisson-Boltzmann equation. Computer Physics Communications, 1998, 111, 59-75.	7.5	500
9	Computations of Standard Binding Free Energies with Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2009, 113, 2234-2246.	2.6	481
10	An Integral Equation To Describe the Solvation of Polar Molecules in Liquid Water. Journal of Physical Chemistry B, 1997, 101, 7821-7826.	2.6	465
11	An Empirical Polarizable Force Field Based on the Classical Drude Oscillator Model: Development History and Recent Applications. Chemical Reviews, 2016, 116, 4983-5013.	47.7	434
12	Simulating Monovalent and Divalent Ions in Aqueous Solution Using a Drude Polarizable Force Field. Journal of Chemical Theory and Computation, 2010, 6, 774-786.	5.3	401
13	Molecular determinants of gating at the potassium-channel selectivity filter. Nature Structural and Molecular Biology, 2006, 13, 311-318.	8.2	399
14	Molecular Dynamics Simulations of Ionic Liquids and Electrolytes Using Polarizable Force Fields. Chemical Reviews, 2019, 119, 7940-7995.	47.7	386
15	Energetics of ion conduction through the gramicidin channel. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 117-122.	7.1	371
16	Atomic Radii for Continuum Electrostatics Calculations Based on Molecular Dynamics Free Energy Simulations. Journal of Physical Chemistry B, 1997, 101, 5239-5248.	2.6	369
17	Dynamic Coupling between the SH2 and SH3 Domains of c-Src and Hck Underlies Their Inactivation by C-Terminal Tyrosine Phosphorylation. Cell, 2001, 105, 115-126.	28.9	366
18	Theoretical and computational models of biological ion channels. Quarterly Reviews of Biophysics, 2004, 37, 15-103.	5.7	362

#	Article	IF	Citations
19	Absolute Hydration Free Energy Scale for Alkali and Halide Ions Established from Simulations with a Polarizable Force Field. Journal of Physical Chemistry B, 2006, 110, 3308-3322.	2.6	357
20	Ion Permeation and Selectivity of OmpF Porin: A Theoretical Study Based on Molecular Dynamics, Brownian Dynamics, and Continuum Electrodiffusion Theory. Journal of Molecular Biology, 2002, 322, 851-869.	4.2	353
21	Polarizable Force Field for Peptides and Proteins Based on the Classical Drude Oscillator. Journal of Chemical Theory and Computation, 2013, 9, 5430-5449.	5.3	329
22	Absolute Binding Free Energy Calculations Using Molecular Dynamics Simulations with Restraining Potentials. Biophysical Journal, 2006, 91, 2798-2814.	0.5	316
23	Molecular Dynamics of the KcsA K+ Channel in a Bilayer Membrane. Biophysical Journal, 2000, 78, 2900-2917.	0.5	314
24	Molecular modeling and dynamics studies with explicit inclusion of electronic polarizability: theory and applications. Theoretical Chemistry Accounts, 2009, 124, 11-28.	1.4	314
25	Finding Transition Pathways Using the String Method with Swarms of Trajectories. Journal of Physical Chemistry B, 2008, 112, 3432-3440.	2.6	313
26	Activation pathway of Src kinase reveals intermediate states as targets for drug design. Nature Communications, 2014, 5, 3397.	12.8	300
27	Standard Binding Free Energies from Computer Simulations: What Is the Best Strategy?. Journal of Chemical Theory and Computation, 2013, 9, 794-802.	5.3	298
28	Molecular Dynamics Study of Hydration in Ethanolâ˜Water Mixtures Using a Polarizable Force Fieldâ€. Journal of Physical Chemistry B, 2005, 109, 6705-6713.	2.6	275
29	Structure, energetics, and dynamics of lipidâ€“protein interactions: A molecular dynamics study of the gramicidin A channel in a DMPC bilayer. , 1996, 24, 92-114.		274
30	Closing In on the Resting State of the Shaker K+ Channel. Neuron, 2007, 56, 124-140.	8.1	270
31	Structural basis for the coupling between activation and inactivation gates in K+ channels. Nature, 2010, 466, 272-275.	27.8	267
32	Simulation of Osmotic Pressure in Concentrated Aqueous Salt Solutions. Journal of Physical Chemistry Letters, 2010, 1, 183-189.	4.6	266
33	Calculation of Standard Binding Free Energies:â€‰Aromatic Molecules in the T4 Lysozyme L99A Mutant. Journal of Chemical Theory and Computation, 2006, 2, 1255-1273.	5.3	265
34	Gating charge displacement in voltage-gated ion channels involves limited transmembrane movement. Nature, 2005, 436, 852-856.	27.8	263
35	Determination of Electrostatic Parameters for a Polarizable Force Field Based on the Classical Drude Oscillator. Journal of Chemical Theory and Computation, 2005, 1, 153-168.	5.3	260
36	Ions and Counterions in a Biological Channel: A Molecular Dynamics Simulation of OmpF Porin from Escherichia coli in an Explicit Membrane with 1M KCl Aqueous Salt Solution. Journal of Molecular Biology, 2002, 319, 1177-1197.	4.2	252

#	Article	IF	Citations
37	Molecular Mechanism of H+ Conduction in the Single-File Water Chain of the Gramicidin Channel. Biophysical Journal, 2002, 82, 2304-2316.	0.5	250
38	High-Performance Scalable Molecular Dynamics Simulations of a Polarizable Force Field Based on Classical Drude Oscillators in NAMD. Journal of Physical Chemistry Letters, 2011, 2, 87-92.	4.6	233
39	Molecular basis for the Born model of ion solvation. The Journal of Physical Chemistry, 1990, 94, 4683-4688.	2.9	229
40	Structural mechanism of voltage-dependent gating in an isolated voltage-sensing domain. Nature Structural and Molecular Biology, 2014, 21, 244-252.	8.2	228
41	A Grand Canonical Monte Carloâ€“Brownian Dynamics Algorithm for Simulating Ion Channels. Biophysical Journal, 2000, 79, 788-801.	0.5	226
42	CHARMMâ€GUI 10 years for biomolecular modeling and simulation. Journal of Computational Chemistry, 2017, 38, 1114-1124.	3.3	224
43	A microscopic view of ion conduction through the K+ channel. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 8644-8648.	7.1	222
44	Molecular driving forces determining potassium channel slow inactivation. Nature Structural and Molecular Biology, 2007, 14, 1062-1069.	8.2	216
45	CHARMM-GUI PDB Manipulator for Advanced Modeling and Simulations of Proteins Containing Nonstandard Residues. Advances in Protein Chemistry and Structural Biology, 2014, 96, 235-265.	2.3	214
46	Automated Force Field Parameterization for Nonpolarizable and Polarizable Atomic Models Based on Ab Initio Target Data. Journal of Chemical Theory and Computation, 2013, 9, 3543-3556.	5.3	212
47	Free Energy Perturbation Hamiltonian Replica-Exchange Molecular Dynamics (FEP/H-REMD) for Absolute Ligand Binding Free Energy Calculations. Journal of Chemical Theory and Computation, 2010, 6, 2559-2565.	5.3	211
48	Molecular Dynamics Simulation of Melittin in a Dimyristoylphosphatidylcholine Bilayer Membrane. Biophysical Journal, 1998, 75, 1603-1618.	0.5	209
49	Hydration of Amino Acid Side Chains:Â Nonpolar and Electrostatic Contributions Calculated from Staged Molecular Dynamics Free Energy Simulations with Explicit Water Molecules. Journal of Physical Chemistry B, 2004, 108, 16567-16576.	2.6	206
50	Free Energy Profiles for H+ Conduction along Hydrogen-Bonded Chains of Water Molecules. Biophysical Journal, 1998, 75, 33-40.	0.5	199
51	Multidomain assembled states of Hck tyrosine kinase in solution. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 15757-15762.	7.1	195
52	PBEQ-Solver for online visualization of electrostatic potential of biomolecules. Nucleic Acids Research, 2008, 36, W270-W275.	14.5	194
53	The Solvation Structure of Na⁺ and K⁺ in Liquid Water Determined from High Level ab Initio Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2012, 8, 3526-3535.	5.3	191
54	A Gate in the Selectivity Filter of Potassium Channels. Structure, 2005, 13, 591-600.	3.3	190

#	Article	IF	Citations
55	The Membrane Potential and its Representation by a Constant Electric Field in Computer Simulations. Biophysical Journal, 2008, 95, 4205-4216.	0.5	188
56	Efficient Determination of Proteinâ€“Protein Standard Binding Free Energies from First Principles. Journal of Chemical Theory and Computation, 2013, 9, 3789-3798.	5.3	188
57	Force Field Bias in Protein Folding Simulations. Biophysical Journal, 2009, 96, 3772-3780.	0.5	185
58	Molecular dynamics â€" potential of mean force calculations as a tool for understanding ion permeation and selectivity in narrow channels. Biophysical Chemistry, 2006, 124, 251-267.	2.8	181
59	Control of Ion Selectivity in LeuT: Two Na+ Binding Sites with Two Different Mechanisms. Journal of Molecular Biology, 2008, 377, 804-818.	4.2	181
60	Simulations of Anionic Lipid Membranes: Development of Interaction-Specific Ion Parameters and Validation Using NMR Data. Journal of Physical Chemistry B, 2013, 117, 10183-10192.	2.6	181
61	Atomic Proximity between S4 Segment and Pore Domain in Shaker Potassium Channels. Neuron, 2003, 39, 467-481.	8.1	179
62	Ion Permeation through the Î±-Hemolysin Channel: Theoretical Studies Based on Brownian Dynamics and Poisson-Nernst-Plank Electrodiffusion Theory. Biophysical Journal, 2004, 87, 2299-2309.	0.5	179
63	An emerging consensus on voltage-dependent gating from computational modeling and molecular dynamics simulations. Journal of General Physiology, 2012, 140, 587-594.	1.9	179
64	Importance of Hydration and Dynamics on the Selectivity of the KcsA and NaK Channels. Journal of General Physiology, 2007, 129, 135-143.	1.9	178
65	Ion selectivity in potassium channels. Biophysical Chemistry, 2006, 124, 279-291.	2.8	174
66	Instantaneous ion configurations in the K ⁺ ion channel selectivity filter revealed by 2D IR spectroscopy. Science, 2016, 353, 1040-1044.	12.6	174
67	Ion transport in a gramicidin-like channel: dynamics and mobility. The Journal of Physical Chemistry, 1991, 95, 4856-4868.	2.9	171
68	Recovery from slow inactivation in K+ channels is controlled by water molecules. Nature, 2013, 501, 121-124.	27.8	171
69	Constant electric field simulations of the membrane potential illustrated with simple systems. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 294-302.	2.6	169
70	Solvation of complex molecules in a polar liquid: An integral equation theory. Journal of Chemical Physics, 1996, 104, 8678-8689.	3.0	168
71	Ion Channels, Permeation, and Electrostatics: Insight into the Function of KcsA. Biochemistry, 2000, 39, 13295-13306.	2.5	167
72	Ion Conduction and Selectivity in K+ Channels. Annual Review of Biophysics and Biomolecular Structure, 2005, 34, 153-171.	18.3	167

#	Article	IF	Citations
73	On the statistical equivalence of restrained-ensemble simulations with the maximum entropy method. Journal of Chemical Physics, 2013, 138, 084107.	3.0	166
74	Two atomic constraints unambiguously position the S4 segment relative to S1 and S2 segments in the closed state of Shaker K channel. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 7904-7909.	7.1	164
75	A Polarizable Force Field of Dipalmitoylphosphatidylcholine Based on the Classical Drude Model for Molecular Dynamics Simulations of Lipids. Journal of Physical Chemistry B, 2013, 117, 9142-9160.	2.6	159
76	Polarizable Empirical Force Field for Aromatic Compounds Based on the Classical Drude Oscillator. Journal of Physical Chemistry B, 2007, 111, 2873-2885.	2.6	149
77	The Theory of Ultra-Coarse-Graining. 1. General Principles. Journal of Chemical Theory and Computation, 2013, 9, 2466-2480.	5.3	149
78	Molecular Basis of Proton Blockage in Aquaporins. Structure, 2004, 12, 65-74.	3.3	142
79	Atomic Level Anisotropy in the Electrostatic Modeling of Lone Pairs for a Polarizable Force Field Based on the Classical Drude Oscillator. Journal of Chemical Theory and Computation, 2006, 2, 1587-1597.	5.3	142
80	Ion selectivity in channels and transporters. Journal of General Physiology, 2011, 137, 415-426.	1.9	142
81	On the Importance of Atomic Fluctuations, Protein Flexibility, and Solvent in Ion Permeation. Journal of General Physiology, 2004, 124, 679-690.	1.9	141
82	Molecular Dynamics Study of a Polymeric Reverse Osmosis Membrane. Journal of Physical Chemistry B, 2009, 113, 10177-10182.	2.6	139
83	Recent Advances in Polarizable Force Fields for Macromolecules: Microsecond Simulations of Proteins Using the Classical Drude Oscillator Model. Journal of Physical Chemistry Letters, 2014, 5, 3144-3150.	4.6	139
84	Constant-pH Molecular Dynamics Simulations for Large Biomolecular Systems. Journal of Chemical Theory and Computation, 2017, 13, 5933-5944.	5.3	139
85	Dynamics of the Kv1.2 Voltage-Gated K+ Channel in a Membrane Environment. Biophysical Journal, 2007, 93, 3070-3082.	0.5	138
86	Building Markov state models along pathways to determine free energies and rates of transitions. Journal of Chemical Physics, 2008, 129, 064107.	3.0	137
87	Computational Studies of Membrane Channels. Structure, 2004, 12, 1343-1351.	3.3	136
88	Polarizable Empirical Force Field for the Primary and Secondary Alcohol Series Based on the Classical Drude Model. Journal of Chemical Theory and Computation, 2007, 3, 1927-1946.	5.3	136
89	Computations of Absolute Solvation Free Energies of Small Molecules Using Explicit and Implicit Solvent Model. Journal of Chemical Theory and Computation, 2009, 5, 919-930.	5.3	136
90	Explaining why Gleevec is a specific and potent inhibitor of Abl kinase. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 1664-1669.	7.1	136

#	Article	IF	Citations
91	Conformational dynamics of ligand-dependent alternating access in LeuT. Nature Structural and Molecular Biology, 2014, 21, 472-479.	8.2	136
92	Calculation of the Gating Charge for the Kv1.2 Voltage-Activated Potassium Channel. Biophysical Journal, 2010, 98, 2189-2198.	0.5	135
93	Ion Permeation through a Narrow Channel: Using Gramicidin to Ascertain All-Atom Molecular Dynamics Potential of Mean Force Methodology and Biomolecular Force Fields. Biophysical Journal, 2006, 90, 3447-3468.	0.5	133
94	Solvation thermodynamics: An approach from analytic temperature derivatives. Journal of Chemical Physics, 1990, 92, 5020-5033.	3.0	132
95	Solvation Free Energy of Polar and Nonpolar Molecules in Water:â€‰ An Extended Interaction Site Integral Equation Theory in Three Dimensions. Journal of Physical Chemistry B, 2000, 104, 796-805.	2.6	132
96	Computational Studies of the Gramicidin Channel. Accounts of Chemical Research, 2002, 35, 366-375.	15.6	131
97	Accurate Calculation of Hydration Free Energies using Pair-Specific Lennard-Jones Parameters in the CHARMM Drude Polarizable Force Field. Journal of Chemical Theory and Computation, 2010, 6, 1181-1198.	5.3	131
98	Numerical solution of the hypernetted chain equation for a solute of arbitrary geometry in three dimensions. Journal of Chemical Physics, 1995, 103, 360-364.	3.0	130
99	Statistical Mechanical Equilibrium Theory of Selective Ion Channels. Biophysical Journal, 1999, 77, 139-153.	0.5	130
100	The Binding of Antibiotics in OmpF Porin. Structure, 2013, 21, 76-87.	3.3	128
101	Modeling the Structure of Agitoxin in Complex with the Shaker K+ Channel: A Computational Approach Based on Experimental Distance Restraints Extracted from Thermodynamic Mutant Cycles. Biophysical Journal, 2002, 83, 2595-2609.	0.5	124
102	Structure of Gramicidin A in a Lipid Bilayer Environment Determined Using Molecular Dynamics Simulations and Solid-State NMR Data. Journal of the American Chemical Society, 2003, 125, 9868-9877.	13.7	123
103	Computation of binding free energy with molecular dynamics and grand canonical Monte Carlo simulations. Journal of Chemical Physics, 2008, 128, 115103.	3.0	123
104	Theoretical Study of H+Translocation along a Model Proton Wire. The Journal of Physical Chemistry, 1996, 100, 2519-2527.	2.9	122
105	Free Energy Landscape of A-DNA to B-DNA Conversion in Aqueous Solution. Journal of the American Chemical Society, 2005, 127, 6866-6876.	13.7	122
106	Understanding the Dielectric Properties of Liquid Amides from a Polarizable Force Field. Journal of Physical Chemistry B, 2008, 112, 3509-3521.	2.6	122
107	Computation of Absolute Hydration and Binding Free Energy with Free Energy Perturbation Distributed Replica-Exchange Molecular Dynamics. Journal of Chemical Theory and Computation, 2009, 5, 2583-2588.	5.3	120
108	Ion transport in the gramicidin channel: free energy of the solvated right-handed dimer in a model membrane. Journal of the American Chemical Society, 1993, 115, 3250-3262.	13.7	118

#	Article	IF	Citations
109	An Overview of Electrostatic Free Energy Computations for Solutions and Proteins. Journal of Chemical Theory and Computation, 2014, 10, 2690-2709.	5.3	118
110	Conformational Flexibility of o-Phosphorylcholine and o-Phosphorylethanolamine: A Molecular Dynamics Study of Solvation Effects. Journal of the American Chemical Society, 1994, 116, 5916-5926.	13.7	117
111	A Rapid Coarse Residue-Based Computational Method for X-Ray Solution Scattering Characterization of Protein Folds and Multiple Conformational States of Large Protein Complexes. Biophysical Journal, 2009, 96, 4449-4463.	0.5	117
112	Architecture and assembly of the <scp>G</scp>ramâ€positive cell wall. Molecular Microbiology, 2013, 88, 664-672.	2.5	116
113	Gramicidin Channels. IEEE Transactions on Nanobioscience, 2005, 4, 10-20.	3.3	115
114	Generalized scalable multiple copy algorithms for molecular dynamics simulations in NAMD. Computer Physics Communications, 2014, 185, 908-916.	7.5	115
115	Grand canonical Monte Carlo simulations of water in protein environments. Journal of Chemical Physics, 2004, 121, 6392-6400.	3.0	112
116	The hidden energetics of ligand binding and activation in a glutamate receptor. Nature Structural and Molecular Biology, 2011, 18, 283-287.	8.2	112
117	Exploring the Conformational Transitions of Biomolecular Systems Using a Simple Two-State Anisotropic Network Model. PLoS Computational Biology, 2014, 10, e1003521.	3.2	112
118	Electrostatics of Ion Stabilization in a ClC Chloride Channel Homologue from Escherichia coli. Journal of Molecular Biology, 2004, 339, 981-1000.	4.2	111
119	Theoretical and computational models of ion channels. Current Opinion in Structural Biology, 2002, 12, 182-189.	5.7	109
120	Mapping the conformational transition in Src activation by cumulating the information from multiple molecular dynamics trajectories. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 3776-3781.	7.1	106
121	Structural Determinants of Proton Blockage in Aquaporins. Journal of Molecular Biology, 2004, 343, 493-510.	4.2	105
122	Machine Learning Force Field Parameters from Ab Initio Data. Journal of Chemical Theory and Computation, 2017, 13, 4492-4503.	5.3	105
123	The Free Energy Landscapes Governing Conformational Changes in a Glutamate Receptor Ligand-Binding Domain. Structure, 2007, 15, 1203-1214.	3.3	104
124	Six-site polarizable model of water based on the classical Drude oscillator. Journal of Chemical Physics, 2013, 138, 034508.	3.0	103
125	Simulation study of ion pairing in concentrated aqueous salt solutions with a polarizable force field. Faraday Discussions, 2013, 160, 135-149.	3.2	102
126	Modeling the structure of the StART domains of MLN64 and StAR proteins in complex with cholesterol. Journal of Lipid Research, 2006, 47, 2614-2630.	4.2	101

#	Article	IF	Citations
127	Representation of Ionâ€“Protein Interactions Using the Drude Polarizable Force-Field. Journal of Physical Chemistry B, 2015, 119, 9401-9416.	2.6	101
128	Parametrization, Molecular Dynamics Simulation, and Calculation of Electron Spin Resonance Spectra of a Nitroxide Spin Label on a Polyalanine Î±-Helix. Journal of Physical Chemistry B, 2008, 112, 5755-5767.	2.6	98
129	Many-Body Polarization Effects and the Membrane Dipole Potential. Journal of the American Chemical Society, 2009, 131, 2760-2761.	13.7	98
130	In Search of a Consensus Model of the Resting State of a Voltage-Sensing Domain. Neuron, 2011, 72, 713-720.	8.1	93
131	Escherichia coli Peptidoglycan Structure and Mechanics as Predicted by Atomic-Scale Simulations. PLoS Computational Biology, 2014, 10, e1003475.	3.2	92
132	Structural basis of two-stage voltage-dependent activation in K+ channels. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 2935-2940.	7.1	91
133	Src Kinase Conformational Activation: Thermodynamics, Pathways, and Mechanisms. PLoS Computational Biology, 2008, 4, e1000047.	3.2	91
134	Imaging the Electrostatic Potential of Transmembrane Channels: Atomic Probe Microscopy of OmpF Porin. Biophysical Journal, 2002, 82, 1667-1676.	0.5	90
135	Ion Selectivity of the KcsA Channel: A Perspective from Multi-Ion Free Energy Landscapes. Journal of Molecular Biology, 2010, 401, 831-842.	4.2	90
136	Drude Polarizable Force Field for Molecular Dynamics Simulations of Saturated and Unsaturated Zwitterionic Lipids. Journal of Chemical Theory and Computation, 2017, 13, 4535-4552.	5.3	90
137	Calculation of Free Energy Landscape in Multi-Dimensions with Hamiltonian-Exchange Umbrella Sampling on Petascale Supercomputer. Journal of Chemical Theory and Computation, 2012, 8, 4672-4680.	5.3	89
138	On the origin of the electrostatic potential difference at a liquid-vacuum interface. Journal of Chemical Physics, 2008, 129, 234706.	3.0	88
139	Structural Refinement from Restrained-Ensemble Simulations Based on EPR/DEER Data: Application to T4 Lysozyme. Journal of Physical Chemistry B, 2013, 117, 4740-4754.	2.6	88
140	Theoretical Study of Aqueous Solvation of K⁺ Comparing ab Initio, Polarizable, and Fixed-Charge Models. Journal of Chemical Theory and Computation, 2007, 3, 2068-2082.	5.3	87
141	Computer simulations of water flux and salt permeability of the reverse osmosis FT-30 aromatic polyamide membrane. Journal of Membrane Science, 2011, 384, 1-9.	8.2	87
142	The Ionization State and the Conformation of Glu-71 in the KcsA K+ Channel. Biophysical Journal, 2002, 82, 772-780.	0.5	85
143	Ion channels and ion selectivity. Essays in Biochemistry, 2017, 61, 201-209.	4.7	85
144	Atomistic View of the Conformational Activation of Src Kinase Using the String Method with Swarms-of-Trajectories. Biophysical Journal, 2009, 97, L8-L10.	0.5	84

#	Article	IF	Citations
145	Molecular Dynamics Simulations of the Influenza Hemagglutinin Fusion Peptide in Micelles and Bilayers: Conformational Analysis of Peptide and Lipids. Journal of Molecular Biology, 2005, 354, 1129-1141.	4.2	83
146	Two mechanisms of ion selectivity in protein binding sites. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 20329-20334.	7.1	83
147	Conformational cycle and ion-coupling mechanism of the Na ⁺ /hydantoin transporter Mhp1. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 14752-14757.	7.1	83
148	Lipid-Mediated Interactions between Intrinsic Membrane Proteins: Dependence on Protein Size and Lipid Composition. Biophysical Journal, 2001, 81, 276-284.	0.5	82
149	Three-Dimensional Architecture of Membrane-Embedded MscS in the Closed Conformation. Journal of Molecular Biology, 2008, 378, 55-70.	4.2	82
150	Nanosculpting reversed wavelength sensitivity into a photoswitchable iGluR. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 6814-6819.	7.1	82
151	Constant-pH Hybrid Nonequilibrium Molecular Dynamicsâ€“Monte Carlo Simulation Method. Journal of Chemical Theory and Computation, 2015, 11, 3919-3931.	5.3	82
152	Self-Learning Adaptive Umbrella Sampling Method for the Determination of Free Energy Landscapes in Multiple Dimensions. Journal of Chemical Theory and Computation, 2013, 9, 1885-1895.	5.3	80
153	Implementation of extended <scp>L</scp>agrangian dynamics in <scp>GROMACS</scp> for polarizable simulations using the classical <scp>D</scp>rude oscillator model. Journal of Computational Chemistry, 2015, 36, 1473-1479.	3.3	79
154	On the Potential Functions used in Molecular Dynamics Simulations of Ion Channels. Biophysical Journal, 2002, 82, 1681-1684.	0.5	76
155	Locking the Active Conformation of c-Src Kinase through the Phosphorylation of the Activation Loop. Journal of Molecular Biology, 2014, 426, 423-435.	4.2	74
156	Multifrequency Electron Spin Resonance Spectra of a Spin-Labeled Protein Calculated from Molecular Dynamics Simulations. Journal of the American Chemical Society, 2009, 131, 2597-2605.	13.7	73
157	Extracellular Blockade of K+ Channels by Tea. Journal of General Physiology, 2001, 118, 207-218.	1.9	71
158	On the structural basis of modal gating behavior in K+ channels. Nature Structural and Molecular Biology, 2011, 18, 67-74.	8.2	71
159	CHARMM-GUI Ligand Binder for Absolute Binding Free Energy Calculations and Its Application. Journal of Chemical Information and Modeling, 2013, 53, 267-277.	5.4	71
160	Quantitative Analysis of the Water Occupancy around the Selectivity Filter of a K⁺ Channel in Different Gating Modes. Journal of the American Chemical Society, 2014, 136, 2000-2007.	13.7	70
161	Kinetics of peptide folding: computer simulations of SYPFDV and peptide variants in water 1 1Edited by G. von Heijne. Journal of Molecular Biology, 1997, 272, 423-442.	4.2	69
162	Molecular dynamics study of calbindin D9k in the apo and singly and doubly calcium-loaded states. , 1998, 33, 265-284.		69

#	Article	IF	Citations
163	Atomic Radii for Continuum Electrostatics Calculations on Nucleic Acids. Journal of Physical Chemistry B, 2002, 106, 11026-11035.	2.6	69
164	Dominant solvation effects from the primary shell of hydration: Approximation for molecular dynamics simulations. Biopolymers, 1995, 35, 171-178.	2.4	68
165	Transition path theory analysis of c-Src kinase activation. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 9193-9198.	7.1	67
166	Spatial dependence of timeâ€dependent friction for pair diffusion in a simple fluid. Journal of Chemical Physics, 1990, 93, 6804-6812.	3.0	66
167	Restrained-Ensemble Molecular Dynamics Simulations Based on Distance Histograms from Double Electronâ€“Electron Resonance Spectroscopy. Journal of Physical Chemistry B, 2013, 117, 4733-4739.	2.6	66
168	Reproducibility of Free Energy Calculations across Different Molecular Simulation Software Packages. Journal of Chemical Theory and Computation, 2018, 14, 5567-5582.	5.3	66
169	Shifts in the selectivity filter dynamics cause modal gating in K+ channels. Nature Communications, 2019, 10, 123.	12.8	66
170	A Combined Molecular Dynamics and Diffusion Model of Single Proton Conduction through Gramicidin. Biophysical Journal, 2000, 79, 2840-2857.	0.5	65
171	Rapid constriction of the selectivity filter underlies C-type inactivation in the KcsA potassium channel. Journal of General Physiology, 2018, 150, 1408-1420.	1.9	64
172	Quantum effects on the structure and energy of a protonated linear chain of hydrogen-bonded water molecules. Chemical Physics Letters, 1995, 234, 416-424.	2.6	63
173	Free Energy and Kinetics of Conformational Transitions from Voronoi Tessellated Milestoning with Restraining Potentials. Journal of Chemical Theory and Computation, 2009, 5, 2589-2594.	5.3	62
174	Electrostatics of the Intracellular Vestibule of K+ Channels. Journal of Molecular Biology, 2005, 354, 272-288.	4.2	58
175	RNA Structure Determination Using SAXS Data. Journal of Physical Chemistry B, 2010, 114, 10039-10048.	2.6	58
176	Mechanism of Intracellular Block of the KcsA K+ Channel by Tetrabutylammonium: Insights from X-ray Crystallography, Electrophysiology and Replica-exchange Molecular Dynamics Simulations. Journal of Molecular Biology, 2007, 365, 649-662.	4.2	57
177	Mechanism of potassium ion uptake by the Na+/K+-ATPase. Nature Communications, 2015, 6, 7622.	12.8	57
178	CHARMM-GUI Free Energy Calculator for Absolute and Relative Ligand Solvation and Binding Free Energy Simulations. Journal of Chemical Theory and Computation, 2020, 16, 7207-7218.	5.3	57
179	Potential energy function for cation-peptide interactions: Anab initio study. Journal of Computational Chemistry, 1995, 16, 690-704.	3.3	56
180	Computational Study of the â€œDFG-Flipâ€•Conformational Transition in c-Abl and c-Src Tyrosine Kinases. Journal of Physical Chemistry B, 2015, 119, 1443-1456.	2.6	56

#	Article	IF	Citations
181	Accurate determination of protein:ligand standard binding free energies from molecular dynamics simulations. Nature Protocols, 2022, 17, 1114-1141.	12.0	56
182	Simulating electron spin resonance spectra of nitroxide spin labels from molecular dynamics and stochastic trajectories. Journal of Chemical Physics, 2008, 128, 165106.	3.0	55
183	Local Deformations Revealed by Dynamics Simulations of DNA Polymerase Î² with DNA Mismatches at the Primer Terminus. Journal of Molecular Biology, 2002, 321, 459-478.	4.2	54
184	On the importance of a funneled energy landscape for the assembly and regulation of multidomain Src tyrosine kinases. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 13643-13648.	7.1	54
185	Protonation of key acidic residues is critical for the K+-selectivity of the Na/K pump. Nature Structural and Molecular Biology, 2011, 18, 1159-1163.	8.2	54
186	Relative Free Energies for Hydration of Monovalent Ions from QM and QM/MM Simulations. Journal of Chemical Theory and Computation, 2013, 9, 4165-4175.	5.3	54
187	Tyrosine Kinase Activation and Conformational Flexibility: Lessons from Src-Family Tyrosine Kinases. Accounts of Chemical Research, 2017, 50, 1193-1201.	15.6	53
188	Computing Relative Binding Affinity of Ligands to Receptor: An Effective Hybrid Single-Dual-Topology Free-Energy Perturbation Approach in NAMD. Journal of Chemical Information and Modeling, 2019, 59, 3794-3802.	5.4	52
189	Molecular dynamics simulations of membrane proteins under asymmetric ionic concentrations. Journal of General Physiology, 2013, 142, 465-475.	1.9	51
190	Dynamics transitions at the outer vestibule of the KcsA potassium channel during gating. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 1831-1836.	7.1	51
191	Absolute Binding Free Energy Calculations of Sparsomycin Analogs to the Bacterial Ribosome. Journal of Physical Chemistry B, 2010, 114, 9525-9539.	2.6	50
192	Ouabain Binding Site in a Functioning Na+/K+ ATPase. Journal of Biological Chemistry, 2011, 286, 38177-38183.	3.4	50
193	Intermediate state trapping of a voltage sensor. Journal of General Physiology, 2012, 140, 635-652.	1.9	50
194	Anchoring of a monotopic membrane protein: the binding of prostaglandin H2 synthase-1 to the surface of a phospholipid bilayer. European Biophysics Journal, 2000, 29, 439-454.	2.2	49
195	Thermodynamic coupling between activation and inactivation gating in potassium channels revealed by free energy molecular dynamics simulations. Journal of General Physiology, 2011, 138, 571-580.	1.9	49
196	Determination of Membrane-Insertion Free Energies by Molecular Dynamics Simulations. Biophysical Journal, 2012, 102, 795-801.	0.5	49
197	Computational Analysis of the Binding Specificity of Gleevec to Abl, c-Kit, Lck, and c-Src Tyrosine Kinases. Journal of the American Chemical Society, 2013, 135, 14741-14753.	13.7	49
198	New Coarse Variables for the Accurate Determination of Standard Binding Free Energies. Journal of Chemical Theory and Computation, 2017, 13, 5173-5178.	5.3	49

#	Article	IF	Citations
199	Rapid Intracellular TEA Block of the KcsA Potassium Channel. Biophysical Journal, 2005, 88, 1018-1029.	0.5	48
200	Non-additivity in cationâ€"peptide interactions. A molecular dynamics and ab initio study of Na+ in the gramicidin channel. Chemical Physics Letters, 1993, 212, 231-240.	2.6	47
201	Lipid-Mediated Interactions between Intrinsic Membrane Proteins: A Theoretical Study Based on Integral Equations. Biophysical Journal, 2000, 79, 2867-2879.	0.5	47
202	Using Markov Models to Simulate Electron Spin Resonance Spectra from Molecular Dynamics Trajectories. Journal of Physical Chemistry B, 2008, 112, 11014-11027.	2.6	47
203	Molecular Dynamics Investigation of the Ï‰-Current in the Kv1.2 Voltage Sensor Domains. Biophysical Journal, 2012, 102, 258-267.	0.5	47
204	Predicting the Conformational Variability of Abl Tyrosine Kinase using Molecular Dynamics Simulations and Markov State Models. Journal of Chemical Theory and Computation, 2018, 14, 2721-2732.	5.3	47
205	Long-pore Electrostatics in Inward-rectifier Potassium Channels. Journal of General Physiology, 2008, 132, 613-632.	1.9	46
206	Binding specificity of SH2 domains: Insight from free energy simulations. Proteins: Structure, Function and Bioinformatics, 2009, 74, 996-1007.	2.6	46
207	The activated state of a sodium channel voltage sensor in a membrane environment. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 5435-5440.	7.1	46
208	Simulating the Distance Distribution between Spin-Labels Attached to Proteins. Journal of Physical Chemistry B, 2015, 119, 3901-3911.	2.6	46
209	Graphâ€"Theoretic Analysis of Monomethyl Phosphate Clustering in Ionic Solutions. Journal of Physical Chemistry B, 2018, 122, 1484-1494.	2.6	46
210	The N-Terminal End of the Catalytic Domain of Src Kinase Hck Is a Conformational Switch Implicated in Long-Range Allosteric Regulation. Structure, 2005, 13, 1715-1723.	3.3	45
211	Polarizable Force Field for Molecular Ions Based on the Classical Drude Oscillator. Journal of Chemical Information and Modeling, 2018, 58, 993-1004.	5.4	45
212	Characterization of conformational equilibria through Hamiltonian and temperature replica-exchange simulations: Assessing entropic and environmental effects. Journal of Computational Chemistry, 2007, 28, 1634-1647.	3.3	44
213	Optimized Lennard-Jones Parameters for Druglike Small Molecules. Journal of Chemical Theory and Computation, 2018, 14, 3121-3131.	5.3	44
214	A potential function for computer simulation studies of proton transfer in acetylacetone. Journal of Computational Chemistry, 1997, 18, 368-380.	3.3	43
215	Web interface for brownian dynamics simulation of ion transport and its applications to betaâ€barrel pores. Journal of Computational Chemistry, 2012, 33, 331-339.	3.3	43
216	Framework Model For Single Proton Conduction through Gramicidin. Biophysical Journal, 2001, 80, 12-30.	0.5	42

#	Article	IF	Citations
217	A Variable Residue in the Pore of Kv1 Channels Is Critical for the High Affinity of Blockers from Sea Anemones and Scorpions. Journal of Biological Chemistry, 2005, 280, 27093-27102.	3.4	42
218	Quantum Effects in Cation Interactions with First and Second Coordination Shell Ligands in Metalloproteins. Journal of Chemical Theory and Computation, 2015, 11, 4992-5001.	5.3	42
219	Reconciling the Roles of Kinetic and Thermodynamic Factors in Membraneâ€"Protein Insertion. Journal of the American Chemical Society, 2013, 135, 2291-2297.	13.7	41
220	Computational Study of Gleevec and G6G Reveals Molecular Determinants of Kinase Inhibitor Selectivity. Journal of the American Chemical Society, 2014, 136, 14753-14762.	13.7	41
221	The Activation of c-Src Tyrosine Kinase: Conformational Transition Pathway and Free Energy Landscape. Journal of Physical Chemistry B, 2017, 121, 3352-3363.	2.6	41
222	Anatomy of a structural pathway for activation of the catalytic domain of Src kinase Hck. Proteins: Structure, Function and Bioinformatics, 2007, 67, 1096-1112.	2.6	39
223	A Conformational Intermediate in Glutamate Receptor Activation. Neuron, 2013, 79, 492-503.	8.1	39
224	Flexibility and charge asymmetry in the activation loop of Src tyrosine kinases. Proteins: Structure, Function and Bioinformatics, 2009, 74, 378-389.	2.6	38
225	Ion Selectivity of Î±-Hemolysin with Î²-Cyclodextrin Adapter. II. Multi-Ion Effects Studied with Grand Canonical Monte Carlo/Brownian Dynamics Simulations. Journal of Physical Chemistry B, 2010, 114, 2901-2909.	2.6	38
226	Comparison between Mean Forces and Swarms-of-Trajectories String Methods. Journal of Chemical Theory and Computation, 2014, 10, 524-533.	5.3	38
227	Ion Selectivity of Î±-Hemolysin with a Î²-Cyclodextrin Adapter. I. Single Ion Potential of Mean Force and Diffusion Coefficient. Journal of Physical Chemistry B, 2010, 114, 952-958.	2.6	37
228	Conformational Transitions and Alternating-Access Mechanism in the Sarcoplasmic Reticulum Calcium Pump. Journal of Molecular Biology, 2017, 429, 647-666.	4.2	37
229	A structural model for K2P potassium channels based on 23 pairs of interacting sites and continuum electrostatics. Journal of General Physiology, 2009, 134, 53-68.	1.9	36
230	QM/MM molecular dynamics simulations of the hydration of Mg(II) and Zn(II) ions. Canadian Journal of Chemistry, 2013, 91, 552-558.	1.1	36
231	Critical assessment of a proposed model of Shaker. FEBS Letters, 2004, 564, 257-263.	2.8	35
232	A Combined Experimental and Theoretical Study of Ion Solvation in Liquid N-Methylacetamide. Journal of the American Chemical Society, 2010, 132, 10847-10856.	13.7	35
233	Molecular Dynamics Simulations of the Cx26 Hemichannel: Insights into Voltage-Dependent Loop-Gating. Biophysical Journal, 2012, 102, 1341-1351.	0.5	35
234	Hydration Number, Topological Control, and Ion Selectivity. Journal of Physical Chemistry B, 2009, 113, 8725-8730.	2.6	34

#	Article	IF	Citations
235	Multi-ion free energy landscapes underscore the microscopic mechanism of ion selectivity in the KcsA channel. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1722-1732.	2.6	34
236	Simulation Analysis of the Retinal Conformational Equilibrium in Dark-Adapted Bacteriorhodopsin. Biophysical Journal, 1999, 76, 1909-1917.	0.5	33
237	The selectivity of the Na+/K+-pump is controlled by binding site protonation and self-correcting occlusion. ELife, 2016, 5, .	6.0	33
238	Reduced Free Energy Perturbation/Hamiltonian Replica Exchange Molecular Dynamics Method with Unbiased Alchemical Thermodynamic Axis. Journal of Physical Chemistry B, 2018, 122, 9435-9442.	2.6	33
239	String Method for Proteinâ€"Protein Binding Free-Energy Calculations. Journal of Chemical Theory and Computation, 2019, 15, 5829-5844.	5.3	33
240	Free Energy Simulations:â€‰ Thermodynamic Reversibility and Variability. Journal of Physical Chemistry B, 2000, 104, 5179-5190.	2.6	32
241	Lonely Arginine Seeks Friendly Environment. Journal of General Physiology, 2007, 130, 233-236.	1.9	32
242	The backbone 15N chemical shift tensor of the gramicidin channel. A molecular dynamics and density functional study. Chemical Physics Letters, 1995, 239, 186-194.	2.6	31
243	Selectivity of externally facing ion-binding sites in the Na/K pump to alkali metals and organic cations. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 18718-18723.	7.1	31
244	Gramicidin A Backbone and Side Chain Dynamics Evaluated by Molecular Dynamics Simulations and Nuclear Magnetic Resonance Experiments. I: Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2011, 115, 7417-7426.	2.6	31
245	Kirkwood-Buff analysis of aqueous N-methylacetamide and acetamide solutions modeled by the CHARMM additive and Drude polarizable force fields. Journal of Chemical Physics, 2013, 139, 084509.	3.0	31
246	Understanding Atomic-Scale Behavior of Liquid Crystals at Aqueous Interfaces. Journal of Chemical Theory and Computation, 2017, 13, 237-244.	5.3	31
247	Quantum Chemical Methods for Modeling Covalent Modification of Biological Thiols. Journal of Computational Chemistry, 2020, 41, 427-438.	3.3	31
248	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
249	Structural Dynamics of the Magnesium-Bound Conformation of CorA in a Lipid Bilayer. Structure, 2010, 18, 868-878.	3.3	30
250	Permeation Redux: Thermodynamics and Kinetics of Ion Movement through Potassium Channels. Biophysical Journal, 2014, 106, 1859-1863.	0.5	30
251	Concepts and protocols for electrostatic free energies. Molecular Simulation, 2016, 42, 1090-1101.	2.0	30
252	Probing the Effects of Gating on the Ion Occupancy of the K⁺ Channel Selectivity Filter Using Two-Dimensional Infrared Spectroscopy. Journal of the American Chemical Society, 2017, 139, 8837-8845.	13.7	30

#	Article	IF	Citations
253	Exploring the Ion Selectivity Properties of a Large Number of Simplified Binding Site Models. Biophysical Journal, 2010, 98, 2877-2885.	0.5	29
254	Cation-selective Pathway of OmpF Porin Revealed by Anomalous X-ray Diffraction. Journal of Molecular Biology, 2010, 396, 293-300.	4.2	29
255	Chemical substitutions in the selectivity filter of potassium channels do not rule out constricted-like conformations for C-type inactivation. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 11145-11150.	7.1	29
256	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.	3.3	28
257	Classical molecular dynamics. Journal of Chemical Physics, 2021, 154, 100401.	3.0	28
258	Atomic Constraints between the Voltage Sensor and the Pore Domain in a Voltage-gated K+ Channel of Known Structure. Journal of General Physiology, 2008, 131, 549-561.	1.9	27
259	Biogenesis of the pore architecture of a voltage-gated potassium channel. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 3240-3245.	7.1	27
260	Protein inclusion in lipid membranes: A theory based on the hypernetted chain integral equation. Faraday Discussions, 1999, 111, 165-172.	3.2	26
261	Eppur Si Muove! The 2013 Nobel Prize in Chemistry. Structure, 2013, 21, 2102-2105.	3.3	26
262	Structural Refinement of Proteins by Restrained Molecular Dynamics Simulations with Non-interacting Molecular Fragments. PLoS Computational Biology, 2015, 11, e1004368.	3.2	26
263	Enhanced configurational sampling with hybrid non-equilibrium molecular dynamicsâ€“Monte Carlo propagator. Journal of Chemical Physics, 2018, 148, 014101.	3.0	26
264	Molecular Dynamics of Ion Conduction through the Selectivity Filter of the Na_VAb Sodium Channel. Journal of Physical Chemistry B, 2018, 122, 10126-10142.	2.6	26
265	Polarization Effects in Water-Mediated Selective Cation Transport across a Narrow Transmembrane Channel. Journal of Chemical Theory and Computation, 2021, 17, 1726-1741.	5.3	26
266	Mechanism of C-type inactivation in the hERG potassium channel. Science Advances, 2021, 7, .	10.3	26
267	Interaction of K+with a Phospholipid Bilayer:Â A Molecular Dynamics Study. Journal of Physical Chemistry B, 1997, 101, 6066-6072.	2.6	24
268	Assessing the accuracy of approximate treatments of ion hydration based on primitive quasichemical theory. Journal of Chemical Physics, 2010, 132, 234101.	3.0	24
269	String Method with Swarms-of-Trajectories, Mean Drifts, Lag Time, and Committor. Journal of Physical Chemistry A, 2021, 125, 7558-7571.	2.5	24
270	Free Energy Methods in Drug Discoveryâ€”Introduction. ACS Symposium Series, 0, , 1-38.	0.5	24

#	Article	IF	Citations
271	Cysteine Mutagenesis and Computer Modeling of the S6 Region of an Intermediate Conductance IKCa Channel. Journal of General Physiology, 2002, 120, 99-116.	1.9	23
272	Structural Refinement of Membrane Proteins by Restrained Molecular Dynamics and Solvent Accessibility Data. Biophysical Journal, 2008, 95, 5349-5361.	0.5	23
273	Computing conformational free energy by deactivated morphing. Journal of Chemical Physics, 2008, 129, 134102.	3.0	23
274	Mechanism of Cd2+ Coordination during Slow Inactivation in Potassium Channels. Structure, 2012, 20, 1332-1342.	3.3	23
275	A Structural Study of Ion Permeation in OmpF Porin from Anomalous X-ray Diffraction and Molecular Dynamics Simulations. Journal of the American Chemical Society, 2013, 135, 16561-16568.	13.7	23
276	Achieving ergodic sampling using replica-exchange free-energy calculations. Molecular Simulation, 2014, 40, 218-228.	2.0	23
277	Efficient Determination of Free Energy Landscapes in Multiple Dimensions from Biased Umbrella Sampling Simulations Using Linear Regression. Journal of Chemical Theory and Computation, 2015, 11, 3523-3529.	5.3	23
278	Amphiphile-Induced Phase Transition of Liquid Crystals at Aqueous Interfaces. ACS Applied Materials & Interfaces, 2018, 10, 37618-37624.	8.0	23
279	Classical Drude Polarizable Force Field Model for Methyl Phosphate and Its Interactions with Mg²⁺. Journal of Physical Chemistry A, 2018, 122, 6147-6155.	2.5	23
280	Crystal structure of an archaeal CorB magnesium transporter. Nature Communications, 2021, 12, 4028.	12.8	23
281	Atomic mutagenesis in ion channels with engineered stoichiometry. ELife, 2016, 5, .	6.0	23
282	Nucleotide Regulation of the Structure and Dynamics of G-Actin. Biophysical Journal, 2014, 106, 1710-1720.	0.5	22
283	Comment on â€œFree energy simulations of single and double ion occupancy in gramicidin Aâ€•[J. Chem. Phys. 126, 105103 (2007)]. Journal of Chemical Physics, 2008, 128, 227101.	3.0	21
284	Generalized Metropolis acceptance criterion for hybrid non-equilibrium molecular dynamicsâ€”Monte Carlo simulations. Journal of Chemical Physics, 2015, 142, 024101.	3.0	21
285	Efficient hybrid non-equilibrium molecular dynamics - Monte Carlo simulations with symmetric momentum reversal. Journal of Chemical Physics, 2014, 141, 114107.	3.0	20
286	Transition rate theory, spectral analysis, and reactive paths. Journal of Chemical Physics, 2022, 156, 134111.	3.0	20
287	CHARMMâ€GUI DEER facilitator for spinâ€pair distance distribution calculations and preparation of restrainedâ€ensemble molecular dynamics simulations. Journal of Computational Chemistry, 2020, 41, 415-420.	3.3	19
288	Mixing quantum-classical molecular dynamics methods applied to intramolecular proton transfer in acetylacetone. Journal of Computational Chemistry, 1997, 18, 1760-1772.	3.3	18

#	Article	IF	Citations
289	Accurate Molecular Polarizabilities Based on Continuum Electrostatics. Journal of Chemical Theory and Computation, 2008, 4, 1480-1493.	5.3	18
290	Integrated Continuum Dielectric Approaches To Treat Molecular Polarizability and the Condensed Phase: Refractive Index and Implicit Solvation. Journal of Chemical Theory and Computation, 2009, 5, 1785-1802.	5.3	18
291	Voltage Profile along the Permeation Pathway of an Open Channel. Biophysical Journal, 2010, 99, 2863-2869.	0.5	18
292	Enhanced Sampling of an Atomic Model with Hybrid Nonequilibrium Molecular Dynamicsâ€"Monte Carlo Simulations Guided by a Coarse-Grained Model. Journal of Chemical Theory and Computation, 2015, 11, 3572-3583.	5.3	18
293	On the Utilization of Energy Minimization to the Study of Ion Selectivity. Biophysical Journal, 2009, 97, L15-L17.	0.5	17
294	Calculation of the standard binding free energy of sparsomycin to the ribosomal peptidylâ€transferase Pâ€site using molecular dynamics simulations with restraining potentials. Journal of Molecular Recognition, 2010, 23, 128-141.	2.1	16
295	Ion Binding Sites and Their Representations by Reduced Models. Journal of Physical Chemistry B, 2012, 116, 6966-6979.	2.6	16
296	A computational study of barium blockades in the KcsA potassium channel based on multi-ion potential of mean force calculations and free energy perturbation. Journal of General Physiology, 2013, 142, 451-463.	1.9	16
297	Identification of Druggable Kinase Target Conformations Using Markov Model Metastable States Analysis of apo-Abl. Journal of Chemical Theory and Computation, 2020, 16, 1896-1912.	5.3	16
298	Structure and electrostatic property of cytoplasmic domain of ZntB transporter. Protein Science, 2009, 18, 2043-2052.	7.6	15
299	Energetics of Double-Ion Occupancy in the Gramicidin A Channel. Journal of Physical Chemistry B, 2010, 114, 13881-13888.	2.6	15
300	Nano-Positioning System for Structural Analysis of Functional Homomeric Proteins in Multiple Conformations. Structure, 2012, 20, 1629-1640.	3.3	15
301	Efficiency in nonequilibrium molecular dynamics Monte Carlo simulations. Journal of Chemical Physics, 2016, 145, 134109.	3.0	15
302	Equivalence of M- and P-Summation in Calculations of Ionic Solvation Free Energies. Journal of Physical Chemistry A, 2017, 121, 1525-1530.	2.5	15
303	Proton Countertransport and Coupled Gating in the Sarcoplasmic Reticulum Calcium Pump. Journal of Molecular Biology, 2018, 430, 5050-5065.	4.2	15
304	Combining the polarizable Drude force field with a continuum electrostatic Poissonâ€"Boltzmann implicit solvation model. Journal of Computational Chemistry, 2018, 39, 1707-1719.	3.3	15
305	Leveraging the Information from Markov State Models To Improve the Convergence of Umbrella Sampling Simulations. Journal of Physical Chemistry B, 2016, 120, 8733-8742.	2.6	14
306	Modeling induction phenomena in amino acid cationâ€" $$pi $$ Ï€ interactions. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	14

#	Article	IF	Citations
307	Open and Closed Structures of a Barium-Blocked Potassium Channel. Journal of Molecular Biology, 2020, 432, 4783-4798.	4.2	14
308	Diversity of Long-Lived Intermediates along the Binding Pathway of Imatinib to Abl Kinase Revealed by MD Simulations. Journal of Chemical Theory and Computation, 2020, 16, 7852-7865.	5.3	14
309	pKa Calculations with the Polarizable Drude Force Field and Poissonâ€“Boltzmann Solvation Model. Journal of Chemical Theory and Computation, 2020, 16, 4655-4668.	5.3	14
310	Computational study of non-conductive selectivity filter conformations and C-type inactivation in a voltage-dependent potassium channel. Journal of General Physiology, 2021, 153, .	1.9	14
311	Gramicidin Channels: Versatile Tools. , 2007, , 33-80.		14
312	A Companion Guide to the String Method with Swarms of Trajectories: Characterization, Performance, and Pitfalls. Journal of Chemical Theory and Computation, 2022, 18, 1406-1422.	5.3	14
313	Perspectives on: Molecular dynamics and computational methods. Journal of General Physiology, 2010, 135, 547-548.	1.9	13
314	Molecular Dynamics Simulations of Ion Channels: How Far Have We Gone and Where Are We Heading?. Biophysical Journal, 1998, 74, 2744-2745.	0.5	12
315	Molecular Dynamics Simulations Based on Polarizable Models Show that Ion Permeation Interconverts between Different Mechanisms as a Function of Membrane Thickness. Journal of Physical Chemistry B, 2021, 125, 1020-1035.	2.6	12
316	Molecular Dynamics of Pf1 Coat Protein in a Phospholipid Bilayer. , 1996, , 555-587.		12
317	Virtual High-Throughput Ligand Screening. Methods in Molecular Biology, 2014, 1140, 251-261.	0.9	12
318	Using multiscale preconditioning to accelerate the convergence of iterative molecular calculations. Journal of Chemical Physics, 2014, 140, 184114.	3.0	11
319	Efficient Determination of Relative Entropy Using Combined Temperature and Hamiltonian Replica-Exchange Molecular Dynamics. Journal of Chemical Theory and Computation, 2015, 11, 2234-2244.	5.3	11
320	Computational study of the <scp>W</scp>260<scp>A</scp> activating mutant of <scp>S</scp>rc tyrosine kinase. Protein Science, 2016, 25, 219-230.	7.6	11
321	Structural and functional characterization of a calcium-activated cation channel from Tsukamurella paurometabola. Nature Communications, 2016, 7, 12753.	12.8	11
322	Statistical mechanics of polarizable force fields based on classical Drude oscillators with dynamical propagation by the dual-thermostat extended Lagrangian. Journal of Chemical Physics, 2020, 153, 114108.	3.0	11
323	Implicit Solvent Models. , 2001, , .		11
324	A distinct mechanism of C-type inactivation in the Kv-like KcsA mutant E71V. Nature Communications, 2022, 13, 1574.	12.8	11

#	Article	IF	Citations
325	Dissecting the Coupling between the Voltage Sensor and Pore Domains. Neuron, 2006, 52, 568-569.	8.1	10
326	EROS: Better than SAXS!. Structure, 2011, 19, 3-4.	3.3	10
327	A Structural Rearrangement of the Na+/K+-ATPase Traps Ouabain within the External Ion Permeation Pathway. Journal of Molecular Biology, 2015, 427, 1335-1344.	4.2	10
328	A Catalytically Disabled Double Mutant of Src Tyrosine Kinase Can Be Stabilized into an Active-Like Conformation. Journal of Molecular Biology, 2018, 430, 881-889.	4.2	10
329	Membrane Anchoring of Hck Kinase via the Intrinsically Disordered SH4-U and Length Scale Associated with Subcellular Localization. Journal of Molecular Biology, 2020, 432, 2985-2997.	4.2	10
330	Global Optimization of the Lennard-Jones Parameters for the Drude Polarizable Force Field. Journal of Chemical Theory and Computation, 2021, 17, 7085-7095.	5.3	10
331	Hazardous Shortcuts in Standard Binding Free Energy Calculations. Journal of Physical Chemistry Letters, 2022, 13, 6250-6258.	4.6	10
332	Multiple Time-Step Dual-Hamiltonian Hybrid Molecular Dynamics â€“ Monte Carlo Canonical Propagation Algorithm. Journal of Chemical Theory and Computation, 2016, 12, 1449-1458.	5.3	9
333	Water Flux Induced Reorientation of Liquid Crystals. ACS Central Science, 2017, 3, 1345-1349.	11.3	9
334	Using electronic polarization from the internal continuum (EPIC) for intermolecular interactions. Journal of Computational Chemistry, 2010, 31, 811-824.	3.3	8
335	Formalisms for the Explicit Inclusion of Electronic Polarizability in Molecular Modeling and Dynamics Studies. Challenges and Advances in Computational Chemistry and Physics, 2009, , 219-257.	0.6	8
336	A generalized linear response framework for expanded ensemble and replica exchange simulations. Journal of Chemical Physics, 2018, 149, 072315.	3.0	7
337	Theoretical studies of activated processes in biological ion channels. , 1998, , .		6
338	One Channel: Open and Closed. Structure, 2005, 13, 1398-1400.	3.3	6
339	What Can Be Deduced about the Structure of Shaker from Available Data?. Novartis Foundation Symposium, 2008, , 84-108.	1.1	6
340	Molecular Mechanisms of K+ Selectivity in Na/K Pump. Australian Journal of Chemistry, 2012, 65, 448.	0.9	6
341	Computational Modeling and Simulations of Biomolecular Systems. , 2021, , .		6
342	Computational Assessment of Proteinâ€“Protein Binding Specificity within a Family of Synaptic Surface Receptors. Journal of Physical Chemistry B, 2022, 126, 7510-7527.	2.6	6

#	Article	IF	Citations
343	The Art of Dissecting the Function of a Potassium Channel. Neuron, 2005, 47, 777-778.	8.1	5
344	Gramicidin A Backbone and Side Chain Dynamics Evaluated by Molecular Dynamics Simulations and Nuclear Magnetic Resonance Experiments. II: Nuclear Magnetic Resonance Experiments. Journal of Physical Chemistry B, 2011, 115, 7427-7432.	2.6	5
345	Folding and misfolding of potassium channel monomers during assembly and tetramerization. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	5
346	Theory of Transport in Ion Channels. , 0, , 133-169.		4
347	Extracellular Blockade of Potassium Channels by TEA+: The Tip of the Iceberg?. Journal of General Physiology, 2006, 128, 635-636.	1.9	4
348	Computational Electrophysiology: The Molecular Dynamics of Ion Channel Permeation and Selectivity in Atomistic Detail. Biophysical Journal, 2011, 101, 755-756.	0.5	4
349	Perspective on computational and structural aspects of kinase discovery from IPK2014. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2015, 1854, 1595-1604.	2.3	4
350	What can be deduced about the structure of Shaker from available data?. Novartis Foundation Symposium, 2002, 245, 84-101; discussion 101-8, 165-8.	1.1	4
351	1H, 15N, and 13C resonance assignments of the intrinsically disordered SH4 and Unique domains of Hck. Biomolecular NMR Assignments, 2019, 13, 71-74.	0.8	3
352	Continuum Electrostatic Behavior of a 3D-RISM Theory. Journal of Physical Chemistry B, 2020, 124, 7444-7451.	2.6	3
353	Glycine substitution in SH3-SH2 connector of Hck tyrosine kinase causes population shift from assembled to disassembled state. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129604.	2.4	3
354	Elusive Intermediate State Key in the Conversion of ATP Hydrolysis into Useful Work Driving the Ca2+ Pump SERCA. Journal of Physical Chemistry B, 2021, 125, 2921-2928.	2.6	3
355	Markov State and Diffusive Stochastic Models in Electron Spin Resonance. Advances in Experimental Medicine and Biology, 2014, 797, 115-138.	1.6	3
356	Tyrosine kinases: complex molecular systems challenging computational methodologies. European Physical Journal B, 2021, 94, 1.	1.5	3
357	Proton Wires Are Different. Biophysical Journal, 1999, 77, 2331-2332.	0.5	2
358	A proton-controlled check valve for sodium ion transport. Nature Chemical Biology, 2007, 3, 609-610.	8.0	2
359	Chapter 13 A Brief Introduction to Voltage-Gated K+ Channels. Current Topics in Membranes, 2008, , 369-384.	0.9	2
360	One domain, multiple conformations. Nature Chemical Biology, 2011, 7, 130-131.	8.0	2

#	Article	IF	Citations
361	The Binding Site of Sodium in the Gramicidin A Channel. Novartis Foundation Symposium, 1999, 225, 113-127.	1.1	2
362	A bas les barriÃ¨resâ€¦ dâ€™Ã©nergie dans les canaux potassiquesÂ!. Medecine/Sciences, 2002, 18, 605-609.	0.2	1
363	Voltage-Gated Ion Channels: The Machines Responsible for the Nerve Impulse. , 2011, , 231-248.		1
364	Comment on â€œProbing the Thermodynamics of Competitive Ion Binding Using Minimum Energy Structuresâ€• Journal of Physical Chemistry B, 2012, 116, 7991-7993.	2.6	1
365	Barium blockade of the KcsA channel in open and closed conformation datasets. Data in Brief, 2020, 32, 106135.	1.0	1
366	Virtual Issue on Ion Channels and Ion Permeation. Journal of Physical Chemistry B, 2021, 125, 7575-7577.	2.6	1
367	From Sequence to Structure and Function. , 2002, , 141-148.		0
368	Perspectives on: Molecular dynamics and computational methods. Journal of Cell Biology, 2010, 189, i16-i16.	5.2	0
369	Explicit Inclusion of Induced Polarization in Atomistic Force Fields Based on the Classical Drude Oscillator Model. , 2016, , 191-232.		0
370	Engineering of a synthetic antibody fragment for structural and functional studies of K+ channels. Journal of General Physiology, 2022, 154, .	1.9	0