BenoÄ±Ì‚t Roux

List of Publications by Year
in descending order

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326 papers	44,917 citations	1459 107 h-index	2277 200 g-index
338 all docs	338 docs citations	338 times ranked	27159 citing authors

#	Article	IF	Citations
1	CHARMM: The biomolecular simulation program. Journal of Computational Chemistry, 2009, 30, 1545-1614.	1.5	7,077
2	Scalable molecular dynamics on CPU and GPU architectures with NAMD. Journal of Chemical Physics, 2020, 153, 044130.	1.2	1,548
3	The calculation of the potential of mean force using computer simulations. Computer Physics Communications, 1995, 91, 275-282.	3.0	1,496
4	Finite representation of an infinite bulk system: Solvent boundary potential for computer simulations. Journal of Chemical Physics, 1994, 100, 9050-9063.	1.2	911
5	Extension to the weighted histogram analysis method: combining umbrella sampling with free energy calculations. Computer Physics Communications, 2001, 135, 40-57.	3.0	816
6	Implicit solvent models. Biophysical Chemistry, 1999, 78, 1-20.	1.5	793
7	Energetics of ion conduction through the K+ channel. Nature, 2001, 414, 73-77.	13.7	745
8	A simple polarizable model of water based on classical Drude oscillators. Journal of Chemical Physics, 2003, 119, 5185-5197.	1.2	635
9	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.	3.3	594
10	Modeling induced polarization with classical Drude oscillators: Theory and molecular dynamics simulation algorithm. Journal of Chemical Physics, 2003, 119, 3025-3039.	1.2	584
11	A polarizable model of water for molecular dynamics simulations of biomolecules. Chemical Physics Letters, 2006, 418, 245-249.	1.2	548
12	Control of ion selectivity in potassium channels by electrostatic and dynamic properties of carbonyl ligands. Nature, 2004, 431, 830-834.	13.7	528
13	Continuum solvation model: Computation of electrostatic forces from numerical solutions to the Poisson-Boltzmann equation. Computer Physics Communications, 1998, 111, 59-75.	3.0	500
14	Computations of Standard Binding Free Energies with Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2009, 113, 2234-2246.	1.2	481
15	An Integral Equation To Describe the Solvation of Polar Molecules in Liquid Water. Journal of Physical Chemistry B, 1997, 101, 7821-7826.	1.2	465
16	An Empirical Polarizable Force Field Based on the Classical Drude Oscillator Model: Development History and Recent Applications. Chemical Reviews, 2016, 116, 4983-5013.	23.0	434
17	Simulating Monovalent and Divalent Ions in Aqueous Solution Using a Drude Polarizable Force Field. Journal of Chemical Theory and Computation, 2010, 6, 774-786.	2.3	401
18	Molecular determinants of gating at the potassium-channel selectivity filter. Nature Structural and Molecular Biology, 2006, 13, 311-318.	3.6	399

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19	Molecular Dynamics Simulations of Ionic Liquids and Electrolytes Using Polarizable Force Fields. Chemical Reviews, 2019, 119, 7940-7995.	23.0	386
20	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.	3.3	371
21	Atomic Radii for Continuum Electrostatics Calculations Based on Molecular Dynamics Free Energy Simulations. Journal of Physical Chemistry B, 1997, 101, 5239-5248.	1.2	369
22	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.	13.5	366
23	Theoretical and computational models of biological ion channels. Quarterly Reviews of Biophysics, 2004, 37, 15-103.	2.4	362
24	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.	1.2	357
25	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.	2.0	353
26	Polarizable Force Field for Peptides and Proteins Based on the Classical Drude Oscillator. Journal of Chemical Theory and Computation, 2013, 9, 5430-5449.	2.3	329
27	Absolute Binding Free Energy Calculations Using Molecular Dynamics Simulations with Restraining Potentials. Biophysical Journal, 2006, 91, 2798-2814.	0.2	316
28	Molecular Dynamics of the KcsA K+ Channel in a Bilayer Membrane. Biophysical Journal, 2000, 78, 2900-2917.	0.2	314
29	Molecular modeling and dynamics studies with explicit inclusion of electronic polarizability: theory and applications. Theoretical Chemistry Accounts, 2009, 124, 11-28.	0.5	314
30	Finding Transition Pathways Using the String Method with Swarms of Trajectories. Journal of Physical Chemistry B, 2008, 112, 3432-3440.	1.2	313
31	Activation pathway of Src kinase reveals intermediate states as targets for drug design. Nature Communications, 2014, 5, 3397.	5.8	300
32	Standard Binding Free Energies from Computer Simulations: What Is the Best Strategy?. Journal of Chemical Theory and Computation, 2013, 9, 794-802.	2.3	298
33	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
34	Closing In on the Resting State of the Shaker K+ Channel. Neuron, 2007, 56, 124-140.	3.8	270
35	Structural basis for the coupling between activation and inactivation gates in K+ channels. Nature, 2010, 466, 272-275.	13.7	267
36	Simulation of Osmotic Pressure in Concentrated Aqueous Salt Solutions. Journal of Physical Chemistry Letters, 2010, 1, 183-189.	2.1	266

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37	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.	2.3	265
38	Gating charge displacement in voltage-gated ion channels involves limited transmembrane movement. Nature, 2005, 436, 852-856.	13.7	263
39	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.	2.3	260
40	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.	2.0	252
41	Molecular Mechanism of H+ Conduction in the Single-File Water Chain of the Gramicidin Channel. Biophysical Journal, 2002, 82, 2304-2316.	0.2	250
42	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.	2.1	233
43	Molecular basis for the Born model of ion solvation. The Journal of Physical Chemistry, 1990, 94, 4683-4688.	2.9	229
44	Structural mechanism of voltage-dependent gating in an isolated voltage-sensing domain. Nature Structural and Molecular Biology, 2014, 21, 244-252.	3.6	228
45	A Grand Canonical Monte Carloâ€“Brownian Dynamics Algorithm for Simulating Ion Channels. Biophysical Journal, 2000, 79, 788-801.	0.2	226
46	CHARMMâ€GUI 10 years for biomolecular modeling and simulation. Journal of Computational Chemistry, 2017, 38, 1114-1124.	1.5	224
47	Generalized solvent boundary potential for computer simulations. Journal of Chemical Physics, 2001, 114, 2924-2937.	1.2	223
48	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.	3.3	222
49	Molecular driving forces determining potassium channel slow inactivation. Nature Structural and Molecular Biology, 2007, 14, 1062-1069.	3.6	216
50	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.	1.0	214
51	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.	2.3	212
52	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.	2.3	211
53	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.	1.2	206
54	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.	3.3	195

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55	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.	2.3	191
56	A Gate in the Selectivity Filter of Potassium Channels. Structure, 2005, 13, 591-600.	1.6	190
57	The Membrane Potential and its Representation by a Constant Electric Field in Computer Simulations. Biophysical Journal, 2008, 95, 4205-4216.	0.2	188
58	Efficient Determination of Proteinâ€“Protein Standard Binding Free Energies from First Principles. Journal of Chemical Theory and Computation, 2013, 9, 3789-3798.	2.3	188
59	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.	1.5	181
60	Control of Ion Selectivity in LeuT: Two Na+ Binding Sites with Two Different Mechanisms. Journal of Molecular Biology, 2008, 377, 804-818.	2.0	181
61	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.	1.2	181
62	An emerging consensus on voltage-dependent gating from computational modeling and molecular dynamics simulations. Journal of General Physiology, 2012, 140, 587-594.	0.9	179
63	Importance of Hydration and Dynamics on the Selectivity of the KcsA and NaK Channels. Journal of General Physiology, 2007, 129, 135-143.	0.9	178
64	Ion selectivity in potassium channels. Biophysical Chemistry, 2006, 124, 279-291.	1.5	174
65	Instantaneous ion configurations in the K ⁺ ion channel selectivity filter revealed by 2D IR spectroscopy. Science, 2016, 353, 1040-1044.	6.0	174
66	Ion transport in a gramicidin-like channel: dynamics and mobility. The Journal of Physical Chemistry, 1991, 95, 4856-4868.	2.9	171
67	Recovery from slow inactivation in K+ channels is controlled by water molecules. Nature, 2013, 501, 121-124.	13.7	171
68	Constant electric field simulations of the membrane potential illustrated with simple systems. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 294-302.	1.4	169
69	Solvation of complex molecules in a polar liquid: An integral equation theory. Journal of Chemical Physics, 1996, 104, 8678-8689.	1.2	168
70	Ion Channels, Permeation, and Electrostatics: Insight into the Function of KcsA. Biochemistry, 2000, 39, 13295-13306.	1.2	167
71	Ion Conduction and Selectivity in K+ Channels. Annual Review of Biophysics and Biomolecular Structure, 2005, 34, 153-171.	18.3	167
72	On the statistical equivalence of restrained-ensemble simulations with the maximum entropy method. Journal of Chemical Physics, 2013, 138, 084107.	1.2	166

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73	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.	3.3	164
74	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.	1.2	159
75	Polarizable Empirical Force Field for Aromatic Compounds Based on the Classical Drude Oscillator. Journal of Physical Chemistry B, 2007, 111, 2873-2885.	1.2	149
76	The Theory of Ultra-Coarse-Graining. 1. General Principles. Journal of Chemical Theory and Computation, 2013, 9, 2466-2480.	2.3	149
77	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.	2.3	142
78	Ion selectivity in channels and transporters. Journal of General Physiology, 2011, 137, 415-426.	0.9	142
79	On the Importance of Atomic Fluctuations, Protein Flexibility, and Solvent in Ion Permeation. Journal of General Physiology, 2004, 124, 679-690.	0.9	141
80	Molecular Dynamics Study of a Polymeric Reverse Osmosis Membrane. Journal of Physical Chemistry B, 2009, 113, 10177-10182.	1.2	139
81	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.	2.1	139
82	Constant-pH Molecular Dynamics Simulations for Large Biomolecular Systems. Journal of Chemical Theory and Computation, 2017, 13, 5933-5944.	2.3	139
83	Dynamics of the Kv1.2 Voltage-Gated K+ Channel in a Membrane Environment. Biophysical Journal, 2007, 93, 3070-3082.	0.2	138
84	Building Markov state models along pathways to determine free energies and rates of transitions. Journal of Chemical Physics, 2008, 129, 064107.	1.2	137
85	Computational Studies of Membrane Channels. Structure, 2004, 12, 1343-1351.	1.6	136
86	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.	2.3	136
87	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.	2.3	136
88	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.	3.3	136
89	Conformational dynamics of ligand-dependent alternating access in LeuT. Nature Structural and Molecular Biology, 2014, 21, 472-479.	3.6	136
90	Calculation of the Gating Charge for the Kv1.2 Voltage-Activated Potassium Channel. Biophysical Journal, 2010, 98, 2189-2198.	0.2	135

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91	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.	0.2	133
92	Solvation thermodynamics: An approach from analytic temperature derivatives. Journal of Chemical Physics, 1990, 92, 5020-5033.	1.2	132
93	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.	1.2	132
94	Computational Studies of the Gramicidin Channel. Accounts of Chemical Research, 2002, 35, 366-375.	7.6	131
95	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.	2.3	131
96	Numerical solution of the hypernetted chain equation for a solute of arbitrary geometry in three dimensions. Journal of Chemical Physics, 1995, 103, 360-364.	1.2	130
97	Statistical Mechanical Equilibrium Theory of Selective Ion Channels. Biophysical Journal, 1999, 77, 139-153.	0.2	130
98	The Binding of Antibiotics in OmpF Porin. Structure, 2013, 21, 76-87.	1.6	128
99	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.	0.2	124
100	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.	6.6	123
101	Computation of binding free energy with molecular dynamics and grand canonical Monte Carlo simulations. Journal of Chemical Physics, 2008, 128, 115103.	1.2	123
102	Free Energy Landscape of A-DNA to B-DNA Conversion in Aqueous Solution. Journal of the American Chemical Society, 2005, 127, 6866-6876.	6.6	122
103	Understanding the Dielectric Properties of Liquid Amides from a Polarizable Force Field. Journal of Physical Chemistry B, 2008, 112, 3509-3521.	1.2	122
104	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.	2.3	120
105	An Overview of Electrostatic Free Energy Computations for Solutions and Proteins. Journal of Chemical Theory and Computation, 2014, 10, 2690-2709.	2.3	118
106	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.	6.6	117
107	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.	0.2	117
108	Architecture and assembly of the <scp>G</scp>ramâ€positive cell wall. Molecular Microbiology, 2013, 88, 664-672.	1.2	116

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109	Generalized scalable multiple copy algorithms for molecular dynamics simulations in NAMD. Computer Physics Communications, 2014, 185, 908-916.	3.0	115
110	Grand canonical Monte Carlo simulations of water in protein environments. Journal of Chemical Physics, 2004, 121, 6392-6400.	1.2	112
111	Exploring the Conformational Transitions of Biomolecular Systems Using a Simple Two-State Anisotropic Network Model. PLoS Computational Biology, 2014, 10, e1003521.	1.5	112
112	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.	3.3	106
113	Machine Learning Force Field Parameters from Ab Initio Data. Journal of Chemical Theory and Computation, 2017, 13, 4492-4503.	2.3	105
114	Six-site polarizable model of water based on the classical Drude oscillator. Journal of Chemical Physics, 2013, 138, 034508.	1.2	103
115	Simulation study of ion pairing in concentrated aqueous salt solutions with a polarizable force field. Faraday Discussions, 2013, 160, 135-149.	1.6	102
116	Representation of Ionâ€“Protein Interactions Using the Drude Polarizable Force-Field. Journal of Physical Chemistry B, 2015, 119, 9401-9416.	1.2	101
117	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.	1.2	98
118	Many-Body Polarization Effects and the Membrane Dipole Potential. Journal of the American Chemical Society, 2009, 131, 2760-2761.	6.6	98
119	In Search of a Consensus Model of the Resting State of a Voltage-Sensing Domain. Neuron, 2011, 72, 713-720.	3.8	93
120	Escherichia coli Peptidoglycan Structure and Mechanics as Predicted by Atomic-Scale Simulations. PLoS Computational Biology, 2014, 10, e1003475.	1.5	92
121	Src Kinase Conformational Activation: Thermodynamics, Pathways, and Mechanisms. PLoS Computational Biology, 2008, 4, e1000047.	1.5	91
122	Ion Selectivity of the KcsA Channel: A Perspective from Multi-Ion Free Energy Landscapes. Journal of Molecular Biology, 2010, 401, 831-842.	2.0	90
123	Drude Polarizable Force Field for Molecular Dynamics Simulations of Saturated and Unsaturated Zwitterionic Lipids. Journal of Chemical Theory and Computation, 2017, 13, 4535-4552.	2.3	90
124	Phosphoantigen-induced conformational change of butyrophilin 3A1 (BTN3A1) and its implication on Vî39Vî2 T cell activation. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E7311-E7320.	3.3	90
125	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.	2.3	89
126	On the origin of the electrostatic potential difference at a liquid-vacuum interface. Journal of Chemical Physics, 2008, 129, 234706.	1.2	88

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127	Structural Refinement from Restrained-Ensemble Simulations Based on EPR/DEER Data: Application to T4 Lysozyme. Journal of Physical Chemistry B, 2013, 117, 4740-4754.	1.2	88
128	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.	2.3	87
129	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.	4.1	87
130	Ion channels and ion selectivity. Essays in Biochemistry, 2017, 61, 201-209.	2.1	85
131	Atomistic View of the Conformational Activation of Src Kinase Using the String Method with Swarms-of-Trajectories. Biophysical Journal, 2009, 97, L8-L10.	0.2	84
132	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.	3.3	83
133	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.	3.3	83
134	Lipid-Mediated Interactions between Intrinsic Membrane Proteins: Dependence on Protein Size and Lipid Composition. Biophysical Journal, 2001, 81, 276-284.	0.2	82
135	Constant-pH Hybrid Nonequilibrium Molecular Dynamicsâ€“Monte Carlo Simulation Method. Journal of Chemical Theory and Computation, 2015, 11, 3919-3931.	2.3	82
136	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.	2.3	80
137	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.	1.5	79
138	On the Potential Functions used in Molecular Dynamics Simulations of Ion Channels. Biophysical Journal, 2002, 82, 1681-1684.	0.2	76
139	Locking the Active Conformation of c-Src Kinase through the Phosphorylation of the Activation Loop. Journal of Molecular Biology, 2014, 426, 423-435.	2.0	74
140	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.	6.6	73
141	Extracellular Blockade of K+ Channels by Tea. Journal of General Physiology, 2001, 118, 207-218.	0.9	71
142	On the structural basis of modal gating behavior in K+ channels. Nature Structural and Molecular Biology, 2011, 18, 67-74.	3.6	71
143	CHARMM-GUI Ligand Binder for Absolute Binding Free Energy Calculations and Its Application. Journal of Chemical Information and Modeling, 2013, 53, 267-277.	2.5	71
144	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.	6.6	70

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145	Brownian dynamics simulations of ions channels: A general treatment of electrostatic reaction fields for molecular pores of arbitrary geometry. Journal of Chemical Physics, 2001, 115, 4850-4861.	1.2	69
146	Atomic Radii for Continuum Electrostatics Calculations on Nucleic Acids. Journal of Physical Chemistry B, 2002, 106, 11026-11035.	1.2	69
147	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.	3.3	67
148	Spatial dependence of timeâ€dependent friction for pair diffusion in a simple fluid. Journal of Chemical Physics, 1990, 93, 6804-6812.	1.2	66
149	Restrained-Ensemble Molecular Dynamics Simulations Based on Distance Histograms from Double Electronâ€“Electron Resonance Spectroscopy. Journal of Physical Chemistry B, 2013, 117, 4733-4739.	1.2	66
150	Reproducibility of Free Energy Calculations across Different Molecular Simulation Software Packages. Journal of Chemical Theory and Computation, 2018, 14, 5567-5582.	2.3	66
151	Shifts in the selectivity filter dynamics cause modal gating in K+ channels. Nature Communications, 2019, 10, 123.	5.8	66
152	Rapid constriction of the selectivity filter underlies C-type inactivation in the KcsA potassium channel. Journal of General Physiology, 2018, 150, 1408-1420.	0.9	64
153	Free Energy and Kinetics of Conformational Transitions from Voronoi Tessellated Milestoning with Restraining Potentials. Journal of Chemical Theory and Computation, 2009, 5, 2589-2594.	2.3	62
154	Electrostatics of the Intracellular Vestibule of K+ Channels. Journal of Molecular Biology, 2005, 354, 272-288.	2.0	58
155	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.	2.0	57
156	Mechanism of potassium ion uptake by the Na+/K+-ATPase. Nature Communications, 2015, 6, 7622.	5.8	57
157	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.	2.3	57
158	Potential energy function for cation-peptide interactions: Anab initio study. Journal of Computational Chemistry, 1995, 16, 690-704.	1.5	56
159	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.	1.2	56
160	Molecular Structure of Canonical Liquid Crystal Interfaces. Journal of the American Chemical Society, 2017, 139, 3841-3850.	6.6	56
161	Accurate determination of protein:ligand standard binding free energies from molecular dynamics simulations. Nature Protocols, 2022, 17, 1114-1141.	5.5	56
162	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.	3.3	54

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163	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.	3.6	54
164	Relative Free Energies for Hydration of Monovalent Ions from QM and QM/MM Simulations. Journal of Chemical Theory and Computation, 2013, 9, 4165-4175.	2.3	54
165	Tyrosine Kinase Activation and Conformational Flexibility: Lessons from Src-Family Tyrosine Kinases. Accounts of Chemical Research, 2017, 50, 1193-1201.	7.6	53
166	Further Optimization and Validation of the Classical Drude Polarizable Protein Force Field. Journal of Chemical Theory and Computation, 2020, 16, 3221-3239.	2.3	53
167	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.	2.5	52
168	Molecular dynamics simulations of membrane proteins under asymmetric ionic concentrations. Journal of General Physiology, 2013, 142, 465-475.	0.9	51
169	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.	3.3	51
170	Absolute Binding Free Energy Calculations of Sparsomycin Analogs to the Bacterial Ribosome. Journal of Physical Chemistry B, 2010, 114, 9525-9539.	1.2	50
171	Ouabain Binding Site in a Functioning Na+/K+ ATPase. Journal of Biological Chemistry, 2011, 286, 38177-38183.	1.6	50
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