Benoit Roux

List of Publications by Year
in descending order

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370 papers	38,830 citations	1233 110 h-index	3725 179 g-index
378 all docs	378 docs citations	378 times ranked	21853 citing authors

#	Article	IF	Citations
1	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.	2.3	14
2	Engineering of a synthetic antibody fragment for structural and functional studies of K+ channels. Journal of General Physiology, 2022, 154, .	0.9	0
3	A distinct mechanism of C-type inactivation in the Kv-like KcsA mutant E71V. Nature Communications, 2022, 13, 1574.	5.8	11
4	Accurate determination of protein:ligand standard binding free energies from molecular dynamics simulations. Nature Protocols, 2022, 17, 1114-1141.	5.5	56
5	Transition rate theory, spectral analysis, and reactive paths. Journal of Chemical Physics, 2022, 156, 134111.	1.2	20
6	Hazardous Shortcuts in Standard Binding Free Energy Calculations. Journal of Physical Chemistry Letters, 2022, 13, 6250-6258.	2.1	10
7	Computational Assessment of Proteinâ€“Protein Binding Specificity within a Family of Synaptic Surface Receptors. Journal of Physical Chemistry B, 2022, 126, 7510-7527.	1.2	6
8	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.	1.2	12
9	Polarization Effects in Water-Mediated Selective Cation Transport across a Narrow Transmembrane Channel. Journal of Chemical Theory and Computation, 2021, 17, 1726-1741.	2.3	26
10	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.	1.2	3
11	Classical molecular dynamics. Journal of Chemical Physics, 2021, 154, 100401.	1.2	28
12	Crystal structure of an archaeal CorB magnesium transporter. Nature Communications, 2021, 12, 4028.	5.8	23
13	Virtual Issue on Ion Channels and Ion Permeation. Journal of Physical Chemistry B, 2021, 125, 7575-7577.	1.2	1
14	String Method with Swarms-of-Trajectories, Mean Drifts, Lag Time, and Committor. Journal of Physical Chemistry A, 2021, 125, 7558-7571.	1.1	24
15	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, .	3.3	5
16	Computational study of non-conductive selectivity filter conformations and C-type inactivation in a voltage-dependent potassium channel. Journal of General Physiology, 2021, 153, .	0.9	14
17	Computational Modeling and Simulations of Biomolecular Systems. , 2021, , .		6
18	Mechanism of C-type inactivation in the hERG potassium channel. Science Advances, 2021, 7, .	4.7	26

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19	Global Optimization of the Lennard-Jones Parameters for the Drude Polarizable Force Field. Journal of Chemical Theory and Computation, 2021, 17, 7085-7095.	2.3	10
20	Tyrosine kinases: complex molecular systems challenging computational methodologies. European Physical Journal B, 2021, 94, 1.	0.6	3
21	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.	1.5	19
22	Quantum Chemical Methods for Modeling Covalent Modification of Biological Thiols. Journal of Computational Chemistry, 2020, 41, 427-438.	1.5	31
23	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.	2.0	10
24	Barium blockade of the KcsA channel in open and closed conformation datasets. Data in Brief, 2020, 32, 106135.	0.5	1
25	Open and Closed Structures of a Barium-Blocked Potassium Channel. Journal of Molecular Biology, 2020, 432, 4783-4798.	2.0	14
26	Continuum Electrostatic Behavior of a 3D-RISM Theory. Journal of Physical Chemistry B, 2020, 124, 7444-7451.	1.2	3
27	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.	2.3	16
28	Scalable molecular dynamics on CPU and GPU architectures with NAMD. Journal of Chemical Physics, 2020, 153, 044130.	1.2	1,548
29	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
30	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.	1.2	11
31	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.	2.3	14
32	pKa Calculations with the Polarizable Drude Force Field and Poissonâ€“Boltzmann Solvation Model. Journal of Chemical Theory and Computation, 2020, 16, 4655-4668.	2.3	14
33	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.	1.1	3
34	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
35	String Method for Proteinâ€“Protein Binding Free-Energy Calculations. Journal of Chemical Theory and Computation, 2019, 15, 5829-5844.	2.3	33
36	Molecular Dynamics Simulations of Ionic Liquids and Electrolytes Using Polarizable Force Fields. Chemical Reviews, 2019, 119, 7940-7995.	23.0	386

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37	Shifts in the selectivity filter dynamics cause modal gating in K+ channels. Nature Communications, 2019, 10, 123.	5.8	66
38	1H, 15N, and 13C resonance assignments of the intrinsically disordered SH4 and Unique domains of Hck. Biomolecular NMR Assignments, 2019, 13, 71-74.	0.4	3
39	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.	2.3	47
40	Polarizable Force Field for Molecular Ions Based on the Classical Drude Oscillator. Journal of Chemical Information and Modeling, 2018, 58, 993-1004.	2.5	45
41	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.	2.0	10
42	Graphâ€“Theoretic Analysis of Monomethyl Phosphate Clustering in Ionic Solutions. Journal of Physical Chemistry B, 2018, 122, 1484-1494.	1.2	46
43	Enhanced configurational sampling with hybrid non-equilibrium molecular dynamicsâ€“Monte Carlo propagator. Journal of Chemical Physics, 2018, 148, 014101.	1.2	26
44	Optimized Lennard-Jones Parameters for Druglike Small Molecules. Journal of Chemical Theory and Computation, 2018, 14, 3121-3131.	2.3	44
45	Modeling induction phenomena in amino acid cationâ€“ $$pi $$ Ï€ interactions. Theoretical Chemistry Accounts, 2018, 137, 1.	0.5	14
46	Reproducibility of Free Energy Calculations across Different Molecular Simulation Software Packages. Journal of Chemical Theory and Computation, 2018, 14, 5567-5582.	2.3	66
47	Amphiphile-Induced Phase Transition of Liquid Crystals at Aqueous Interfaces. ACS Applied Materials & Interfaces, 2018, 10, 37618-37624.	4.0	23
48	Reduced Free Energy Perturbation/Hamiltonian Replica Exchange Molecular Dynamics Method with Unbiased Alchemical Thermodynamic Axis. Journal of Physical Chemistry B, 2018, 122, 9435-9442.	1.2	33
49	Proton Countertransport and Coupled Gating in the Sarcoplasmic Reticulum Calcium Pump. Journal of Molecular Biology, 2018, 430, 5050-5065.	2.0	15
50	Molecular Dynamics of Ion Conduction through the Selectivity Filter of the Na_VAb Sodium Channel. Journal of Physical Chemistry B, 2018, 122, 10126-10142.	1.2	26
51	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
52	Classical Drude Polarizable Force Field Model for Methyl Phosphate and Its Interactions with Mg²⁺. Journal of Physical Chemistry A, 2018, 122, 6147-6155.	1.1	23
53	A generalized linear response framework for expanded ensemble and replica exchange simulations. Journal of Chemical Physics, 2018, 149, 072315.	1.2	7
54	Combining the polarizable Drude force field with a continuum electrostatic Poissonâ€“Boltzmann implicit solvation model. Journal of Computational Chemistry, 2018, 39, 1707-1719.	1.5	15

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55	Conformational Transitions and Alternating-Access Mechanism in the Sarcoplasmic Reticulum Calcium Pump. Journal of Molecular Biology, 2017, 429, 647-666.	2.0	37
56	Equivalence of M- and P-Summation in Calculations of Ionic Solvation Free Energies. Journal of Physical Chemistry A, 2017, 121, 1525-1530.	1.1	15
57	Tyrosine Kinase Activation and Conformational Flexibility: Lessons from Src-Family Tyrosine Kinases. Accounts of Chemical Research, 2017, 50, 1193-1201.	7.6	53
58	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.	6.6	30
59	New Coarse Variables for the Accurate Determination of Standard Binding Free Energies. Journal of Chemical Theory and Computation, 2017, 13, 5173-5178.	2.3	49
60	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.	3.3	29
61	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
62	Machine Learning Force Field Parameters from Ab Initio Data. Journal of Chemical Theory and Computation, 2017, 13, 4492-4503.	2.3	105
63	Water Flux Induced Reorientation of Liquid Crystals. ACS Central Science, 2017, 3, 1345-1349.	5.3	9
64	Constant-pH Molecular Dynamics Simulations for Large Biomolecular Systems. Journal of Chemical Theory and Computation, 2017, 13, 5933-5944.	2.3	139
65	The Activation of c-Src Tyrosine Kinase: Conformational Transition Pathway and Free Energy Landscape. Journal of Physical Chemistry B, 2017, 121, 3352-3363.	1.2	41
66	CHARMMâ€GUI 10 years for biomolecular modeling and simulation. Journal of Computational Chemistry, 2017, 38, 1114-1124.	1.5	224
67	Understanding Atomic-Scale Behavior of Liquid Crystals at Aqueous Interfaces. Journal of Chemical Theory and Computation, 2017, 13, 237-244.	2.3	31
68	Ion channels and ion selectivity. Essays in Biochemistry, 2017, 61, 201-209.	2.1	85
69	The selectivity of the Na+/K+-pump is controlled by binding site protonation and self-correcting occlusion. ELife, 2016, 5, .	2.8	33
70	Concepts and protocols for electrostatic free energies. Molecular Simulation, 2016, 42, 1090-1101.	0.9	30
71	Efficiency in nonequilibrium molecular dynamics Monte Carlo simulations. Journal of Chemical Physics, 2016, 145, 134109.	1.2	15
72	Multiple Time-Step Dual-Hamiltonian Hybrid Molecular Dynamics â€“ Monte Carlo Canonical Propagation Algorithm. Journal of Chemical Theory and Computation, 2016, 12, 1449-1458.	2.3	9

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73	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.	3.1	11
74	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
75	Instantaneous ion configurations in the K ⁺ ion channel selectivity filter revealed by 2D IR spectroscopy. Science, 2016, 353, 1040-1044.	6.0	174
76	Leveraging the Information from Markov State Models To Improve the Convergence of Umbrella Sampling Simulations. Journal of Physical Chemistry B, 2016, 120, 8733-8742.	1.2	14
77	Structural and functional characterization of a calcium-activated cation channel from Tsukamurella paurometabola. Nature Communications, 2016, 7, 12753.	5.8	11
78	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
79	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.	1.4	34
80	Atomic mutagenesis in ion channels with engineered stoichiometry. ELife, 2016, 5, .	2.8	23
81	Explicit Inclusion of Induced Polarization in Atomistic Force Fields Based on the Classical Drude Oscillator Model. , 2016, , 191-232.		0
82	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
83	Structural Refinement of Proteins by Restrained Molecular Dynamics Simulations with Non-interacting Molecular Fragments. PLoS Computational Biology, 2015, 11, e1004368.	1.5	26
84	Simulating the Distance Distribution between Spin-Labels Attached to Proteins. Journal of Physical Chemistry B, 2015, 119, 3901-3911.	1.2	46
85	Representation of Ionâ€"Protein Interactions Using the Drude Polarizable Force-Field. Journal of Physical Chemistry B, 2015, 119, 9401-9416.	1.2	101
86	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
87	A Structural Rearrangement of the Na+/K+-ATPase Traps Ouabain within the External Ion Permeation Pathway. Journal of Molecular Biology, 2015, 427, 1335-1344.	2.0	10
88	Generalized Metropolis acceptance criterion for hybrid non-equilibrium molecular dynamicsâ€"Monte Carlo simulations. Journal of Chemical Physics, 2015, 142, 024101.	1.2	21
89	Constant-pH Hybrid Nonequilibrium Molecular Dynamicsâ€"Monte Carlo Simulation Method. Journal of Chemical Theory and Computation, 2015, 11, 3919-3931.	2.3	82
90	Mechanism of potassium ion uptake by the Na+/K+-ATPase. Nature Communications, 2015, 6, 7622.	5.8	57

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91	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.	2.3	18
92	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.	2.3	23
93	Perspective on computational and structural aspects of kinase discovery from IPK2014. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2015, 1854, 1595-1604.	1.1	4
94	Efficient Determination of Relative Entropy Using Combined Temperature and Hamiltonian Replica-Exchange Molecular Dynamics. Journal of Chemical Theory and Computation, 2015, 11, 2234-2244.	2.3	11
95	Quantum Effects in Cation Interactions with First and Second Coordination Shell Ligands in Metalloproteins. Journal of Chemical Theory and Computation, 2015, 11, 4992-5001.	2.3	42
96	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
97	Achieving ergodic sampling using replica-exchange free-energy calculations. Molecular Simulation, 2014, 40, 218-228.	0.9	23
98	Conformational dynamics of ligand-dependent alternating access in LeuT. Nature Structural and Molecular Biology, 2014, 21, 472-479.	3.6	136
99	Exploring the Conformational Transitions of Biomolecular Systems Using a Simple Two-State Anisotropic Network Model. PLoS Computational Biology, 2014, 10, e1003521.	1.5	112
100	Escherichia coli Peptidoglycan Structure and Mechanics as Predicted by Atomic-Scale Simulations. PLoS Computational Biology, 2014, 10, e1003475.	1.5	92
101	Using multiscale preconditioning to accelerate the convergence of iterative molecular calculations. Journal of Chemical Physics, 2014, 140, 184114.	1.2	11
102	Efficient hybrid non-equilibrium molecular dynamics - Monte Carlo simulations with symmetric momentum reversal. Journal of Chemical Physics, 2014, 141, 114107.	1.2	20
103	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
104	Activation pathway of Src kinase reveals intermediate states as targets for drug design. Nature Communications, 2014, 5, 3397.	5.8	300
105	Structural mechanism of voltage-dependent gating in an isolated voltage-sensing domain. Nature Structural and Molecular Biology, 2014, 21, 244-252.	3.6	228
106	Permeation Redux: Thermodynamics and Kinetics of Ion Movement through Potassium Channels. Biophysical Journal, 2014, 106, 1859-1863.	0.2	30
107	Computational Study of Gleevec and G6G Reveals Molecular Determinants of Kinase Inhibitor Selectivity. Journal of the American Chemical Society, 2014, 136, 14753-14762.	6.6	41
108	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

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109	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
110	Comparison between Mean Forces and Swarms-of-Trajectories String Methods. Journal of Chemical Theory and Computation, 2014, 10, 524-533.	2.3	38
111	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
112	Nucleotide Regulation of the Structure and Dynamics of G-Actin. Biophysical Journal, 2014, 106, 1710-1720.	0.2	22
113	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
114	Generalized scalable multiple copy algorithms for molecular dynamics simulations in NAMD. Computer Physics Communications, 2014, 185, 908-916.	3.0	115
115	An Overview of Electrostatic Free Energy Computations for Solutions and Proteins. Journal of Chemical Theory and Computation, 2014, 10, 2690-2709.	2.3	118
116	Virtual High-Throughput Ligand Screening. Methods in Molecular Biology, 2014, 1140, 251-261.	0.4	12
117	Markov State and Diffusive Stochastic Models in Electron Spin Resonance. Advances in Experimental Medicine and Biology, 2014, 797, 115-138.	0.8	3
118	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
119	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
120	A Conformational Intermediate in Glutamate Receptor Activation. Neuron, 2013, 79, 492-503.	3.8	39
121	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
122	Reconciling the Roles of Kinetic and Thermodynamic Factors in Membraneâ€“Protein Insertion. Journal of the American Chemical Society, 2013, 135, 2291-2297.	6.6	41
123	Recovery from slow inactivation in K+ channels is controlled by water molecules. Nature, 2013, 501, 121-124.	13.7	171
124	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.	6.6	49
125	Simulation study of ion pairing in concentrated aqueous salt solutions with a polarizable force field. Faraday Discussions, 2013, 160, 135-149.	1.6	102
126	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

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127	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.	6.6	23
128	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
129	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.	1.2	31
130	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
131	The Binding of Antibiotics in OmpF Porin. Structure, 2013, 21, 76-87.	1.6	128
132	Eppur Si Muove! The 2013 Nobel Prize in Chemistry. Structure, 2013, 21, 2102-2105.	1.6	26
133	Six-site polarizable model of water based on the classical Drude oscillator. Journal of Chemical Physics, 2013, 138, 034508.	1.2	103
134	On the statistical equivalence of restrained-ensemble simulations with the maximum entropy method. Journal of Chemical Physics, 2013, 138, 084107.	1.2	166
135	The Theory of Ultra-Coarse-Graining. 1. General Principles. Journal of Chemical Theory and Computation, 2013, 9, 2466-2480.	2.3	149
136	Architecture and assembly of the <scp>G</scp>ramâ€positive cell wall. Molecular Microbiology, 2013, 88, 664-672.	1.2	116
137	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
138	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
139	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
140	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
141	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
142	QM/MM molecular dynamics simulations of the hydration of Mg(II) and Zn(II) ions. Canadian Journal of Chemistry, 2013, 91, 552-558.	0.6	36
143	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.	0.9	16
144	Molecular dynamics simulations of membrane proteins under asymmetric ionic concentrations. Journal of General Physiology, 2013, 142, 465-475.	0.9	51

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145	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
146	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
147	Intermediate state trapping of a voltage sensor. Journal of General Physiology, 2012, 140, 635-652.	0.9	50
148	Molecular Dynamics Simulations of the Cx26 Hemichannel: Insights into Voltage-Dependent Loop-Gating. Biophysical Journal, 2012, 102, 1341-1351.	0.2	35
149	Ion Binding Sites and Their Representations by Reduced Models. Journal of Physical Chemistry B, 2012, 116, 6966-6979.	1.2	16
150	Comment on â€œProbing the Thermodynamics of Competitive Ion Binding Using Minimum Energy Structuresâ€• Journal of Physical Chemistry B, 2012, 116, 7991-7993.	1.2	1
151	Mechanism of Cd2+ Coordination during Slow Inactivation in Potassium Channels. Structure, 2012, 20, 1332-1342.	1.6	23
152	Constant electric field simulations of the membrane potential illustrated with simple systems. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 294-302.	1.4	169
153	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
154	Molecular Dynamics Investigation of the Ï‰-Current in the Kv1.2 Voltage Sensor Domains. Biophysical Journal, 2012, 102, 258-267.	0.2	47
155	Determination of Membrane-Insertion Free Energies by Molecular Dynamics Simulations. Biophysical Journal, 2012, 102, 795-801.	0.2	49
156	Nano-Positioning System for Structural Analysis of Functional Homomeric Proteins in Multiple Conformations. Structure, 2012, 20, 1629-1640.	1.6	15
157	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
158	Molecular Mechanisms of K+ Selectivity in Na/K Pump. Australian Journal of Chemistry, 2012, 65, 448.	0.5	6
159	Web interface for brownian dynamics simulation of ion transport and its applications to betaâ€barrel pores. Journal of Computational Chemistry, 2012, 33, 331-339.	1.5	43
160	Voltage-Gated Ion Channels: The Machines Responsible for the Nerve Impulse. , 2011, , 231-248.		1
161	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.	1.2	5
162	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.	1.2	31

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163	Computational Electrophysiology: The Molecular Dynamics of Ion Channel Permeation and Selectivity in Atomistic Detail. Biophysical Journal, 2011, 101, 755-756.	0.2	4
164	In Search of a Consensus Model of the Resting State of a Voltage-Sensing Domain. Neuron, 2011, 72, 713-720.	3.8	93
165	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
166	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.	0.9	49
167	One domain, multiple conformations. Nature Chemical Biology, 2011, 7, 130-131.	3.9	2
168	On the structural basis of modal gating behavior in K+ channels. Nature Structural and Molecular Biology, 2011, 18, 67-74.	3.6	71
169	The hidden energetics of ligand binding and activation in a glutamate receptor. Nature Structural and Molecular Biology, 2011, 18, 283-287.	3.6	112
170	EROS: Better than SAXS!. Structure, 2011, 19, 3-4.	1.6	10
171	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
172	Ouabain Binding Site in a Functioning Na+/K+ ATPase. Journal of Biological Chemistry, 2011, 286, 38177-38183.	1.6	50
173	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.	3.3	27
174	Ion selectivity in channels and transporters. Journal of General Physiology, 2011, 137, 415-426.	0.9	142
175	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
176	Using electronic polarization from the internal continuum (EPIC) for intermolecular interactions. Journal of Computational Chemistry, 2010, 31, 811-824.	1.5	8
177	Simulation of Osmotic Pressure in Concentrated Aqueous Salt Solutions. Journal of Physical Chemistry Letters, 2010, 1, 183-189.	2.1	266
178	Structural Dynamics of the Magnesium-Bound Conformation of CorA in a Lipid Bilayer. Structure, 2010, 18, 868-878.	1.6	30
179	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.	1.1	16
180	Structural basis for the coupling between activation and inactivation gates in K+ channels. Nature, 2010, 466, 272-275.	13.7	267

#	Article	IF	Citations
181	Perspectives on: Molecular dynamics and computational methods. Journal of General Physiology, 2010, 135, 547-548.	0.9	13
182	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
183	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.	3.3	46
184	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.	3.3	31
185	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
186	Assessing the accuracy of approximate treatments of ion hydration based on primitive quasichemical theory. Journal of Chemical Physics, 2010, 132, 234101.	1.2	24
187	A Combined Experimental and Theoretical Study of Ion Solvation in Liquid N-Methylacetamide. Journal of the American Chemical Society, 2010, 132, 10847-10856.	6.6	35
188	Calculation of the Gating Charge for the Kv1.2 Voltage-Activated Potassium Channel. Biophysical Journal, 2010, 98, 2189-2198.	0.2	135
189	Exploring the Ion Selectivity Properties of a Large Number of Simplified Binding Site Models. Biophysical Journal, 2010, 98, 2877-2885.	0.2	29
190	Voltage Profile along the Permeation Pathway of an Open Channel. Biophysical Journal, 2010, 99, 2863-2869.	0.2	18
191	RNA Structure Determination Using SAXS Data. Journal of Physical Chemistry B, 2010, 114, 10039-10048.	1.2	58
192	Absolute Binding Free Energy Calculations of Sparsomycin Analogs to the Bacterial Ribosome. Journal of Physical Chemistry B, 2010, 114, 9525-9539.	1.2	50
193	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.	1.2	38
194	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.	1.2	37
195	Energetics of Double-Ion Occupancy in the Gramicidin A Channel. Journal of Physical Chemistry B, 2010, 114, 13881-13888.	1.2	15
196	Cation-selective Pathway of OmpF Porin Revealed by Anomalous X-ray Diffraction. Journal of Molecular Biology, 2010, 396, 293-300.	2.0	29
197	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
198	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

#	Article	IF	Citations
199	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
200	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
201	Perspectives on: Molecular dynamics and computational methods. Journal of Cell Biology, 2010, 189, i16-i16.	2.3	0
202	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.	3.3	82
203	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
204	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.	0.9	36
205	Molecular modeling and dynamics studies with explicit inclusion of electronic polarizability: theory and applications. Theoretical Chemistry Accounts, 2009, 124, 11-28.	0.5	314
206	Binding specificity of SH2 domains: Insight from free energy simulations. Proteins: Structure, Function and Bioinformatics, 2009, 74, 996-1007.	1.5	46
207	Structure and electrostatic property of cytoplasmic domain of ZntB transporter. Protein Science, 2009, 18, 2043-2052.	3.1	15
208	Computations of Standard Binding Free Energies with Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2009, 113, 2234-2246.	1.2	481
209	Hydration Number, Topological Control, and Ion Selectivity. Journal of Physical Chemistry B, 2009, 113, 8725-8730.	1.2	34
210	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
211	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.	2.3	18
212	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
213	Force Field Bias in Protein Folding Simulations. Biophysical Journal, 2009, 96, 3772-3780.	0.2	185
214	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
215	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
216	On the Utilization of Energy Minimization to the Study of Ion Selectivity. Biophysical Journal, 2009, 97, L15-L17.	0.2	17

#	Article	IF	Citations
217	Molecular Dynamics Study of a Polymeric Reverse Osmosis Membrane. Journal of Physical Chemistry B, 2009, 113, 10177-10182.	1.2	139
218	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
219	Many-Body Polarization Effects and the Membrane Dipole Potential. Journal of the American Chemical Society, 2009, 131, 2760-2761.	6.6	98
220	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
221	Flexibility and charge asymmetry in the activation loop of Src tyrosine kinases. Proteins: Structure, Function and Bioinformatics, 2009, 74, 378-389.	1.5	38
222	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
223	Computation of binding free energy with molecular dynamics and grand canonical Monte Carlo simulations. Journal of Chemical Physics, 2008, 128, 115103.	1.2	123
224	Structural Refinement of Membrane Proteins by Restrained Molecular Dynamics and Solvent Accessibility Data. Biophysical Journal, 2008, 95, 5349-5361.	0.2	23
225	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
226	Three-Dimensional Architecture of Membrane-Embedded MscS in the Closed Conformation. Journal of Molecular Biology, 2008, 378, 55-70.	2.0	82
227	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
228	On the origin of the electrostatic potential difference at a liquid-vacuum interface. Journal of Chemical Physics, 2008, 129, 234706.	1.2	88
229	The Membrane Potential and its Representation by a Constant Electric Field in Computer Simulations. Biophysical Journal, 2008, 95, 4205-4216.	0.2	188
230	Accurate Molecular Polarizabilities Based on Continuum Electrostatics. Journal of Chemical Theory and Computation, 2008, 4, 1480-1493.	2.3	18
231	Understanding the Dielectric Properties of Liquid Amides from a Polarizable Force Field. Journal of Physical Chemistry B, 2008, 112, 3509-3521.	1.2	122
232	Finding Transition Pathways Using the String Method with Swarms of Trajectories. Journal of Physical Chemistry B, 2008, 112, 3432-3440.	1.2	313
233	Using Markov Models to Simulate Electron Spin Resonance Spectra from Molecular Dynamics Trajectories. Journal of Physical Chemistry B, 2008, 112, 11014-11027.	1.2	47
234	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.	0.9	27

#	Article	IF	Citations
235	Building Markov state models along pathways to determine free energies and rates of transitions. Journal of Chemical Physics, 2008, 129, 064107.	1.2	137
236	PBEQ-Solver for online visualization of electrostatic potential of biomolecules. Nucleic Acids Research, 2008, 36, W270-W275.	6.5	194
237	Simulating electron spin resonance spectra of nitroxide spin labels from molecular dynamics and stochastic trajectories. Journal of Chemical Physics, 2008, 128, 165106.	1.2	55
238	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.	1.2	21
239	Computing conformational free energy by deactivated morphing. Journal of Chemical Physics, 2008, 129, 134102.	1.2	23
240	Src Kinase Conformational Activation: Thermodynamics, Pathways, and Mechanisms. PLoS Computational Biology, 2008, 4, e1000047.	1.5	91
241	Long-pore Electrostatics in Inward-rectifier Potassium Channels. Journal of General Physiology, 2008, 132, 613-632.	0.9	46
242	Chapter 13 A Brief Introduction to Voltage-Gated K+ Channels. Current Topics in Membranes, 2008, , 369-384.	0.5	2
243	What Can Be Deduced about the Structure of Shaker from Available Data?. Novartis Foundation Symposium, 2008, , 84-108.	1.2	6
244	Lonely Arginine Seeks Friendly Environment. Journal of General Physiology, 2007, 130, 233-236.	0.9	32
245	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
246	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
247	Closing In on the Resting State of the Shaker K+ Channel. Neuron, 2007, 56, 124-140.	3.8	270
248	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
249	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
250	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
251	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
252	Dynamics of the Kv1.2 Voltage-Gated K+ Channel in a Membrane Environment. Biophysical Journal, 2007, 93, 3070-3082.	0.2	138

#	Article	IF	Citations
253	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
254	Characterization of conformational equilibria through Hamiltonian and temperature replica-exchange simulations: Assessing entropic and environmental effects. Journal of Computational Chemistry, 2007, 28, 1634-1647.	1.5	44
255	Anatomy of a structural pathway for activation of the catalytic domain of Src kinase Hck. Proteins: Structure, Function and Bioinformatics, 2007, 67, 1096-1112.	1.5	39
256	A proton-controlled check valve for sodium ion transport. Nature Chemical Biology, 2007, 3, 609-610.	3.9	2
257	Molecular driving forces determining potassium channel slow inactivation. Nature Structural and Molecular Biology, 2007, 14, 1062-1069.	3.6	216
258	The Free Energy Landscapes Governing Conformational Changes in a Glutamate Receptor Ligand-Binding Domain. Structure, 2007, 15, 1203-1214.	1.6	104
259	Gramicidin Channels: Versatile Tools. , 2007, , 33-80.		14
260	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
261	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
262	Absolute Binding Free Energy Calculations Using Molecular Dynamics Simulations with Restraining Potentials. Biophysical Journal, 2006, 91, 2798-2814.	0.2	316
263	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
264	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
265	Dissecting the Coupling between the Voltage Sensor and Pore Domains. Neuron, 2006, 52, 568-569.	3.8	10
266	Molecular determinants of gating at the potassium-channel selectivity filter. Nature Structural and Molecular Biology, 2006, 13, 311-318.	3.6	399
267	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
268	Ion selectivity in potassium channels. Biophysical Chemistry, 2006, 124, 279-291.	1.5	174
269	A polarizable model of water for molecular dynamics simulations of biomolecules. Chemical Physics Letters, 2006, 418, 245-249.	1.2	548
270	Modeling the structure of the StART domains of MLN64 and StAR proteins in complex with cholesterol. Journal of Lipid Research, 2006, 47, 2614-2630.	2.0	101

#	Article	IF	Citations
271	Extracellular Blockade of Potassium Channels by TEA+: The Tip of the Iceberg?. Journal of General Physiology, 2006, 128, 635-636.	0.9	4
272	Gating charge displacement in voltage-gated ion channels involves limited transmembrane movement. Nature, 2005, 436, 852-856.	13.7	263
273	A Gate in the Selectivity Filter of Potassium Channels. Structure, 2005, 13, 591-600.	1.6	190
274	One Channel: Open and Closed. Structure, 2005, 13, 1398-1400.	1.6	6
275	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.	1.6	45
276	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.	1.6	42
277	Gramicidin Channels. IEEE Transactions on Nanobioscience, 2005, 4, 10-20.	2.2	115
278	Ion Conduction and Selectivity in K+ Channels. Annual Review of Biophysics and Biomolecular Structure, 2005, 34, 153-171.	18.3	167
279	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
280	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
281	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
282	Electrostatics of the Intracellular Vestibule of K+ Channels. Journal of Molecular Biology, 2005, 354, 272-288.	2.0	58
283	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.	2.0	83
284	The Art of Dissecting the Function of a Potassium Channel. Neuron, 2005, 47, 777-778.	3.8	5
285	Rapid Intracellular TEA Block of the KcsA Potassium Channel. Biophysical Journal, 2005, 88, 1018-1029.	0.2	48
286	Molecular Dynamics Study of Hydration in Ethanolâ^'Water Mixtures Using a Polarizable Force Fieldâ€. Journal of Physical Chemistry B, 2005, 109, 6705-6713.	1.2	275
287	Grand canonical Monte Carlo simulations of water in protein environments. Journal of Chemical Physics, 2004, 121, 6392-6400.	1.2	112
288	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

#	Article	IF	Citations
289	Theoretical and computational models of biological ion channels. Quarterly Reviews of Biophysics, 2004, 37, 15-103.	2.4	362
290	Control of ion selectivity in potassium channels by electrostatic and dynamic properties of carbonyl ligands. Nature, 2004, 431, 830-834.	13.7	528
291	Molecular Basis of Proton Blockage in Aquaporins. Structure, 2004, 12, 65-74.	1.6	142
292	Computational Studies of Membrane Channels. Structure, 2004, 12, 1343-1351.	1.6	136
293	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.	0.2	179
294	Electrostatics of Ion Stabilization in a ClC Chloride Channel Homologue from Escherichia coli. Journal of Molecular Biology, 2004, 339, 981-1000.	2.0	111
295	Structural Determinants of Proton Blockage in Aquaporins. Journal of Molecular Biology, 2004, 343, 493-510.	2.0	105
296	Critical assessment of a proposed model of Shaker. FEBS Letters, 2004, 564, 257-263.	1.3	35
297	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
298	On the Importance of Atomic Fluctuations, Protein Flexibility, and Solvent in Ion Permeation. Journal of General Physiology, 2004, 124, 679-690.	0.9	141
299	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
300	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
301	Atomic Proximity between S4 Segment and Pore Domain in Shaker Potassium Channels. Neuron, 2003, 39, 467-481.	3.8	179
302	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.	3.3	91
303	Cysteine Mutagenesis and Computer Modeling of the S6 Region of an Intermediate Conductance IKCa Channel. Journal of General Physiology, 2002, 120, 99-116.	0.9	23
304	Atomic Radii for Continuum Electrostatics Calculations on Nucleic Acids. Journal of Physical Chemistry B, 2002, 106, 11026-11035.	1.2	69
305	Computational Studies of the Gramicidin Channel. Accounts of Chemical Research, 2002, 35, 366-375.	7.6	131
306	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

#	Article	IF	Citations
307	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.	2.0	54
308	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
309	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
310	The Ionization State and the Conformation of Glu-71 in the KcsA K+ Channel. Biophysical Journal, 2002, 82, 772-780.	0.2	85
311	Imaging the Electrostatic Potential of Transmembrane Channels: Atomic Probe Microscopy of OmpF Porin. Biophysical Journal, 2002, 82, 1667-1676.	0.2	90
312	On the Potential Functions used in Molecular Dynamics Simulations of Ion Channels. Biophysical Journal, 2002, 82, 1681-1684.	0.2	76
313	Molecular Mechanism of H+ Conduction in the Single-File Water Chain of the Gramicidin Channel. Biophysical Journal, 2002, 82, 2304-2316.	0.2	250
314	A bas les barriÃ¨resâ€¦ dâ€™Ã©nergie dans les canaux potassiquesÂ!. Medecine/Sciences, 2002, 18, 605-609.	0.0	1
315	Theoretical and computational models of ion channels. Current Opinion in Structural Biology, 2002, 12, 182-189.	2.6	109
316	From Sequence to Structure and Function. , 2002, , 141-148.		0
317	What can be deduced about the structure of Shaker from available data?. Novartis Foundation Symposium, 2002, 245, 84-101; discussion 101-8, 165-8.	1.2	4
318	Lipid-Mediated Interactions between Intrinsic Membrane Proteins: Dependence on Protein Size and Lipid Composition. Biophysical Journal, 2001, 81, 276-284.	0.2	82
319	Framework Model For Single Proton Conduction through Gramicidin. Biophysical Journal, 2001, 80, 12-30.	0.2	42
320	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
321	Energetics of ion conduction through the K+ channel. Nature, 2001, 414, 73-77.	13.7	745
322	Extracellular Blockade of K+ Channels by Tea. Journal of General Physiology, 2001, 118, 207-218.	0.9	71
323	Implicit Solvent Models. , 2001, , .		11
324	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.	1.2	49

#	Article	IF	Citations
325	A Grand Canonical Monte Carloâ€“Brownian Dynamics Algorithm for Simulating Ion Channels. Biophysical Journal, 2000, 79, 788-801.	0.2	226
326	A Combined Molecular Dynamics and Diffusion Model of Single Proton Conduction through Gramicidin. Biophysical Journal, 2000, 79, 2840-2857.	0.2	65
327	Lipid-Mediated Interactions between Intrinsic Membrane Proteins: A Theoretical Study Based on Integral Equations. Biophysical Journal, 2000, 79, 2867-2879.	0.2	47
328	Molecular Dynamics of the KcsA K+ Channel in a Bilayer Membrane. Biophysical Journal, 2000, 78, 2900-2917.	0.2	314
329	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
330	Free Energy Simulations:â€‰ Thermodynamic Reversibility and Variability. Journal of Physical Chemistry B, 2000, 104, 5179-5190.	1.2	32
331	Ion Channels, Permeation, and Electrostatics: Insight into the Function of KcsA. Biochemistry, 2000, 39, 13295-13306.	1.2	167
332	Efficient calculation of two-dimensional adiabatic and free energy maps: Application to the isomerization of the C13?C14 and C15?N16 bonds in the retinal of bacteriorhodopsin. Journal of Computational Chemistry, 1999, 20, 1644-1658.	1.5	28
333	Protein inclusion in lipid membranes: A theory based on the hypernetted chain integral equation. Faraday Discussions, 1999, 111, 165-172.	1.6	26
334	Statistical Mechanical Equilibrium Theory of Selective Ion Channels. Biophysical Journal, 1999, 77, 139-153.	0.2	130
335	Proton Wires Are Different. Biophysical Journal, 1999, 77, 2331-2332.	0.2	2
336	Simulation Analysis of the Retinal Conformational Equilibrium in Dark-Adapted Bacteriorhodopsin. Biophysical Journal, 1999, 76, 1909-1917.	0.2	33
337	The Binding Site of Sodium in the Gramicidin A Channel. Novartis Foundation Symposium, 1999, 225, 113-127.	1.2	2
338	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
339	Molecular dynamics study of calbindin D9k in the apo and singly and doubly calcium-loaded states. , 1998, 33, 265-284.		69
340	Free Energy Profiles for H+ Conduction along Hydrogen-Bonded Chains of Water Molecules. Biophysical Journal, 1998, 75, 33-40.	0.2	199
341	Molecular Dynamics Simulation of Melittin in a Dimyristoylphosphatidylcholine Bilayer Membrane. Biophysical Journal, 1998, 75, 1603-1618.	0.2	209
342	Molecular Dynamics Simulations of Ion Channels: How Far Have We Gone and Where Are We Heading?. Biophysical Journal, 1998, 74, 2744-2745.	0.2	12

#	Article	IF	Citations
343	Theoretical studies of activated processes in biological ion channels. , 1998, , .		6
344	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
345	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
346	Interaction of K+with a Phospholipid Bilayer:Â A Molecular Dynamics Study. Journal of Physical Chemistry B, 1997, 101, 6066-6072.	1.2	24
347	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
348	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.	2.0	69
349	A potential function for computer simulation studies of proton transfer in acetylacetone. Journal of Computational Chemistry, 1997, 18, 368-380.	1.5	43
350	Mixing quantum-classical molecular dynamics methods applied to intramolecular proton transfer in acetylacetone. Journal of Computational Chemistry, 1997, 18, 1760-1772.	1.5	18
351	Solvation of complex molecules in a polar liquid: An integral equation theory. Journal of Chemical Physics, 1996, 104, 8678-8689.	1.2	168
352	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
353	Theoretical Study of H+Translocation along a Model Proton Wire. The Journal of Physical Chemistry, 1996, 100, 2519-2527.	2.9	122
354	Molecular Dynamics of Pf1 Coat Protein in a Phospholipid Bilayer. , 1996, , 555-587.		12
355	Dominant solvation effects from the primary shell of hydration: Approximation for molecular dynamics simulations. Biopolymers, 1995, 35, 171-178.	1.2	68
356	Quantum effects on the structure and energy of a protonated linear chain of hydrogen-bonded water molecules. Chemical Physics Letters, 1995, 234, 416-424.	1.2	63
357	The backbone 15N chemical shift tensor of the gramicidin channel. A molecular dynamics and density functional study. Chemical Physics Letters, 1995, 239, 186-194.	1.2	31
358	The calculation of the potential of mean force using computer simulations. Computer Physics Communications, 1995, 91, 275-282.	3.0	1,496
359	Potential energy function for cation-peptide interactions: Anab initio study. Journal of Computational Chemistry, 1995, 16, 690-704.	1.5	56
360	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

#	Article	IF	Citations
361	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
362	Finite representation of an infinite bulk system: Solvent boundary potential for computer simulations. Journal of Chemical Physics, 1994, 100, 9050-9063.	1.2	911
363	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.	1.2	47
364	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.	6.6	118
365	Ion transport in a gramicidin-like channel: dynamics and mobility. The Journal of Physical Chemistry, 1991, 95, 4856-4868.	2.9	171
366	Solvation thermodynamics: An approach from analytic temperature derivatives. Journal of Chemical Physics, 1990, 92, 5020-5033.	1.2	132
367	Spatial dependence of timeâ€dependent friction for pair diffusion in a simple fluid. Journal of Chemical Physics, 1990, 93, 6804-6812.	1.2	66
368	Molecular basis for the Born model of ion solvation. The Journal of Physical Chemistry, 1990, 94, 4683-4688.	2.9	229
369	Theory of Transport in Ion Channels. , 0, , 133-169.		4
370	Free Energy Methods in Drug Discoveryâ€"Introduction. ACS Symposium Series, 0, , 1-38.	0.5	24