

# Benoît 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	A Companion Guide to the String Method with Swarms of Trajectories: Characterization, Performance, and Pitfalls. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 1406-1422.	2.3	14
2	Challenges and Advantages of Accounting for Backbone Flexibility in Prediction of Protein-Protein Complexes. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2016-2032.	2.3	2
3	Engineering of a synthetic antibody fragment for structural and functional studies of K <sup>+</sup> channels. <i>Journal of General Physiology</i> , 2022, 154, .	0.9	0
4	A distinct mechanism of C-type inactivation in the Kv-like KcsA mutant E71V. <i>Nature Communications</i> , 2022, 13, 1574.	5.8	11
5	Accurate determination of protein:ligand standard binding free energies from molecular dynamics simulations. <i>Nature Protocols</i> , 2022, 17, 1114-1141.	5.5	56
6	Transition rate theory, spectral analysis, and reactive paths. <i>Journal of Chemical Physics</i> , 2022, 156, 134111.	1.2	20
7	Metal-responsive regulation of enzyme catalysis using genetically encoded chemical switches. <i>Nature Communications</i> , 2022, 13, 1864.	5.8	15
8	Hazardous Shortcuts in Standard Binding Free Energy Calculations. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 6250-6258.	2.1	10
9	Computational Assessment of Protein-Protein Binding Specificity within a Family of Synaptic Surface Receptors. <i>Journal of Physical Chemistry B</i> , 2022, 126, 7510-7527.	1.2	6
10	Molecular Dynamics Simulations Based on Polarizable Models Show that Ion Permeation Interconverts between Different Mechanisms as a Function of Membrane Thickness. <i>Journal of Physical Chemistry B</i> , 2021, 125, 1020-1035.	1.2	12
11	Polarization Effects in Water-Mediated Selective Cation Transport across a Narrow Transmembrane Channel. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 1726-1741.	2.3	26
12	A critical perspective on Markov state model treatments of protein-protein association using coarse-grained simulations. <i>Journal of Chemical Physics</i> , 2021, 154, 084101.	1.2	17
13	Elusive Intermediate State Key in the Conversion of ATP Hydrolysis into Useful Work Driving the Ca <sup>2+</sup> Pump SERCA. <i>Journal of Physical Chemistry B</i> , 2021, 125, 2921-2928.	1.2	3
14	Classical molecular dynamics. <i>Journal of Chemical Physics</i> , 2021, 154, 100401.	1.2	28
15	Synthesis, Characterization, and Simulation of Four-Armed Megamolecules. <i>Biomacromolecules</i> , 2021, 22, 2363-2372.	2.6	4
16	Crystal structure of an archaeal CorB magnesium transporter. <i>Nature Communications</i> , 2021, 12, 4028.	5.8	23
17	Editorial: Advances in computational molecular biophysics. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2021, 1865, 129888.	1.1	0
18	The breakthrough of a quantum chemist by classical dynamics: Martin Karplus and the birth of computer simulations of chemical reactions. <i>European Physical Journal H</i> , 2021, 46, 1.	0.5	1

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19	Virtual Issue on Ion Channels and Ion Permeation. Journal of Physical Chemistry B, 2021, 125, 7575-7577.	1.2	1
20	String Method with Swarms-of-Trajectories, Mean Drifts, Lag Time, and Commitor. Journal of Physical Chemistry A, 2021, 125, 7558-7571.	1.1	24
21	Engineering Dirhodium Artificial Metalloenzymes for Diazo Coupling Cascade Reactions**. Angewandte Chemie - International Edition, 2021, 60, 23672-23677.	7.2	10
22	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
23	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
24	Computational Modeling and Simulations of Biomolecular Systems. , 2021, , .		6
25	Mechanism of C-type inactivation in the hERG potassium channel. Science Advances, 2021, 7, .	4.7	26
26	Frontispiz: Engineering Dirhodium Artificial Metalloenzymes for Diazo Coupling Cascade Reactions. Angewandte Chemie, 2021, 133, .	1.6	0
27	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
28	Tyrosine kinases: complex molecular systems challenging computational methodologies. European Physical Journal B, 2021, 94, 1.	0.6	3
29	Frontispiece: Engineering Dirhodium Artificial Metalloenzymes for Diazo Coupling Cascade Reactions. Angewandte Chemie - International Edition, 2021, 60, .	7.2	0
30	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
31	Quantum Chemical Methods for Modeling Covalent Modification of Biological Thiols. Journal of Computational Chemistry, 2020, 41, 427-438.	1.5	31
32	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
33	Barium blockade of the KcsA channel in open and closed conformation datasets. Data in Brief, 2020, 32, 106135.	0.5	1
34	Open and Closed Structures of a Barium-Blocked Potassium Channel. Journal of Molecular Biology, 2020, 432, 4783-4798.	2.0	14
35	Continuum Electrostatic Behavior of a 3D-RISM Theory. Journal of Physical Chemistry B, 2020, 124, 7444-7451.	1.2	3
36	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

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37	Scalable molecular dynamics on CPU and GPU architectures with NAMD. <i>Journal of Chemical Physics</i> , 2020, 153, 044130.	1.2	1,548
38	CHARMM-GUI Free Energy Calculator for Absolute and Relative Ligand Solvation and Binding Free Energy Simulations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7207-7218.	2.3	57
39	Statistical mechanics of polarizable force fields based on classical Drude oscillators with dynamical propagation by the dual-thermostat extended Lagrangian. <i>Journal of Chemical Physics</i> , 2020, 153, 114108.	1.2	11
40	Diversity of Long-Lived Intermediates along the Binding Pathway of Imatinib to Abl Kinase Revealed by MD Simulations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7852-7865.	2.3	14
41	pKa Calculations with the Polarizable Drude Force Field and Poisson-Boltzmann Solvation Model. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 4655-4668.	2.3	14
42	Glycine substitution in SH3-SH2 connector of Hck tyrosine kinase causes population shift from assembled to disassembled state. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2020, 1864, 129604.	1.1	3
43	Characteristics of Impactful Computational Contributions to <i>The Journal of Physical Chemistry B</i> . <i>Journal of Physical Chemistry B</i> , 2020, 124, 5093-5094.	1.2	3
44	Further Optimization and Validation of the Classical Drude Polarizable Protein Force Field. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3221-3239.	2.3	53
45	Biochemical patterns of antibody polyreactivity revealed through a bioinformatics-based analysis of CDR loops. <i>ELife</i> , 2020, 9, .	2.8	29
46	Computing Relative Binding Affinity of Ligands to Receptor: An Effective Hybrid Single-Dual-Topology Free-Energy Perturbation Approach in NAMD. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3794-3802.	2.5	52
47	String Method for Protein-Protein Binding Free-Energy Calculations. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5829-5844.	2.3	33
48	Molecular Dynamics Simulations of Ionic Liquids and Electrolytes Using Polarizable Force Fields. <i>Chemical Reviews</i> , 2019, 119, 7940-7995.	23.0	386
49	Crystal Structure and Conformational Dynamics of <i>Pyrococcus furiosus</i> Prolyl Oligopeptidase. <i>Biochemistry</i> , 2019, 58, 1616-1626.	1.2	19
50	Calculating the Effect of Membrane Thickness on the Lifetime of the Gramicidin A Channel: A Landmark. <i>Biophysical Journal</i> , 2019, 117, 1779-1780.	0.2	0
51	Shifts in the selectivity filter dynamics cause modal gating in K <sup>+</sup> channels. <i>Nature Communications</i> , 2019, 10, 123.	5.8	66
52	<sup>1</sup> H, <sup>15</sup> N, and <sup>13</sup> C resonance assignments of the intrinsically disordered SH4 and Unique domains of Hck. <i>Biomolecular NMR Assignments</i> , 2019, 13, 71-74.	0.4	3
53	Predicting the Conformational Variability of Abl Tyrosine Kinase using Molecular Dynamics Simulations and Markov State Models. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2721-2732.	2.3	47
54	Polarizable Force Field for Molecular Ions Based on the Classical Drude Oscillator. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 993-1004.	2.5	45

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55	A Catalytically Disabled Double Mutant of Src Tyrosine Kinase Can Be Stabilized into an Active-Like Conformation. <i>Journal of Molecular Biology</i> , 2018, 430, 881-889.	2.0	10
56	Graphical Theoretic Analysis of Monomethyl Phosphate Clustering in Ionic Solutions. <i>Journal of Physical Chemistry B</i> , 2018, 122, 1484-1494.	1.2	46
57	Enhanced configurational sampling with hybrid non-equilibrium molecular dynamics Monte Carlo propagator. <i>Journal of Chemical Physics</i> , 2018, 148, 014101.	1.2	26
58	Optimized Lennard-Jones Parameters for Druglike Small Molecules. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3121-3131.	2.3	44
59	Modeling induction phenomena in amino acid cation- $\pi$ interactions. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	14
60	Reproducibility of Free Energy Calculations across Different Molecular Simulation Software Packages. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 5567-5582.	2.3	66
61	Amphiphile-Induced Phase Transition of Liquid Crystals at Aqueous Interfaces. <i>ACS Applied Materials &amp; Interfaces</i> , 2018, 10, 37618-37624.	4.0	23
62	Reduced Free Energy Perturbation/Hamiltonian Replica Exchange Molecular Dynamics Method with Unbiased Alchemical Thermodynamic Axis. <i>Journal of Physical Chemistry B</i> , 2018, 122, 9435-9442.	1.2	33
63	Proton Countertransport and Coupled Gating in the Sarcoplasmic Reticulum Calcium Pump. <i>Journal of Molecular Biology</i> , 2018, 430, 5050-5065.	2.0	15
64	Molecular Dynamics of Ion Conduction through the Selectivity Filter of the Na <sup>V</sup> Ab Sodium Channel. <i>Journal of Physical Chemistry B</i> , 2018, 122, 10126-10142.	1.2	26
65	Rapid constriction of the selectivity filter underlies C-type inactivation in the KcsA potassium channel. <i>Journal of General Physiology</i> , 2018, 150, 1408-1420.	0.9	64
66	Classical Drude Polarizable Force Field Model for Methyl Phosphate and Its Interactions with Mg <sup>2+</sup> . <i>Journal of Physical Chemistry A</i> , 2018, 122, 6147-6155.	1.1	23
67	A generalized linear response framework for expanded ensemble and replica exchange simulations. <i>Journal of Chemical Physics</i> , 2018, 149, 072315.	1.2	7
68	Combining the polarizable Drude force field with a continuum electrostatic Poisson-Boltzmann implicit solvation model. <i>Journal of Computational Chemistry</i> , 2018, 39, 1707-1719.	1.5	15
69	Molecular Structure of Canonical Liquid Crystal Interfaces. <i>Journal of the American Chemical Society</i> , 2017, 139, 3841-3850.	6.6	56
70	Conformational Transitions and Alternating-Access Mechanism in the Sarcoplasmic Reticulum Calcium Pump. <i>Journal of Molecular Biology</i> , 2017, 429, 647-666.	2.0	37
71	Equivalence of M- and P-Summation in Calculations of Ionic Solvation Free Energies. <i>Journal of Physical Chemistry A</i> , 2017, 121, 1525-1530.	1.1	15
72	Inversion of the Side-Chain Stereochemistry of Individual Thr or Ile Residues in a Protein Molecule: Impact on the Folding, Stability, and Structure of the ShK Toxin. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 3324-3328.	7.2	17

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73	Perplexing cooperative folding and stability of a low-sequence complexity, polyproline 2 protein lacking a hydrophobic core. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 2241-2246.	3.3	29
74	Tyrosine Kinase Activation and Conformational Flexibility: Lessons from Src-Family Tyrosine Kinases. Accounts of Chemical Research, 2017, 50, 1193-1201.	7.6	53
75	Probing the Effects of Gating on the Ion Occupancy of the K <sup>+</sup> Channel Selectivity Filter Using Two-Dimensional Infrared Spectroscopy. Journal of the American Chemical Society, 2017, 139, 8837-8845.	6.6	30
76	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
77	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
78	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
79	Phosphoantigen-induced conformational change of butyrophilin 3A1 (BTN3A1) and its implication on V $\beta$ 9V $\gamma$ 2 T cell activation. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E7311-E7320.	3.3	90
80	Machine Learning Force Field Parameters from Ab Initio Data. Journal of Chemical Theory and Computation, 2017, 13, 4492-4503.	2.3	105
81	Water Flux Induced Reorientation of Liquid Crystals. ACS Central Science, 2017, 3, 1345-1349.	5.3	9
82	Constant-pH Molecular Dynamics Simulations for Large Biomolecular Systems. Journal of Chemical Theory and Computation, 2017, 13, 5933-5944.	2.3	139
83	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
84	CHARMMâ€“GUI 10 years for biomolecular modeling and simulation. Journal of Computational Chemistry, 2017, 38, 1114-1124.	1.5	224
85	Understanding Atomic-Scale Behavior of Liquid Crystals at Aqueous Interfaces. Journal of Chemical Theory and Computation, 2017, 13, 237-244.	2.3	31
86	Ion channels and ion selectivity. Essays in Biochemistry, 2017, 61, 201-209.	2.1	85
87	The selectivity of the Na <sup>+</sup> /K <sup>+</sup> -pump is controlled by binding site protonation and self-correcting occlusion. ELife, 2016, 5, .	2.8	33
88	Concepts and protocols for electrostatic free energies. Molecular Simulation, 2016, 42, 1090-1101.	0.9	30
89	Efficiency in nonequilibrium molecular dynamics Monte Carlo simulations. Journal of Chemical Physics, 2016, 145, 134109.	1.2	15
90	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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91	Computational study of the W260A activating mutant of Src tyrosine kinase. <i>Protein Science</i> , 2016, 25, 219-230.	3.1	11
92	Transition path theory analysis of c-Src kinase activation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, 9193-9198.	3.3	67
93	Instantaneous ion configurations in the K <sup>+</sup> ion channel selectivity filter revealed by 2D IR spectroscopy. <i>Science</i> , 2016, 353, 1040-1044.	6.0	174
94	Leveraging the Information from Markov State Models To Improve the Convergence of Umbrella Sampling Simulations. <i>Journal of Physical Chemistry B</i> , 2016, 120, 8733-8742.	1.2	14
95	An Empirical Polarizable Force Field Based on the Classical Drude Oscillator Model: Development History and Recent Applications. <i>Chemical Reviews</i> , 2016, 116, 4983-5013.	23.0	434
96	Multi-ion free energy landscapes underscore the microscopic mechanism of ion selectivity in the KcsA channel. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2016, 1858, 1722-1732.	1.4	34
97	Atomic mutagenesis in ion channels with engineered stoichiometry. <i>ELife</i> , 2016, 5, .	2.8	23
98	Implementation of extended Lagrangian dynamics in GROMACS for polarizable simulations using the classical Drude oscillator model. <i>Journal of Computational Chemistry</i> , 2015, 36, 1473-1479.	1.5	79
99	Structural Refinement of Proteins by Restrained Molecular Dynamics Simulations with Non-interacting Molecular Fragments. <i>PLoS Computational Biology</i> , 2015, 11, e1004368.	1.5	26
100	Insights into the molecular foundations of electrical excitation. <i>Journal of Molecular Biology</i> , 2015, 427, 1-2.	2.0	4
101	Simulating the Distance Distribution between Spin-Labels Attached to Proteins. <i>Journal of Physical Chemistry B</i> , 2015, 119, 3901-3911.	1.2	46
102	Representation of Ion-Protein Interactions Using the Drude Polarizable Force-Field. <i>Journal of Physical Chemistry B</i> , 2015, 119, 9401-9416.	1.2	101
103	Computational Study of the $\alpha$ DFG-Flip Conformational Transition in c-Abl and c-Src Tyrosine Kinases. <i>Journal of Physical Chemistry B</i> , 2015, 119, 1443-1456.	1.2	56
104	A Structural Rearrangement of the Na <sup>+</sup> /K <sup>+</sup> -ATPase Traps Ouabain within the External Ion Permeation Pathway. <i>Journal of Molecular Biology</i> , 2015, 427, 1335-1344.	2.0	10
105	Generalized Metropolis acceptance criterion for hybrid non-equilibrium molecular dynamics Monte Carlo simulations. <i>Journal of Chemical Physics</i> , 2015, 142, 024101.	1.2	21
106	Constant-pH Hybrid Nonequilibrium Molecular Dynamics Monte Carlo Simulation Method. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3919-3931.	2.3	82
107	Mechanism of potassium ion uptake by the Na <sup>+</sup> /K <sup>+</sup> -ATPase. <i>Nature Communications</i> , 2015, 6, 7622.	5.8	57
108	Enhanced Sampling of an Atomic Model with Hybrid Nonequilibrium Molecular Dynamics Monte Carlo Simulations Guided by a Coarse-Grained Model. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3572-3583.	2.3	18

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109	Efficient Determination of Free Energy Landscapes in Multiple Dimensions from Biased Umbrella Sampling Simulations Using Linear Regression. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3523-3529.	2.3	23
110	Perspective on computational and structural aspects of kinase discovery from IPK2014. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2015, 1854, 1595-1604.	1.1	4
111	Efficient Determination of Relative Entropy Using Combined Temperature and Hamiltonian Replica-Exchange Molecular Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2234-2244.	2.3	11
112	Quantum Effects in Cation Interactions with First and Second Coordination Shell Ligands in Metalloproteins. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4992-5001.	2.3	42
113	Dynamics transitions at the outer vestibule of the KcsA potassium channel during gating. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 1831-1836.	3.3	51
114	Achieving ergodic sampling using replica-exchange free-energy calculations. <i>Molecular Simulation</i> , 2014, 40, 218-228.	0.9	23
115	Conformational dynamics of ligand-dependent alternating access in LeuT. <i>Nature Structural and Molecular Biology</i> , 2014, 21, 472-479.	3.6	136
116	Exploring the Conformational Transitions of Biomolecular Systems Using a Simple Two-State Anisotropic Network Model. <i>PLoS Computational Biology</i> , 2014, 10, e1003521.	1.5	112
117	<i>Escherichia coli</i> Peptidoglycan Structure and Mechanics as Predicted by Atomic-Scale Simulations. <i>PLoS Computational Biology</i> , 2014, 10, e1003475.	1.5	92
118	Using multiscale preconditioning to accelerate the convergence of iterative molecular calculations. <i>Journal of Chemical Physics</i> , 2014, 140, 184114.	1.2	11
119	Efficient hybrid non-equilibrium molecular dynamics - Monte Carlo simulations with symmetric momentum reversal. <i>Journal of Chemical Physics</i> , 2014, 141, 114107.	1.2	20
120	Locking the Active Conformation of c-Src Kinase through the Phosphorylation of the Activation Loop. <i>Journal of Molecular Biology</i> , 2014, 426, 423-435.	2.0	74
121	Activation pathway of Src kinase reveals intermediate states as targets for drug design. <i>Nature Communications</i> , 2014, 5, 3397.	5.8	300
122	Structural mechanism of voltage-dependent gating in an isolated voltage-sensing domain. <i>Nature Structural and Molecular Biology</i> , 2014, 21, 244-252.	3.6	228
123	Permeation Redux: Thermodynamics and Kinetics of Ion Movement through Potassium Channels. <i>Biophysical Journal</i> , 2014, 106, 1859-1863.	0.2	30
124	Computational Study of Gleevec and G6G Reveals Molecular Determinants of Kinase Inhibitor Selectivity. <i>Journal of the American Chemical Society</i> , 2014, 136, 14753-14762.	6.6	41
125	Recent Advances in Polarizable Force Fields for Macromolecules: Microsecond Simulations of Proteins Using the Classical Drude Oscillator Model. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 3144-3150.	2.1	139
126	CHARMM-GUI PDB Manipulator for Advanced Modeling and Simulations of Proteins Containing Nonstandard Residues. <i>Advances in Protein Chemistry and Structural Biology</i> , 2014, 96, 235-265.	1.0	214



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127	Comparison between Mean Forces and Swarms-of-Trajectories String Methods. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 524-533.	2.3	38
128	Conformational cycle and ion-coupling mechanism of the Na <sup>+</sup> /hydantoin transporter Mhp1. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014, 111, 14752-14757.	3.3	83
129	Nucleotide Regulation of the Structure and Dynamics of G-Actin. <i>Biophysical Journal</i> , 2014, 106, 1710-1720.	0.2	22
130	Quantitative Analysis of the Water Occupancy around the Selectivity Filter of a K <sup>+</sup> Channel in Different Gating Modes. <i>Journal of the American Chemical Society</i> , 2014, 136, 2000-2007.	6.6	70
131	Generalized scalable multiple copy algorithms for molecular dynamics simulations in NAMD. <i>Computer Physics Communications</i> , 2014, 185, 908-916.	3.0	115
132	An Overview of Electrostatic Free Energy Computations for Solutions and Proteins. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2690-2709.	2.3	118
133	Markov State and Diffusive Stochastic Models in Electron Spin Resonance. <i>Advances in Experimental Medicine and Biology</i> , 2014, 797, 115-138.	0.8	3
134	Automated Force Field Parameterization for Nonpolarizable and Polarizable Atomic Models Based on Ab Initio Target Data. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3543-3556.	2.3	212
135	Efficient Determination of Protein-Protein Standard Binding Free Energies from First Principles. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 3789-3798.	2.3	188
136	Simulations of Anionic Lipid Membranes: Development of Interaction-Specific Ion Parameters and Validation Using NMR Data. <i>Journal of Physical Chemistry B</i> , 2013, 117, 10183-10192.	1.2	181
137	Recovery from slow inactivation in K <sup>+</sup> channels is controlled by water molecules. <i>Nature</i> , 2013, 501, 121-124.	13.7	171
138	Computational Analysis of the Binding Specificity of Gleevec to Abl, c-Kit, Lck, and c-Src Tyrosine Kinases. <i>Journal of the American Chemical Society</i> , 2013, 135, 14741-14753.	6.6	49
139	Simulation study of ion pairing in concentrated aqueous salt solutions with a polarizable force field. <i>Faraday Discussions</i> , 2013, 160, 135-149.	1.6	102
140	Polarizable Force Field for Peptides and Proteins Based on the Classical Drude Oscillator. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 5430-5449.	2.3	329
141	A Structural Study of Ion Permeation in OmpF Porin from Anomalous X-ray Diffraction and Molecular Dynamics Simulations. <i>Journal of the American Chemical Society</i> , 2013, 135, 16561-16568.	6.6	23
142	A Polarizable Force Field of Dipalmitoylphosphatidylcholine Based on the Classical Drude Model for Molecular Dynamics Simulations of Lipids. <i>Journal of Physical Chemistry B</i> , 2013, 117, 9142-9160.	1.2	159
143	Kirkwood-Buff analysis of aqueous N-methylacetamide and acetamide solutions modeled by the CHARMM additive and Drude polarizable force fields. <i>Journal of Chemical Physics</i> , 2013, 139, 084509.	1.2	31
144	CHARMM-GUI Ligand Binder for Absolute Binding Free Energy Calculations and Its Application. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 267-277.	2.5	71

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145	The Binding of Antibiotics in OmpF Porin. <i>Structure</i> , 2013, 21, 76-87.	1.6	128
146	Eppur Si Muove! The 2013 Nobel Prize in Chemistry. <i>Structure</i> , 2013, 21, 2102-2105.	1.6	26
147	Six-site polarizable model of water based on the classical Drude oscillator. <i>Journal of Chemical Physics</i> , 2013, 138, 034508.	1.2	103
148	On the statistical equivalence of restrained-ensemble simulations with the maximum entropy method. <i>Journal of Chemical Physics</i> , 2013, 138, 084107.	1.2	166
149	The Theory of Ultra-Coarse-Graining. 1. General Principles. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 2466-2480.	2.3	149
150	Architecture and assembly of the $\gamma$ -positive cell wall. <i>Molecular Microbiology</i> , 2013, 88, 664-672.	1.2	116
151	Restrained-Ensemble Molecular Dynamics Simulations Based on Distance Histograms from Double Electron Resonance Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2013, 117, 4733-4739.	1.2	66
152	Self-Learning Adaptive Umbrella Sampling Method for the Determination of Free Energy Landscapes in Multiple Dimensions. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1885-1895.	2.3	80
153	Standard Binding Free Energies from Computer Simulations: What Is the Best Strategy?. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 794-802.	2.3	298
154	Relative Free Energies for Hydration of Monovalent Ions from QM and QM/MM Simulations. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4165-4175.	2.3	54
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