Beno t Roux

List of Publications by Year in Descending Order

311 papers	36,185 citations	102 h-index	185 g-index
338 ext. papers	41,038 ext. citations	7.3 avg, IF	7.68 L-index

#	Paper	IF	Citations
311	A distinct mechanism of C-type inactivation in the Kv-like KcsA mutant E71V.. *Nature Communications*, **2022**, 13, 1574	17.4	1
310	Accurate determination of protein:ligand standard binding free energies from molecular dynamics simulations.. *Nature Protocols*, **2022**,	18.8	5
309	Transition rate theory, spectral analysis, and reactive paths.. *Journal of Chemical Physics*, **2022**, 156, 134114	3.9	4
308	Metal-responsive regulation of enzyme catalysis using genetically encoded chemical switches.. *Nature Communications*, **2022**, 13, 1864	17.4	1
307	Global Optimization of the Lennard-Jones Parameters for the Drude Polarizable Force Field. *Journal of Chemical Theory and Computation*, **2021**, 17, 7085-7095	6.4	0
306	Tyrosine kinases: complex molecular systems challenging computational methodologies. *European Physical Journal B*, **2021**, 94, 1	1.2	2
305	Elusive Intermediate State Key in the Conversion of ATP Hydrolysis into Useful Work Driving the Ca Pump SERCA. *Journal of Physical Chemistry B*, **2021**, 125, 2921-2928	3.4	2
304	Synthesis, Characterization, and Simulation of Four-Armed Megamolecules. *Biomacromolecules*, **2021**, 22, 2363-2372	6.9	1
303	Crystal structure of an archaeal CorB magnesium transporter. *Nature Communications*, **2021**, 12, 4028	17.4	4
302	The breakthrough of a quantum chemist by classical dynamics: Martin Karplus and the birth of computer simulations of chemical reactions. *European Physical Journal H*, **2021**, 46, 1	0.9	0
301	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	3.4	3
300	Polarization Effects in Water-Mediated Selective Cation Transport across a Narrow Transmembrane Channel. *Journal of Chemical Theory and Computation*, **2021**, 17, 1726-1741	6.4	7
299	A critical perspective on Markov state model treatments of protein-protein association using coarse-grained simulations. *Journal of Chemical Physics*, **2021**, 154, 084101	3.9	2
298	String Method with Swarms-of-Trajectories, Mean Drifts, Lag Time, and Committor. *Journal of Physical Chemistry A*, **2021**, 125, 7558-7571	2.8	7
297	Engineering Dirhodium Artificial Metalloenzymes for Diazo Coupling Cascade Reactions*. *Angewandte Chemie - International Edition*, **2021**, 60, 23672-23677	16.4	3
296	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,	11.5	2
295	Computational study of non-conductive selectivity filter conformations and C-type inactivation in a voltage-dependent potassium channel. *Journal of General Physiology*, **2021**, 153,	3.4	5

294	Mechanism of C-type inactivation in the hERG potassium channel. *Science Advances*, **2021**, 7,	14.3	8
293	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	6.4	6
292	p Calculations with the Polarizable Drude Force Field and Poisson-Boltzmann Solvation Model. *Journal of Chemical Theory and Computation*, **2020**, 16, 4655-4668	6.4	7
291	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	4	2
290	Further Optimization and Validation of the Classical Drude Polarizable Protein Force Field. *Journal of Chemical Theory and Computation*, **2020**, 16, 3221-3239	6.4	22
289	Biochemical patterns of antibody polyreactivity revealed through a bioinformatics-based analysis of CDR loops. *ELife*, **2020**, 9,	8.9	2
288	Quantum Chemical Methods for Modeling Covalent Modification of Biological Thiols. *Journal of Computational Chemistry*, **2020**, 41, 427-438	3.5	18
287	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	6.5	6
286	Barium blockade of the KcsA channel in open and closed conformation datasets. *Data in Brief*, **2020**, 32, 106135	1.2	1
285	Open and Closed Structures of a Barium-Blocked Potassium Channel. *Journal of Molecular Biology*, **2020**, 432, 4783-4798	6.5	6
284	Continuum Electrostatic Behavior of a 3D-RISM Theory. *Journal of Physical Chemistry B*, **2020**, 124, 7444-7451	3.4	2
283	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	6.4	11
282	Scalable molecular dynamics on CPU and GPU architectures with NAMD. *Journal of Chemical Physics* , **2020**, 153, 044130	3.9	483
281	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	6.4	28
280	Statistical mechanics of polarizable force fields based on classical Drude oscillators with dynamical propagation by the dual-thermostat extended Lagrangian. *Journal of Chemical Physics*, **2020**, 153, 114108	3.9	6
279	CHARMM-GUI DEER facilitator for spin-pair distance distribution calculations and preparation of restrained-ensemble molecular dynamics simulations. *Journal of Computational Chemistry*, **2020**, 41, 415-420	3.5	5
278	Molecular Dynamics Simulations of Ionic Liquids and Electrolytes Using Polarizable Force Fields. *Chemical Reviews*, **2019**, 119, 7940-7995	68.1	206
277	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	6.1	29

276	String Method for Protein-Protein Binding Free-Energy Calculations. *Journal of Chemical Theory and Computation*, **2019**, 15, 5829-5844	6.4	17
275	Crystal Structure and Conformational Dynamics of Pyrococcus furiosus Prolyl Oligopeptidase. *Biochemistry*, **2019**, 58, 1616-1626	3.2	10
274	Calculating the Effect of Membrane Thickness on the Lifetime of the Gramicidin A Channel: A Landmark. *Biophysical Journal*, **2019**, 117, 1779-1780	2.9	
273	Shifts in the selectivity filter dynamics cause modal gating in K channels. *Nature Communications*, **2019**, 10, 123	17.4	40
272	H, N, and C resonance assignments of the intrinsically disordered SH4 and Unique domains of Hck. *Biomolecular NMR Assignments*, **2019**, 13, 71-74	0.7	2
271	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	6.4	30
270	Polarizable Force Field for Molecular Ions Based on the Classical Drude Oscillator. *Journal of Chemical Information and Modeling*, **2018**, 58, 993-1004	6.1	27
269	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	6.5	8
268	Graph-Theoretic Analysis of Monomethyl Phosphate Clustering in Ionic Solutions. *Journal of Physical Chemistry B*, **2018**, 122, 1484-1494	3.4	31
267	Enhanced configurational sampling with hybrid non-equilibrium molecular dynamics-Monte Carlo propagator. *Journal of Chemical Physics*, **2018**, 148, 014101	3.9	16
266	Optimized Lennard-Jones Parameters for Druglike Small Molecules. *Journal of Chemical Theory and Computation*, **2018**, 14, 3121-3131	6.4	26
265	Rapid constriction of the selectivity filter underlies C-type inactivation in the KcsA potassium channel. *Journal of General Physiology*, **2018**, 150, 1408-1420	3.4	40
264	Classical Drude Polarizable Force Field Model for Methyl Phosphate and Its Interactions with Mg. *Journal of Physical Chemistry A*, **2018**, 122, 6147-6155	2.8	15
263	A generalized linear response framework for expanded ensemble and replica exchange simulations. *Journal of Chemical Physics*, **2018**, 149, 072315	3.9	6
262	Combining the polarizable Drude force field with a continuum electrostatic Poisson-Boltzmann implicit solvation model. *Journal of Computational Chemistry*, **2018**, 39, 1707-1719	3.5	13
261	Modeling induction phenomena in amino acid cation(pi) interactions. *Theoretical Chemistry Accounts*, **2018**, 137, 1	1.9	11
260	Reproducibility of Free Energy Calculations across Different Molecular Simulation Software Packages. *Journal of Chemical Theory and Computation*, **2018**, 14, 5567-5582	6.4	53
259	Amphiphile-Induced Phase Transition of Liquid Crystals at Aqueous Interfaces. *ACS Applied Materials & Interfaces*, **2018**, 10, 37618-37624	9.5	11

258	Reduced Free Energy Perturbation/Hamiltonian Replica Exchange Molecular Dynamics Method with Unbiased Alchemical Thermodynamic Axis. *Journal of Physical Chemistry B*, **2018**, 122, 9435-9442	3.4	24
257	Proton Countertransport and Coupled Gating in the Sarcoplasmic Reticulum Calcium Pump. *Journal of Molecular Biology*, **2018**, 430, 5050-5065	6.5	10
256	Molecular Dynamics of Ion Conduction through the Selectivity Filter of the NaAb Sodium Channel. *Journal of Physical Chemistry B*, **2018**, 122, 10126-10142	3.4	18
255	Molecular Structure of Canonical Liquid Crystal Interfaces. *Journal of the American Chemical Society*, **2017**, 139, 3841-3850	16.4	44
254	Conformational Transitions and Alternating-Access Mechanism in the Sarcoplasmic Reticulum Calcium Pump. *Journal of Molecular Biology*, **2017**, 429, 647-666	6.5	26
253	Equivalence of M- and P-Summation in Calculations of Ionic Solvation Free Energies. *Journal of Physical Chemistry A*, **2017**, 121, 1525-1530	2.8	12
252	Inversion of the Side-Chain Stereochemistry of Indvidual Thr or Ile Residues in a Protein Molecule: Impact on the Folding, Stability, and Structure of the ShK Toxin. *Angewandte Chemie - International Edition*, **2017**, 56, 3324-3328	16.4	12
251	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	11.5	21
250	Tyrosine Kinase Activation and Conformational Flexibility: Lessons from Src-Family Tyrosine Kinases. *Accounts of Chemical Research*, **2017**, 50, 1193-1201	24.3	37
249	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	16.4	24
248	New Coarse Variables for the Accurate Determination of Standard Binding Free Energies. *Journal of Chemical Theory and Computation*, **2017**, 13, 5173-5178	6.4	30
247	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	11.5	23
246	Drude Polarizable Force Field for Molecular Dynamics Simulations of Saturated and Unsaturated Zwitterionic Lipids. *Journal of Chemical Theory and Computation*, **2017**, 13, 4535-4552	6.4	63
245	Phosphoantigen-induced conformational change of butyrophilin 3A1 (BTN3A1) and its implication on V9V2 T cell activation. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E7311-E7320	11.5	61
244	Machine Learning Force Field Parameters from Ab Initio Data. *Journal of Chemical Theory and Computation*, **2017**, 13, 4492-4503	6.4	73
243	Water Flux Induced Reorientation of Liquid Crystals. *ACS Central Science*, **2017**, 3, 1345-1349	16.8	4
242	Constant-pH Molecular Dynamics Simulations for Large Biomolecular Systems. *Journal of Chemical Theory and Computation*, **2017**, 13, 5933-5944	6.4	84
241	The Activation of c-Src Tyrosine Kinase: Conformational Transition Pathway and Free Energy Landscape. *Journal of Physical Chemistry B*, **2017**, 121, 3352-3363	3.4	27

240	CHARMM-GUI 10 years for biomolecular modeling and simulation. *Journal of Computational Chemistry*, **2017**, 38, 1114-1124	3.5	119
239	Understanding Atomic-Scale Behavior of Liquid Crystals at Aqueous Interfaces. *Journal of Chemical Theory and Computation*, **2017**, 13, 237-244	6.4	23
238	Ion channels and ion selectivity. *Essays in Biochemistry*, **2017**, 61, 201-209	7.6	49
237	Instantaneous ion configurations in the K+ ion channel selectivity filter revealed by 2D IR spectroscopy. *Science*, **2016**, 353, 1040-1044	33.3	142
236	Leveraging the Information from Markov State Models To Improve the Convergence of Umbrella Sampling Simulations. *Journal of Physical Chemistry B*, **2016**, 120, 8733-42	3.4	11
235	An Empirical Polarizable Force Field Based on the Classical Drude Oscillator Model: Development History and Recent Applications. *Chemical Reviews*, **2016**, 116, 4983-5013	68.1	299
234	Multi-ion free energy landscapes underscore the microscopic mechanism of ion selectivity in the KcsA channel. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 1722-32	3.8	25
233	Atomic mutagenesis in ion channels with engineered stoichiometry. *ELife*, **2016**, 5,	8.9	17
232	The selectivity of the Na(+)/K(+)-pump is controlled by binding site protonation and self-correcting occlusion. *ELife*, **2016**, 5,	8.9	20
231	Concepts and protocols for electrostatic free energies. *Molecular Simulation*, **2016**, 42, 1090-1101	2	25
230	Efficiency in nonequilibrium molecular dynamics Monte Carlo simulations. *Journal of Chemical Physics*, **2016**, 145, 134109	3.9	14
229	Multiple Time-Step Dual-Hamiltonian Hybrid Molecular Dynamics - Monte Carlo Canonical Propagation Algorithm. *Journal of Chemical Theory and Computation*, **2016**, 12, 1449-1458	6.4	7
228	Computational study of the W260A activating mutant of Src tyrosine kinase. *Protein Science*, **2016**, 25, 219-30	6.3	10
227	Transition path theory analysis of c-Src kinase activation. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 9193-8	11.5	49
226	Constant-pH Hybrid Nonequilibrium Molecular Dynamics-Monte Carlo Simulation Method. *Journal of Chemical Theory and Computation*, **2015**, 11, 3919-31	6.4	56
225	Mechanism of potassium ion uptake by the Na(+)/K(+)-ATPase. *Nature Communications*, **2015**, 6, 7622	17.4	36
224	Enhanced Sampling of an Atomic Model with Hybrid Nonequilibrium Molecular Dynamics-Monte Carlo Simulations Guided by a Coarse-Grained Model. *Journal of Chemical Theory and Computation*, **2015**, 11, 3572-83	6.4	16
223	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, 3523-9	6.4	17

222	Perspective on computational and structural aspects of kinase discovery from IPK2014. *Biochimica Et Biophysica Acta - Proteins and Proteomics*, **2015**, 1854, 1595-604	4	4
221	Efficient Determination of Relative Entropy Using Combined Temperature and Hamiltonian Replica-Exchange Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2015**, 11, 2234-44	6.4	10
220	Quantum effects in cation interactions with first and second coordination shell ligands in metalloproteins. *Journal of Chemical Theory and Computation*, **2015**, 11, 4992-5001	6.4	36
219	Implementation of extended Lagrangian dynamics in GROMACS for polarizable simulations using the classical Drude oscillator model. *Journal of Computational Chemistry*, **2015**, 36, 1473-9	3.5	60
218	Structural Refinement of Proteins by Restrained Molecular Dynamics Simulations with Non-interacting Molecular Fragments. *PLoS Computational Biology*, **2015**, 11, e1004368	5	19
217	Simulating the distance distribution between spin-labels attached to proteins. *Journal of Physical Chemistry B*, **2015**, 119, 3901-11	3.4	33
216	Representation of Ion-Protein Interactions Using the Drude Polarizable Force-Field. *Journal of Physical Chemistry B*, **2015**, 119, 9401-16	3.4	80
215	Computational study of the "DFG-flip" conformational transition in c-Abl and c-Src tyrosine kinases. *Journal of Physical Chemistry B*, **2015**, 119, 1443-56	3.4	40
214	A structural rearrangement of the Na+/K+-ATPase traps ouabain within the external ion permeation pathway. *Journal of Molecular Biology*, **2015**, 427, 1335-1344	6.5	10
213	Generalized Metropolis acceptance criterion for hybrid non-equilibrium molecular dynamics-Monte Carlo simulations. *Journal of Chemical Physics*, **2015**, 142, 024101	3.9	16
212	Activation pathway of Src kinase reveals intermediate states as targets for drug design. *Nature Communications*, **2014**, 5, 3397	17.4	244
211	Structural mechanism of voltage-dependent gating in an isolated voltage-sensing domain. *Nature Structural and Molecular Biology*, **2014**, 21, 244-52	17.6	173
210	Permeation redux: thermodynamics and kinetics of ion movement through potassium channels. *Biophysical Journal*, **2014**, 106, 1859-63	2.9	21
209	Computational study of Gleevec and G6G reveals molecular determinants of kinase inhibitor selectivity. *Journal of the American Chemical Society*, **2014**, 136, 14753-62	16.4	39
208	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	6.4	111
207	CHARMM-GUI PDB manipulator for advanced modeling and simulations of proteins containing nonstandard residues. *Advances in Protein Chemistry and Structural Biology*, **2014**, 96, 235-65	5.3	96
206	Comparison between Mean Forces and Swarms-of-Trajectories String Methods. *Journal of Chemical Theory and Computation*, **2014**, 10, 524-33	6.4	27
205	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, 14752-7	11.5	61

204	Nucleotide regulation of the structure and dynamics of G-actin. *Biophysical Journal*, **2014**, 106, 1710-20	2.9	16
203	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, 2000-7	16.4	62
202	Generalized Scalable Multiple Copy Algorithms for Molecular Dynamics Simulations in NAMD. *Computer Physics Communications*, **2014**, 185, 908-916	4.2	88
201	An Overview of Electrostatic Free Energy Computations for Solutions and Proteins. *Journal of Chemical Theory and Computation*, **2014**, 10, 2690-709	6.4	103
200	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, 1831-6	11.5	44
199	Achieving ergodic sampling using replica-exchange free-energy calculations. *Molecular Simulation*, **2014**, 40, 218-228	2	19
198	Conformational dynamics of ligand-dependent alternating access in LeuT. *Nature Structural and Molecular Biology*, **2014**, 21, 472-9	17.6	102
197	Exploring the conformational transitions of biomolecular systems using a simple two-state anisotropic network model. *PLoS Computational Biology*, **2014**, 10, e1003521	5	94
196	Escherichia coli peptidoglycan structure and mechanics as predicted by atomic-scale simulations. *PLoS Computational Biology*, **2014**, 10, e1003475	5	66
195	Using multiscale preconditioning to accelerate the convergence of iterative molecular calculations. *Journal of Chemical Physics*, **2014**, 140, 184114	3.9	11
194	Efficient hybrid non-equilibrium molecular dynamics--Monte Carlo simulations with symmetric momentum reversal. *Journal of Chemical Physics*, **2014**, 141, 114107	3.9	18
193	Locking the active conformation of c-Src kinase through the phosphorylation of the activation loop. *Journal of Molecular Biology*, **2014**, 426, 423-35	6.5	62
192	Markov state and diffusive stochastic models in electron spin resonance. *Advances in Experimental Medicine and Biology*, **2014**, 797, 115-38	3.6	3
191	AUTOMATED FORCE FIELD PARAMETERIZATION FOR NON-POLARIZABLE AND POLARIZABLE ATOMIC MODELS BASED ON TARGET DATA. *Journal of Chemical Theory and Computation*, **2013**, 9,	6.4	172
190	Efficient determination of protein-protein standard binding free energies from first principles. *Journal of Chemical Theory and Computation*, **2013**, 9,	6.4	133
189	Simulations of anionic lipid membranes: development of interaction-specific ion parameters and validation using NMR data. *Journal of Physical Chemistry B*, **2013**, 117, 10183-92	3.4	130
188	Recovery from slow inactivation in K+ channels is controlled by water molecules. *Nature*, **2013**, 501, 121-4	40.4	138
187	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, 14741-53	16.4	45

186	Simulation study of ion pairing in concentrated aqueous salt solutions with a polarizable force field. *Faraday Discussions*, **2013**, 160, 135-49; discussion 207-24	3.6	86
185	Force Field for Peptides and Proteins based on the Classical Drude Oscillator. *Journal of Chemical Theory and Computation*, **2013**, 9, 5430-5449	6.4	274
184	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, 16561-8	16.4	15
183	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, 9142-60	3.4	122
182	Kirkwood-Buff analysis of aqueous N-methylacetamide and acetamide solutions modeled by the CHARMM additive and Drude polarizable force fields. *Journal of Chemical Physics*, **2013**, 139, 084509	3.9	29
181	CHARMM-GUI Ligand Binder for absolute binding free energy calculations and its application. *Journal of Chemical Information and Modeling*, **2013**, 53, 267-77	6.1	51
180	The binding of antibiotics in OmpF porin. *Structure*, **2013**, 21, 76-87	5.2	93
179	Eppur si muove! The 2013 Nobel Prize in Chemistry. *Structure*, **2013**, 21, 2102-5	5.2	20
178	Six-site polarizable model of water based on the classical Drude oscillator. *Journal of Chemical Physics*, **2013**, 138, 034508	3.9	92
177	On the statistical equivalence of restrained-ensemble simulations with the maximum entropy method. *Journal of Chemical Physics*, **2013**, 138, 084107	3.9	139
176	The Theory of Ultra-Coarse-Graining. 1. General Principles. *Journal of Chemical Theory and Computation*, **2013**, 9, 2466-80	6.4	114
175	Architecture and assembly of the Gram-positive cell wall. *Molecular Microbiology*, **2013**, 88, 664-72	4.1	85
174	Restrained-ensemble molecular dynamics simulations based on distance histograms from double electron-electron resonance spectroscopy. *Journal of Physical Chemistry B*, **2013**, 117, 4733-9	3.4	56
173	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	6.4	63
172	Standard binding free energies from computer simulations: What is the best strategy?. *Journal of Chemical Theory and Computation*, **2013**, 9, 794-802	6.4	224
171	Relative Free Energies for Hydration of Monovalent Ions from QM and QM/MM Simulations. *Journal of Chemical Theory and Computation*, **2013**, 9, 4165-75	6.4	45
170	Structural refinement from restrained-ensemble simulations based on EPR/DEER data: application to T4 lysozyme. *Journal of Physical Chemistry B*, **2013**, 117, 4740-54	3.4	67
169	QM/MM molecular dynamics simulations of the hydration of Mg(II) and Zn(II) ions. *Canadian Journal of Chemistry*, **2013**, 91, 552-558	0.9	29

168	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, 451-63	3.4	13
167	Molecular dynamics simulations of membrane proteins under asymmetric ionic concentrations. *Journal of General Physiology*, **2013**, 142, 465-75	3.4	38
166	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, 1664-9	11.5	126
165	Web interface for Brownian dynamics simulation of ion transport and its applications to beta-barrel pores. *Journal of Computational Chemistry*, **2012**, 33, 331-9	3.5	38
164	An emerging consensus on voltage-dependent gating from computational modeling and molecular dynamics simulations. *Journal of General Physiology*, **2012**, 140, 587-94	3.4	141
163	Intermediate state trapping of a voltage sensor. *Journal of General Physiology*, **2012**, 140, 635-52	3.4	43
162	Ion binding sites and their representations by reduced models. *Journal of Physical Chemistry B*, **2012** , 116, 6966-79	3.4	16
161	Comment on "Probing the thermodynamics of competitive ion binding using minimum energy structures". *Journal of Physical Chemistry B*, **2012**, 116, 7991-3	3.4	1
160	Constant electric field simulations of the membrane potential illustrated with simple systems. *Biochimica Et Biophysica Acta - Biomembranes*, **2012**, 1818, 294-302	3.8	119
159	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, 3526-35	6.4	162
158	Multi-ion distributions in the cytoplasmic domain of inward rectifier potassium channels. *Biophysical Journal*, **2012**, 103, 434-443	2.9	6
157	Nano-positioning system for structural analysis of functional homomeric proteins in multiple conformations. *Structure*, **2012**, 20, 1629-40	5.2	13
156	Calculation of Free Energy Landscape in Multi-Dimensions with Hamiltonian-Exchange Umbrella Sampling on Petascale Supercomputer. *Journal of Chemical Theory and Computation*, **2012**, 8, 4672-80	6.4	76
155	Molecular Mechanisms of K+ Selectivity in Na/K Pump. *Australian Journal of Chemistry*, **2012**, 65, 448	1.2	6
154	Computational electrophysiology: the molecular dynamics of ion channel permeation and selectivity in atomistic detail. *Biophysical Journal*, **2011**, 101, 755-6	2.9	4
153	In search of a consensus model of the resting state of a voltage-sensing domain. *Neuron*, **2011**, 72, 713-20	13.9	78
152	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	6.4	191
151	Thermodynamic coupling between activation and inactivation gating in potassium channels revealed by free energy molecular dynamics simulations. *Journal of General Physiology*, **2011**, 138, 571-80	3.4	47

150	On the structural basis of modal gating behavior in K(+) channels. *Nature Structural and Molecular Biology*, **2011**, 18, 67-74	17.6	57
149	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	9.6	69
148	Ouabain binding site in a functioning Na+/K+ ATPase. *Journal of Biological Chemistry*, **2011**, 286, 38177-38183	5.4	43
147	Voltage-Gated Ion Channels: The Machines Responsible for the Nerve Impulse **2011**, 231-248		1
146	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, 7417-26	3.4	31
145	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, 3240-5	11.5	18
144	Ion selectivity in channels and transporters. *Journal of General Physiology*, **2011**, 137, 415-26	3.4	127
143	Protonation of key acidic residues is critical for the K+-selectivity of the Na/K pump. *Nature Structural and Molecular Biology*, **2011**, 18, 1159-63	17.6	47
142	Structural basis for the coupling between activation and inactivation gates in K(+) channels. *Nature*, **2010**, 466, 272-5	50.4	227
141	Perspectives on: molecular dynamics and computational methods. *Journal of General Physiology*, **2010**, 135, 547-8	3.4	12
140	Two mechanisms of ion selectivity in protein binding sites. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 20329-34	11.5	69
139	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, 5435-40	11.5	41
138	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, 18718-23	11.5	28
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