Beno t Roux

List of Publications by Citations

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	CHARMM: the biomolecular simulation program. *Journal of Computational Chemistry*, **2009**, 30, 1545-614	3.5	5515
310	The calculation of the potential of mean force using computer simulations. *Computer Physics Communications*, **1995**, 91, 275-282	4.2	1274
309	Finite representation of an infinite bulk system: Solvent boundary potential for computer simulations. *Journal of Chemical Physics*, **1994**, 100, 9050-9063	3.9	796
308	Implicit solvent models. *Biophysical Chemistry*, **1999**, 78, 1-20	3.5	708
307	Energetics of ion conduction through the K+ channel. *Nature*, **2001**, 414, 73-7	50.4	659
306	Extension to the weighted histogram analysis method: combining umbrella sampling with free energy calculations. *Computer Physics Communications*, **2001**, 135, 40-57	4.2	654
305	A simple polarizable model of water based on classical Drude oscillators. *Journal of Chemical Physics*, **2003**, 119, 5185-5197	3.9	584
304	Modeling induced polarization with classical Drude oscillators: Theory and molecular dynamics simulation algorithm. *Journal of Chemical Physics*, **2003**, 119, 3025-3039	3.9	498
303	Scalable molecular dynamics on CPU and GPU architectures with NAMD. *Journal of Chemical Physics* , **2020**, 153, 044130	3.9	483
302	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, 6825-30	11.5	481
301	Continuum solvation model: Computation of electrostatic forces from numerical solutions to the Poisson-Boltzmann equation. *Computer Physics Communications*, **1998**, 111, 59-75	4.2	459
300	Control of ion selectivity in potassium channels by electrostatic and dynamic properties of carbonyl ligands. *Nature*, **2004**, 431, 830-4	50.4	453
299	A polarizable model of water for molecular dynamics simulations of biomolecules. *Chemical Physics Letters*, **2006**, 418, 245-249	2.5	448
298	Computations of standard binding free energies with molecular dynamics simulations. *Journal of Physical Chemistry B*, **2009**, 113, 2234-46	3.4	415
297	An Integral Equation To Describe the Solvation of Polar Molecules in Liquid Water. *Journal of Physical Chemistry B*, **1997**, 101, 7821-7826	3.4	409
296	Molecular determinants of gating at the potassium-channel selectivity filter. *Nature Structural and Molecular Biology*, **2006**, 13, 311-8	17.6	355
295	Atomic Radii for Continuum Electrostatics Calculations Based on Molecular Dynamics Free Energy Simulations. *Journal of Physical Chemistry B*, **1997**, 101, 5239-5248	3.4	352

294	Simulating Monovalent and Divalent Ions in Aqueous Solution Using a Drude Polarizable Force Field. *Journal of Chemical Theory and Computation*, **2010**, 6, 774-786	6.4	336
293	Energetics of ion conduction through the gramicidin channel. *Proceedings of the National Academy of Sciences of the United States of America*, **2004**, 101, 117-22	11.5	335
292	Dynamic coupling between the SH2 and SH3 domains of c-Src and Hck underlies their inactivation by C-terminal tyrosine phosphorylation. *Cell*, **2001**, 105, 115-26	56.2	329
291	Theoretical and computational models of biological ion channels. *Quarterly Reviews of Biophysics*, **2004**, 37, 15-103	7	321
290	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, 3308-22	3.4	320
289	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, 851-69	6.5	312
288	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
287	Molecular dynamics of the KcsA K(+) channel in a bilayer membrane. *Biophysical Journal*, **2000**, 78, 2900-17	4.9	289
286	Molecular modeling and dynamics studies with explicit inclusion of electronic polarizability. Theory and applications. *Theoretical Chemistry Accounts*, **2009**, 124, 11-28	1.9	285
285	Absolute binding free energy calculations using molecular dynamics simulations with restraining potentials. *Biophysical Journal*, **2006**, 91, 2798-814	2.9	284
284	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
283	Finding transition pathways using the string method with swarms of trajectories. *Journal of Physical Chemistry B*, **2008**, 112, 3432-40	3.4	252
282	Structure, energetics, and dynamics of lipid-protein interactions: A molecular dynamics study of the gramicidin A channel in a DMPC bilayer. *Proteins: Structure, Function and Bioinformatics*, **1996**, 24, 92-114	4.2	246
281	Activation pathway of Src kinase reveals intermediate states as targets for drug design. *Nature Communications*, **2014**, 5, 3397	17.4	244
280	Closing in on the resting state of the Shaker K(+) channel. *Neuron*, **2007**, 56, 124-40	13.9	243
279	Determination of Electrostatic Parameters for a Polarizable Force Field Based on the Classical Drude Oscillator. *Journal of Chemical Theory and Computation*, **2005**, 1, 153-68	6.4	237
278	Ions and counterions in a biological channel: a molecular dynamics simulation of OmpF porin from Escherichia coli in an explicit membrane with 1 M KCl aqueous salt solution. *Journal of Molecular Biology*, **2002**, 319, 1177-97	6.5	230
277	Molecular mechanism of H+ conduction in the single-file water chain of the gramicidin channel. *Biophysical Journal*, **2002**, 82, 2304-16	2.9	229

276	Calculation of Standard Binding Free Energies: Aromatic Molecules in the T4 Lysozyme L99A Mutant. *Journal of Chemical Theory and Computation*, **2006**, 2, 1255-73	6.4	228
275	Structural basis for the coupling between activation and inactivation gates in K(+) channels. *Nature*, **2010**, 466, 272-5	50.4	227
274	Gating charge displacement in voltage-gated ion channels involves limited transmembrane movement. *Nature*, **2005**, 436, 852-6	50.4	226
273	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
272	Simulation of Osmotic Pressure in Concentrated Aqueous Salt Solutions. *Journal of Physical Chemistry Letters*, **2010**, 1, 183-189	6.4	208
271	Molecular Dynamics Simulations of Ionic Liquids and Electrolytes Using Polarizable Force Fields. *Chemical Reviews*, **2019**, 119, 7940-7995	68.1	206
270	Generalized solvent boundary potential for computer simulations. *Journal of Chemical Physics*, **2001** , 114, 2924-2937	3.9	206
269	Molecular basis for the Born model of ion solvation. *The Journal of Physical Chemistry*, **1990**, 94, 4683-4688		204
268	Hydration of Amino Acid Side Chains: 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	3.4	196
267	A Grand Canonical Monte Carlo-Brownian dynamics algorithm for simulating ion channels. *Biophysical Journal*, **2000**, 79, 788-801	2.9	192
266	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
265	Molecular driving forces determining potassium channel slow inactivation. *Nature Structural and Molecular Biology*, **2007**, 14, 1062-9	17.6	190
264	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, 8644-8	11.5	189
263	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	6.4	180
262	Multidomain assembled states of Hck tyrosine kinase in solution. *Proceedings of the National Academy of Sciences of the United States of America*, **2010**, 107, 15757-62	11.5	177
261	A gate in the selectivity filter of potassium channels. *Structure*, **2005**, 13, 591-600	5.2	176
260	Structural mechanism of voltage-dependent gating in an isolated voltage-sensing domain. *Nature Structural and Molecular Biology*, **2014**, 21, 244-52	17.6	173
259	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

258	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
257	Control of ion selectivity in LeuT: two Na+ binding sites with two different mechanisms. *Journal of Molecular Biology*, **2008**, 377, 804-18	6.5	160
256	Ion transport in a gramicidin-like channel: dynamics and mobility. *The Journal of Physical Chemistry*, **1991**, 95, 4856-4868		160
255	Importance of hydration and dynamics on the selectivity of the KcsA and NaK channels. *Journal of General Physiology*, **2007**, 129, 135-43	3.4	159
254	Ion channels, permeation, and electrostatics: insight into the function of KcsA. *Biochemistry*, **2000**, 39, 13295-306	3.2	158
253	Molecular dynamics - potential of mean force calculations as a tool for understanding ion permeation and selectivity in narrow channels. *Biophysical Chemistry*, **2006**, 124, 251-67	3.5	155
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251	Ion conduction and selectivity in K(+) channels. *Annual Review of Biophysics and Biomolecular Structure*, **2005**, 34, 153-71		148
250	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, 7904-9	11.5	145
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242	Polarizable empirical force field for aromatic compounds based on the classical drude oscillator. *Journal of Physical Chemistry B*, **2007**, 111, 2873-85	3.4	132
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235	Computational studies of the gramicidin channel. *Accounts of Chemical Research*, **2002**, 35, 366-75	24.3	124
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