Denis Bucher

List of Publications by Citations

27 papers	1,171 citations	18 h-index	29 g-index
29 ext. papers	1,359 ext. citations	5.6 avg, IF	4.39 L-index

#	Paper	IF	Citations
27	Improved Reweighting of Accelerated Molecular Dynamics Simulations for Free Energy Calculation. *Journal of Chemical Theory and Computation*, **2014**, 10, 2677-2689	6.4	225
26	Reaction Mechanism of HIV-1 Protease by Hybrid Car-Parrinello/Classical MD Simulations. *Journal of Physical Chemistry B*, **2004**, 108, 11139-11149	3.4	100
25	Dissociation of NaCl in water from ab initio molecular dynamics simulations. *Journal of Chemical Physics*, **2010**, 132, 114510	3.9	95
24	Accessing a hidden conformation of the maltose binding protein using accelerated molecular dynamics. *PLoS Computational Biology*, **2011**, 7, e1002034	5	92
23	Polarization effects and charge transfer in the KcsA potassium channel. *Biophysical Chemistry*, **2006**, 124, 292-301	3.5	78
22	On the Use of Accelerated Molecular Dynamics to Enhance Configurational Sampling in Ab Initio Simulations. *Journal of Chemical Theory and Computation*, **2011**, 7, 890-897	6.4	67
21	Membranes serve as allosteric activators of phospholipase A2, enabling it to extract, bind, and hydrolyze phospholipid substrates. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, E516-25	11.5	64
20	Coordination numbers of K(+) and Na(+) Ions inside the selectivity filter of the KcsA potassium channel: insights from first principles molecular dynamics. *Biophysical Journal*, **2010**, 98, L47-9	2.9	55
19	The elusive 5′-deoxyadenosyl radical in coenzyme-B12-mediated reactions. *Journal of the American Chemical Society*, **2012**, 134, 1591-9	16.4	48
18	Fluoroketone inhibition of Ca(2+)-independent phospholipase A2 through binding pocket association defined by hydrogen/deuterium exchange and molecular dynamics. *Journal of the American Chemical Society*, **2013**, 135, 1330-7	16.4	41
17	Polarization of water in the first hydration shell of K+ and Ca2+ ions. *Journal of Physical Chemistry B* , **2008**, 112, 10786-90	3.4	35
16	Accelerated Molecular Dynamics Simulations with the AMOEBA Polarizable Force Field on Graphics Processing Units. *Journal of Chemical Theory and Computation*, **2013**, 9, 4684-4691	6.4	32
15	Molecular simulations of ion channels: a quantum chemist's perspective. *Journal of General Physiology*, **2010**, 135, 549-54	3.4	32
14	The protonation state of the Glu-71/Asp-80 residues in the KcsA potassium channel: a first-principles QM/MM molecular dynamics study. *Biophysical Journal*, **2007**, 93, 2315-24	2.9	32
13	Shedding Light on Important Waters for Drug Design: Simulations versus Grid-Based Methods. *Journal of Chemical Information and Modeling*, **2018**, 58, 692-699	6.1	31
12	Insertion of the Ca2+-independent phospholipase A2 into a phospholipid bilayer via coarse-grained and atomistic molecular dynamics simulations. *PLoS Computational Biology*, **2013**, 9, e1003156	5	27
11	Orientational relaxation of water trapped inside C60 fullerenes. *Chemical Physics Letters*, **2012**, 534, 38-42	2.25	24

List of Publications

10	On the importance of ribose orientation in the substrate activation of the coenzyme B12-dependent mutases. *Chemistry - A European Journal*, **2009**, 15, 8578-85	4.8	18
9	Importance of water polarization for ion permeation in narrow pores. *Chemical Physics Letters*, **2009**, 477, 207-210	2.5	18
8	Developing Improved Charge Sets for the Modeling of the KcsA K(+) Channel Using QM/MM Electrostatic Potentials. *Journal of Chemical Theory and Computation*, **2009**, 5, 2173-9	6.4	17
7	Ab Initio Study of Water Polarization in the Hydration Shell of Aqueous Hydroxide: Comparison between Polarizable and Nonpolarizable Water Models. *Journal of Chemical Theory and Computation*, **2010**, 6, 2888-95	6.4	15
6	Dipeptide Aggregation in Aqueous Solution from Fixed Point-Charge Force Fields. *Journal of Chemical Theory and Computation*, **2014**, 10, 1631-1637	6.4	8
5	Exploring the Photophysical Properties of Molecular Systems Using Excited State Accelerated ab Initio Molecular Dynamics. *Journal of Chemical Theory and Computation*, **2012**, 8, 2752-2761	6.4	8
4	Mechanistic Implications of Reductive Co-C Bond Cleavage in B-Dependent Methylmalonyl CoA Mutase. *Journal of Physical Chemistry B*, **2019**, 123, 2210-2216	3.4	4
3	Cryo-EM structural studies of the agonist complexed human TRPV4 ion-channel reveals novel structural rearrangements resulting in an open-conformation		4
2	Insight into Lipopolysaccharide Translocation by Cryo-EM structures of a LptDE Transporter in Complex with Pro-Macrobodies		1
1	Discovery and Optimization of Orally Bioavailable Phthalazone and Cinnolone Carboxylic Acid Derivatives as S1P2 Antagonists against Fibrotic Diseases. *Journal of Medicinal Chemistry*, **2021**, 64, 14557-14586	8.3	0