Denis Bucher

List of Publications by Year
in descending order

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Version: 2024-02-01

26 papers	1,509 citations	430754 18 h-index	580701 25 g-index
29 all docs	29 docs citations	29 times ranked	2148 citing authors

#	Article	IF	Citations
1	Improved Reweighting of Accelerated Molecular Dynamics Simulations for Free Energy Calculation. Journal of Chemical Theory and Computation, 2014, 10, 2677-2689.	2.3	344
2	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.	2.3	116
3	Dissociation of NaCl in water from ab initio molecular dynamics simulations. Journal of Chemical Physics, 2010, 132, 114510.	1.2	111
4	Reaction Mechanism of HIV-1 Protease by Hybrid Car-Parrinello/Classical MD Simulations. Journal of Physical Chemistry B, 2004, 108, 11139-11149.	1.2	106
5	Accessing a Hidden Conformation of the Maltose Binding Protein Using Accelerated Molecular Dynamics. PLoS Computational Biology, 2011, 7, e1002034.	1.5	102
6	Membranes serve as allosteric activators of phospholipase A ₂ , 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.	3.3	85
7	Polarization effects and charge transfer in the KcsA potassium channel. Biophysical Chemistry, 2006, 124, 292-301.	1.5	84
8	Coordination Numbers of K+ and Na+ Ions Inside the Selectivity Filter ofÂtheÂKcsA Potassium Channel: Insights from First Principles MolecularÂDynamics. Biophysical Journal, 2010, 98, L47-L49.	0.2	64
9	The Elusive 5â€²-Deoxyadenosyl Radical in Coenzyme-B₁₂-Mediated Reactions. Journal of the American Chemical Society, 2012, 134, 1591-1599.	6.6	57
10	Fluoroketone Inhibition of Ca²⁺-Independent Phospholipase A₂ through Binding Pocket Association Defined by Hydrogen/Deuterium Exchange and Molecular Dynamics. Journal of the American Chemical Society, 2013, 135, 1330-1337.	6.6	48
11	Polarization of Water in the First Hydration Shell of K+ and Ca2+ Ions. Journal of Physical Chemistry B, 2008, 112, 10786-10790.	1.2	41
12	Shedding Light on Important Waters for Drug Design: Simulations versus Grid-Based Methods. Journal of Chemical Information and Modeling, 2018, 58, 692-699.	2.5	41
13	Accelerated Molecular Dynamics Simulations with the AMOEBA Polarizable Force Field on Graphics Processing Units. Journal of Chemical Theory and Computation, 2013, 9, 4684-4691.	2.3	39
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, 2315-2324.	0.2	38
15	Molecular simulations of ion channels: a quantum chemistâ€™s perspective. Journal of General Physiology, 2010, 135, 549-554.	0.9	35
16	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.	1.5	33
17	Orientational relaxation of water trapped inside C60 fullerenes. Chemical Physics Letters, 2012, 534, 38-42.	1.2	29
18	On the Importance of Ribose Orientation in the Substrate Activation of the Coenzyme B₁₂â€Dependent Mutases. Chemistry - A European Journal, 2009, 15, 8578-8585.	1.7	23

#	Article	IF	Citations
19	Importance of water polarization for ion permeation in narrow pores. Chemical Physics Letters, 2009, 477, 207-210.	1.2	18
20	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, 2173-2179.	2.3	17
21	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, 2888-2895.	2.3	16
22	Mechanistic Implications of Reductive Coâ€“C Bond Cleavage in B₁₂-Dependent Methylmalonyl CoA Mutase. Journal of Physical Chemistry B, 2019, 123, 2210-2216.	1.2	15
23	Dipeptide Aggregation in Aqueous Solution from Fixed Point-Charge Force Fields. Journal of Chemical Theory and Computation, 2014, 10, 1631-1637.	2.3	10
24	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.	2.3	8
25	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.	2.9	8
26	Apo and ligand-bound high resolution Cryo-EM structures of the human Kv3.1 channel reveal a novel binding site for positive modulators. , 2022, 1, .		6