Benjamin T Miller

List of Publications by Year
in descending order

23 papers	654 citations	623574 14 h-index	642610 23 g-index
23 all docs	23 docs citations	23 times ranked	1178 citing authors

#	Article	IF	Citations
1	Reservoir pH replica exchange. Journal of Chemical Physics, 2018, 149, 072321.	1.2	22
2	Computational scheme for pHâ€dependent binding free energy calculation with explicit solvent. Protein Science, 2016, 25, 231-243.	3.1	29
3	Computation of Hydration Free Energies Using the Multiple Environment Single System Quantum Mechanical/Molecular Mechanical Method. Journal of Chemical Theory and Computation, 2016, 12, 332-344.	2.3	42
4	Enhancing Constant-pH Simulation in Explicit Solvent with a Two-Dimensional Replica Exchange Method. Journal of Chemical Theory and Computation, 2015, 11, 2560-2574.	2.3	33
5	Hydrophobic hydration and the anomalous partial molar volumes in ethanol-water mixtures. Journal of Chemical Physics, 2015, 142, 064501.	1.2	29
6	ProBiS-CHARMMing: Web Interface for Prediction and Optimization of Ligands in Protein Binding Sites. Journal of Chemical Information and Modeling, 2015, 55, 2308-2314.	2.5	54
7	Development and implementation of (Q)SAR modeling within the CHARMMing web-user interface. Journal of Computational Chemistry, 2015, 36, 62-67.	1.5	5
8	Web-Based Computational Chemistry Education with CHARMMing I: Lessons and Tutorial. PLoS Computational Biology, 2014, 10, e1003719.	1.5	14
9	Web-Based Computational Chemistry Education with CHARMMing II: Coarse-Grained Protein Folding. PLoS Computational Biology, 2014, 10, e1003738.	1.5	8
10	Web-Based Computational Chemistry Education with CHARMMing III: Reduction Potentials of Electron Transfer Proteins. PLoS Computational Biology, 2014, 10, e1003739.	1.5	10
11	Constant pH Molecular Dynamics in Explicit Solvent with Enveloping Distribution Sampling and Hamiltonian Exchange. Journal of Chemical Theory and Computation, 2014, 10, 2738-2750.	2.3	68
12	Understanding the basis of a class of paradoxical mutations in AraC through simulations. Proteins: Structure, Function and Bioinformatics, 2013, 81, 490-498.	1.5	3
13	Generating Reservoir Conformations for Replica Exchange through the Use of the Conformational Space Annealing Method. Journal of Chemical Theory and Computation, 2013, 9, 1115-1124.	2.3	13
14	Enhanced Sampling in Free Energy Calculations: Combining SGLD with the Bennettâ€™s Acceptance Ratio and Enveloping Distribution Sampling Methods. Journal of Chemical Theory and Computation, 2012, 8, 3650-3662.	2.3	18
15	Comparing normal modes across different models and scales: Hessian reduction versus coarseâ€graining. Journal of Computational Chemistry, 2012, 33, 2250-2275.	1.5	14
16	Implementation of the force decomposition machine for molecular dynamics simulations. Journal of Molecular Graphics and Modelling, 2012, 38, 243-247.	1.3	2
17	Efficient Calculation of QM/MM Frequencies with the Mobile Block Hessian. Journal of Chemical Theory and Computation, 2011, 7, 496-514.	2.3	32
18	MSCALE: A General Utility for Multiscale Modeling. Journal of Chemical Theory and Computation, 2011, 7, 1208-1219.	2.3	41

#	Article	IF	Citations
19	The distributed diagonal force decomposition method for parallelizing molecular dynamics simulations. Journal of Computational Chemistry, 2011, 32, 3005-3013.	1.5	4
20	A parallel implementation of the analytic nuclear gradient for time-dependent density functional theory within the Tammâ€“Dancoff approximation. Molecular Physics, 2010, 108, 2791-2800.	0.8	58
21	CHARMMing: A New, Flexible Web Portal for CHARMM. Journal of Chemical Information and Modeling, 2008, 48, 1920-1929.	2.5	118
22	Langevin Network Model of Myosinâ€. Journal of Physical Chemistry B, 2008, 112, 6274-6281.	1.2	18
23	Open Science Grid Study of the Coupling between Conformation and Water Content in the Interior of a Protein. Journal of Chemical Information and Modeling, 2008, 48, 2021-2029.	2.5	19