

# Benjamin T Miller

## List of Publications by Year in descending order

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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	CHARMMing: A New, Flexible Web Portal for CHARMM. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 1920-1929.	2.5	118
2	Constant pH Molecular Dynamics in Explicit Solvent with Enveloping Distribution Sampling and Hamiltonian Exchange. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 2738-2750.	2.3	68
3	A parallel implementation of the analytic nuclear gradient for time-dependent density functional theory within the Tammâ€“Dancoff approximation. <i>Molecular Physics</i> , 2010, 108, 2791-2800.	0.8	58
4	ProBiS-CHARMMing: Web Interface for Prediction and Optimization of Ligands in Protein Binding Sites. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 2308-2314.	2.5	54
5	Computation of Hydration Free Energies Using the Multiple Environment Single System Quantum Mechanical/Molecular Mechanical Method. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 332-344.	2.3	42
6	MSCALE: A General Utility for Multiscale Modeling. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1208-1219.	2.3	41
7	Enhancing Constant-pH Simulation in Explicit Solvent with a Two-Dimensional Replica Exchange Method. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 2560-2574.	2.3	33
8	Efficient Calculation of QM/MM Frequencies with the Mobile Block Hessian. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 496-514.	2.3	32
9	Hydrophobic hydration and the anomalous partial molar volumes in ethanol-water mixtures. <i>Journal of Chemical Physics</i> , 2015, 142, 064501.	1.2	29
10	Computational scheme for pHâ€“dependent binding free energy calculation with explicit solvent. <i>Protein Science</i> , 2016, 25, 231-243.	3.1	29
11	Reservoir pH replica exchange. <i>Journal of Chemical Physics</i> , 2018, 149, 072321.	1.2	22
12	Open Science Grid Study of the Coupling between Conformation and Water Content in the Interior of a Protein. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 2021-2029.	2.5	19
13	Langevin Network Model of Myosinâ€™. <i>Journal of Physical Chemistry B</i> , 2008, 112, 6274-6281.	1.2	18
14	Enhanced Sampling in Free Energy Calculations: Combining SGLD with the Bennettâ€™s Acceptance Ratio and Enveloping Distribution Sampling Methods. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 3650-3662.	2.3	18
15	Comparing normal modes across different models and scales: Hessian reduction versus coarseâ€“graining. <i>Journal of Computational Chemistry</i> , 2012, 33, 2250-2275.	1.5	14
16	Web-Based Computational Chemistry Education with CHARMMing I: Lessons and Tutorial. <i>PLoS Computational Biology</i> , 2014, 10, e1003719.	1.5	14
17	Generating Reservoir Conformations for Replica Exchange through the Use of the Conformational Space Annealing Method. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1115-1124.	2.3	13
18	Web-Based Computational Chemistry Education with CHARMMing III: Reduction Potentials of Electron Transfer Proteins. <i>PLoS Computational Biology</i> , 2014, 10, e1003739.	1.5	10

#	ARTICLE	IF	CITATIONS
19	Web-Based Computational Chemistry Education with CHARMMing II: Coarse-Grained Protein Folding. PLoS Computational Biology, 2014, 10, e1003738.	1.5	8
20	Development and implementation of (Q)SAR modeling within the CHARMMing web-user interface. Journal of Computational Chemistry, 2015, 36, 62-67.	1.5	5
21	The distributed diagonal force decomposition method for parallelizing molecular dynamics simulations. Journal of Computational Chemistry, 2011, 32, 3005-3013.	1.5	4
22	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
23	Implementation of the force decomposition machine for molecular dynamics simulations. Journal of Molecular Graphics and Modelling, 2012, 38, 243-247.	1.3	2