

Mikolai Fajer

List of Publications by Year in descending order

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Version: 2024-02-01

7
papers

402
citations

1307594

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1720034

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g-index

7
all docs

7
docs citations

7
times ranked

681
citing authors

#	ARTICLE	IF	CITATIONS
1	Generalized scalable multiple copy algorithms for molecular dynamics simulations in NAMD. <i>Computer Physics Communications</i> , 2014, 185, 908-916.	7.5	115
2	Replica-Exchange Accelerated Molecular Dynamics (REXAMD) Applied to Thermodynamic Integration. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1565-1569.	5.3	82
3	Simulated scaling method for localized enhanced sampling and simultaneous "chemical" free energy simulations: A general method for molecular mechanical, quantum mechanical, and quantum mechanical/molecular mechanical simulations. <i>Journal of Chemical Physics</i> , 2007, 126, 024106.	3.0	77
4	The Activation of c-Src Tyrosine Kinase: Conformational Transition Pathway and Free Energy Landscape. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3352-3363.	2.6	41
5	w-REXAMD: A Hamiltonian Replica Exchange Approach to Improve Free Energy Calculations for Systems with Kinetically Trapped Conformations. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 18-23.	5.3	40
6	Using multistate free energy techniques to improve the efficiency of replica exchange accelerated molecular dynamics. <i>Journal of Computational Chemistry</i> , 2009, 30, 1719-1725.	3.3	35
7	Full Atom Simulations of Spin Label Conformations. <i>Methods in Enzymology</i> , 2015, 563, 623-642.	1.0	12