Benjamin R Jagger

List of Publications by Year
in descending order

10	217	1684188 5	1474206 9
papers	citations	h-index	g-index

14	14	14	294
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	SEEKR: Simulation Enabled Estimation of Kinetic Rates, A Computational Tool to Estimate Molecular Kinetics and Its Application to Trypsinâ€“Benzamidine Binding. Journal of Physical Chemistry B, 2017, 121, 3597-3606.	2.6	84
2	Predicting Ligand Binding Kinetics Using a Markovian Milestoning with Voronoi Tessellations Multiscale Approach. Journal of Chemical Theory and Computation, 2020, 16, 5348-5357.	5.3	37
3	Quantitative Ranking of Ligand Binding Kinetics with a Multiscale Milestoning Simulation Approach. Journal of Physical Chemistry Letters, 2018, 9, 4941-4948.	4.6	35
4	Multiscale simulation approaches to modeling drugâ€“protein binding. Current Opinion in Structural Biology, 2020, 61, 213-221.	5.7	29
5	Ranking of Ligand Binding Kinetics Using a Weighted Ensemble Approach and Comparison with a Multiscale Milestoning Approach. Journal of Chemical Information and Modeling, 2020, 60, 5340-5352.	5.4	21
6	Distinguishing the Protonation State of the Histidine Ligand to the Oxidized Ironâ€“Sulfur Cluster from the MitoNEET Family of Proteins. ChemPhysChem, 2017, 18, 39-41.	2.1	3
7	Distinguishing Protonation States of Histidine Ligands to the Oxidized Rieske Ironâ€“Sulfur Cluster through ¹⁵N Vibrational Frequency Shifts. ChemPhysChem, 2016, 17, 216-220.	2.1	2
8	SEEKR: Simulation Enabled Estimation of Kinetic Rates, A Multiscale Approach for the Calculation of Protein-Ligand Association and Dissociation Kinetics. Biophysical Journal, 2018, 114, 42a.	0.5	2
9	Computational Predictions of Drug-Protein Binding Kinetics with a Hybrid Molecular Dynamics, Brownian Dynamics, and Milestoning Approach. Biophysical Journal, 2019, 116, 562a.	0.5	2
10	Benchmarking ensemble docking methods in D3R Grand Challenge 4. Journal of Computer-Aided Molecular Design, 2022, 36, 87-99.	2.9	0