

# Benjamin R Jagger

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/8597559/publications.pdf>

Version: 2024-02-01

10  
papers

217  
citations

1684188

5  
h-index

1474206

9  
g-index

14  
all docs

14  
docs citations

14  
times ranked

294  
citing authors

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