Joseph A Morrone

List of Publications by Year
in descending order

24 papers	1,300 citations	361413 20 h-index	610901 24 g-index
24 all docs	24 docs citations	24 times ranked	1670 citing authors

#	Article	IF	Citations
1	Simplified, interpretable graph convolutional neural networks for small molecule activity prediction. Journal of Computer-Aided Molecular Design, 2022, 36, 391-404.	2.9	10
2	Analysis of Training and Seed Bias in Small Molecules Generated with a Conditional Graph-Based Variational Autoencoderâ”€Insights for Practical AI-Driven Molecule Generation. Journal of Chemical Information and Modeling, 2022, 62, 801-816.	5.4	5
3	Combining Docking Pose Rank and Structure with Deep Learning Improves Proteinâ€“Ligand Binding Mode Prediction over a Baseline Docking Approach. Journal of Chemical Information and Modeling, 2020, 60, 4170-4179.	5.4	64
4	Binding Specificity Determines the Cytochrome P450 3A4 Mediated Enantioselective Metabolism of Metconazole. Journal of Physical Chemistry B, 2018, 122, 1176-1184.	2.6	29
5	Accelerating physical simulations of proteins by leveraging external knowledge. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1309.	14.6	16
6	Computed Binding of Peptides to Proteins with MELD-Accelerated Molecular Dynamics. Journal of Chemical Theory and Computation, 2017, 13, 870-876.	5.3	68
7	Molecular Simulations Identify Binding Poses and Approximate Affinities of Stapled Î±-Helical Peptides to MDM2 and MDMX. Journal of Chemical Theory and Computation, 2017, 13, 863-869.	5.3	49
8	Blind protein structure prediction using accelerated free-energy simulations. Science Advances, 2016, 2, e1601274.	10.3	57
9	Advances in free-energy-based simulations of protein folding and ligand binding. Current Opinion in Structural Biology, 2016, 36, 25-31.	5.7	121
10	Role of water and steric constraints in the kinetics of cavityâ€“ligand unbinding. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 12015-12019.	7.1	74
11	How hydrophobic drying forces impact the kinetics of molecular recognition. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 13277-13282.	7.1	45
12	Are Hydrodynamic Interactions Important in the Kinetics of Hydrophobic Collapse?. Journal of Physical Chemistry B, 2012, 116, 11537-11544.	2.6	29
13	Interplay between Hydrodynamics and the Free Energy Surface in the Assembly of Nanoscale Hydrophobes. Journal of Physical Chemistry B, 2012, 116, 378-389.	2.6	52
14	Structure and Dynamics of Acetonitrile Confined in a Silica Nanopore. Journal of Physical Chemistry C, 2012, 116, 9582-9593.	3.1	38
15	Quantum fluctuations can promote or inhibit glassÂformation. Nature Physics, 2011, 7, 134-137.	16.7	84
16	Correlated Tunneling in Hydrogen Bonds. Journal of Statistical Physics, 2011, 145, 365-384.	1.2	45
17	Displaced Path Integral Formulation for the Momentum Distribution of Quantum Particles. Physical Review Letters, 2010, 105, 110602.	7.8	49
18	Molecular Dynamics with Multiple Time Scales: How to Avoid Pitfalls. Journal of Chemical Theory and Computation, 2010, 6, 1798-1804.	5.3	57

#	Article	IF	Citations
19	Tunneling and delocalization effects in hydrogen bonded systems: A study in position and momentum space. Journal of Chemical Physics, 2009, 130, 204511.	3.0	65
20	Proton momentum distribution in water: an open path integral molecular dynamics study. Journal of Chemical Physics, 2007, 126, 234504.	3.0	66
21	Ab Initio Molecular Dynamics Simulation of the Structure and Proton Transport Dynamics of Methanolâ^'Water Solutionsâ€. Journal of Physical Chemistry B, 2006, 110, 3712-3720.	2.6	101
22	Long range interactions on wires: A reciprocal space based formalism. Journal of Chemical Physics, 2004, 121, 11949-11956.	3.0	24
23	A simple quantum mechanical/molecular mechanical (QM/MM) model for methanol. Chemical Physics Letters, 2003, 370, 406-411.	2.6	17
24	Ab initio molecular dynamics study of proton mobility in liquid methanol. Journal of Chemical Physics, 2002, 117, 4403-4413.	3.0	135