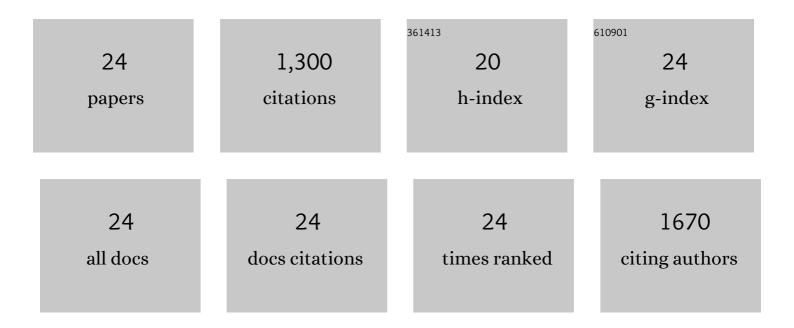
Joseph A Morrone

List of Publications by Year in descending order

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| # | Article | IF | CITATIONS |
|----|---|------|-----------|
| 1 | Ab initio molecular dynamics study of proton mobility in liquid methanol. Journal of Chemical Physics, 2002, 117, 4403-4413. | 3.0 | 135 |
| 2 | Advances in free-energy-based simulations of protein folding and ligand binding. Current Opinion in Structural Biology, 2016, 36, 25-31. | 5.7 | 121 |
| 3 | 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 |
| 4 | Quantum fluctuations can promote or inhibit glassÂformation. Nature Physics, 2011, 7, 134-137. | 16.7 | 84 |
| 5 | Role of water and steric constraints in the kinetics of cavity–ligand unbinding. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 12015-12019. | 7.1 | 74 |
| 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 | Proton momentum distribution in water: an open path integral molecular dynamics study. Journal of Chemical Physics, 2007, 126, 234504. | 3.0 | 66 |
| 8 | 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 |
| 9 | Combining Docking Pose Rank and Structure with Deep Learning Improves Protein–Ligand Binding Mode Prediction over a Baseline Docking Approach. Journal of Chemical Information and Modeling, 2020, 60, 4170-4179. | 5.4 | 64 |
| 10 | Molecular Dynamics with Multiple Time Scales: How to Avoid Pitfalls. Journal of Chemical Theory and Computation, 2010, 6, 1798-1804. | 5.3 | 57 |
| 11 | Blind protein structure prediction using accelerated free-energy simulations. Science Advances, 2016, 2, e1601274. | 10.3 | 57 |
| 12 | 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 |
| 13 | Displaced Path Integral Formulation for the Momentum Distribution of Quantum Particles. Physical Review Letters, 2010, 105, 110602. | 7.8 | 49 |
| 14 | Molecular Simulations Identify Binding Poses and Approximate Affinities of Stapled α-Helical Peptides to MDM2 and MDMX. Journal of Chemical Theory and Computation, 2017, 13, 863-869. | 5.3 | 49 |
| 15 | Correlated Tunneling in Hydrogen Bonds. Journal of Statistical Physics, 2011, 145, 365-384. | 1.2 | 45 |
| 16 | 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 |
| 17 | Structure and Dynamics of Acetonitrile Confined in a Silica Nanopore. Journal of Physical Chemistry C, 2012, 116, 9582-9593. | 3.1 | 38 |
| 18 | Are Hydrodynamic Interactions Important in the Kinetics of Hydrophobic Collapse?. Journal of Physical Chemistry B, 2012, 116, 11537-11544. | 2.6 | 29 |

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| # | Article | IF | CITATIONS |
|----|---|------|-----------|
| 19 | Binding Specificity Determines the Cytochrome P450 3A4 Mediated Enantioselective Metabolism of Metconazole. Journal of Physical Chemistry B, 2018, 122, 1176-1184. | 2.6 | 29 |
| 20 | Long range interactions on wires: A reciprocal space based formalism. Journal of Chemical Physics, 2004, 121, 11949-11956. | 3.0 | 24 |
| 21 | A simple quantum mechanical/molecular mechanical (QM/MM) model for methanol. Chemical Physics Letters, 2003, 370, 406-411. | 2.6 | 17 |
| 22 | Accelerating physical simulations of proteins by leveraging external knowledge. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1309. | 14.6 | 16 |
| 23 | Simplified, interpretable graph convolutional neural networks for small molecule activity prediction. Journal of Computer-Aided Molecular Design, 2022, 36, 391-404. | 2.9 | 10 |
| 24 | Analysis of Training and Seed Bias in Small Molecules Generated with a Conditional Graph-Based Variational Autoencoder─Insights for Practical AI-Driven Molecule Generation. Journal of Chemical Information and Modeling, 2022, 62, 801-816. | 5.4 | 5 |