Joao Marcelo Lamim Ribeiro

List of Publications by Year
in descending order

15 papers	801 citations	759233 12 h-index	996975 15 g-index
17 all docs	17 docs citations	17 times ranked	796 citing authors

#	Article	IF	Citations
1	Differences in interactions between transmembrane domains tune the activation of metabotropic glutamate receptors. ELife, 2021, 10, .	6.0	18
2	A combination of machine learning and infrequent metadynamics to efficiently predict kinetic rates, transition states, and molecular determinants of drug dissociation from G protein-coupled receptors. Journal of Chemical Physics, 2020, 153, 124105.	3.0	26
3	Machine learning approaches for analyzing and enhancing molecular dynamics simulations. Current Opinion in Structural Biology, 2020, 61, 139-145.	5.7	176
4	Pastâ€“future information bottleneck for sampling molecular reaction coordinate simultaneously with thermodynamics and kinetics. Nature Communications, 2019, 10, 3573.	12.8	102
5	Insights From Molecular Dynamics Simulations of a Number of G-Protein Coupled Receptor Targets for the Treatment of Pain and Opioid Use Disorders. Frontiers in Molecular Neuroscience, 2019, 12, 207.	2.9	19
6	Allostery in G protein-coupled receptors investigated by molecular dynamics simulations. Current Opinion in Structural Biology, 2019, 55, 121-128.	5.7	18
7	Toward Achieving Efficient and Accurate Ligand-Protein Unbinding with Deep Learning and Molecular Dynamics through RAVE. Journal of Chemical Theory and Computation, 2019, 15, 708-719.	5.3	61
8	Kinetics of Ligandâ€“Protein Dissociation from All-Atom Simulations: Are We There Yet?. Biochemistry, 2019, 58, 156-165.	2.5	35
9	Reweighted autoencoded variational Bayes for enhanced sampling (RAVE). Journal of Chemical Physics, 2018, 149, 072301.	3.0	219
10	Combined Experimental and Computational Study on the Unimolecular Decomposition of JP-8 Jet Fuel Surrogates. I. n-Decane (n-C₁₀H₂₂). Journal of Physical Chemistry A, 2017, 121, 1261-1280.	2.5	34
11	Combined Experimental and Computational Study on the Unimolecular Decomposition of JP-8 Jet Fuel Surrogates. II: n-Dodecane (n-C₁₂H₂₆). Journal of Physical Chemistry A, 2017, 121, 1281-1297.	2.5	26
12	Reaction mechanism and product branching ratios of the CH + C3H4 reactions: a theoretical study. Physical Chemistry Chemical Physics, 2017, 19, 14543-14554.	2.8	23
13	Reaction Mechanism and Product Branching Ratios of the CH + C₃H₆ Reaction: A Theoretical Study. Journal of Physical Chemistry A, 2016, 120, 1800-1812.	2.5	20
14	Reaction mechanism and rate constants of the CH+CH₄ reaction: a theoretical study. Molecular Physics, 2015, 113, 1865-1872.	1.7	12
15	Reaction Mechanism and Product Branching Ratios of the CH + C₃H₈ Reaction: A Theoretical Study. Journal of Physical Chemistry A, 2014, 118, 9080-9086.	2.5	12