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	Reweighted autoencoded variational Bayes for enhanced sampling (RAVE). Journal of Chemical Physics, 2018, 149, 072301.	3.0	219
2	Machine learning approaches for analyzing and enhancing molecular dynamics simulations. Current Opinion in Structural Biology, 2020, 61, 139-145.	5.7	176
3	Past–future information bottleneck for sampling molecular reaction coordinate simultaneously with thermodynamics and kinetics. Nature Communications, 2019, 10, 3573.	12.8	102
4	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
5	Kinetics of Ligand–Protein Dissociation from All-Atom Simulations: Are We There Yet?. Biochemistry, 2019, 58, 156-165.	2.5	35
6	Combined Experimental and Computational Study on the Unimolecular Decomposition of JP-8 Jet Fuel Surrogates. I. n-Decane (n-$C_{10}H_{22}$). Journal of Physical Chemistry A, 2017, 121, 1261-1280.	2.5	34
7	Combined Experimental and Computational Study on the Unimolecular Decomposition of JP-8 Jet Fuel Surrogates. II. n-Dodecane (n-$C_{12}H_{26}$). Journal of Physical Chemistry A, 2017, 121, 1281-1297.	2.5	26
8	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
9	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
10	Reaction Mechanism and Product Branching Ratios of the CH + C_3H_6 Reaction: A Theoretical Study. Journal of Physical Chemistry A, 2016, 120, 1800-1812.	2.5	20
11	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
12	Allostery in G protein-coupled receptors investigated by molecular dynamics simulations. Current Opinion in Structural Biology, 2019, 55, 121-128.	5.7	18
13	Differences in interactions between transmembrane domains tune the activation of metabotropic glutamate receptors. ELife, 2021, 10, .	6.0	18
14	Reaction Mechanism and Product Branching Ratios of the CH + C_3H_8 Reaction: A Theoretical Study. Journal of Physical Chemistry A, 2014, 118, 9080-9086.	2.5	12
15	Reaction mechanism and rate constants of the CH+CH_4 reaction: a theoretical study. Molecular Physics, 2015, 113, 1865-1872.	1.7	12