Van A Ngo

List of Publications by Year
in descending order

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15 papers	180 citations	1163117 8 h-index	1199594 12 g-index
18 all docs	18 docs citations	18 times ranked	331 citing authors

#	Article	IF	Citations
1	Comparative Analysis of Protein Hydration from MD simulations with Additive and Polarizable Force Fields. Advanced Theory and Simulations, 2019, 2, 1800106.	2.8	22
2	Supercrystals of DNA-Functionalized Gold Nanoparticles: A Million-Atom Molecular Dynamics Simulation Study. Journal of Physical Chemistry C, 2012, 116, 19579-19585.	3.1	20
3	Estimation of Potentials of Mean Force from Nonequilibrium Pulling Simulations Using Both Minh-Adib Estimator and Weighted Histogram Analysis Method. Journal of Chemical Theory and Computation, 2016, 12, 1000-1010.	5.3	20
4	How Anionic Lipids Affect Spatiotemporal Properties of KRAS4B on Model Membranes. Journal of Physical Chemistry B, 2020, 124, 5434-5453.	2.6	18
5	Computational membrane biophysics: From ion channel interactions with drugs to cellular function. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2017, 1865, 1643-1653.	2.3	14
6	Is the G-Quadruplex an Effective Nanoconductor for Ions?. Journal of Physical Chemistry B, 2014, 118, 864-872.	2.6	12
7	Parallel-pulling protocol for free-energy evaluation. Physical Review E, 2012, 85, 036702.	2.1	11
8	Characterizing the Water Wire in the Gramicidin Channel Found by Monte Carlo Sampling Using Continuum Electrostatics and in Molecular Dynamics Trajectories with Conventional or Polarizable Force Fields. Journal of Computational Biophysics and Chemistry, 2021, 20, 111-130.	1.7	11
9	Demonstration of Jarzynski's equality in open quantum systems using a stepwise pulling protocol. Physical Review E, 2012, 86, 031127.	2.1	10
10	Molecular determinants of pro-arrhythmia proclivity of d- and l-sotalol via a multi-scale modeling pipeline. Journal of Molecular and Cellular Cardiology, 2021, 158, 163-177.	1.9	10
11	Mapping Ryanodine Binding Sites in the Pore Cavity of Ryanodine Receptors. Biophysical Journal, 2017, 112, 1645-1653.	0.5	7
12	Molecular Mechanism of Flip-Flop in Triple-Layer Oleic-Acid Membrane: Correlation between Oleic Acid and Water. Journal of Physical Chemistry B, 2012, 116, 13416-13423.	2.6	6
13	Identifying key determinants and dynamics of SARS-CoV-2/ACE2 tight interaction. PLoS ONE, 2021, 16, e0257905.	2.5	6
14	Millisecond molecular dynamics simulations of KRas-dimer formation and interfaces. Biophysical Journal, 2022, 121, 3730-3744.	0.5	6
15	Characterizing the water wire in the Gramicidin channel found by Monte Carlo sampling using continuum electrostatics and in molecular dynamics trajectories with conventional or polarizable force fields. Journal of Theoretical and Computational Chemistry, 0, , 2042001.	1.8	2