Bahaa Jawad

List of Publications by Year
in descending order

11 papers	347 citations	1163117 8 h-index	1281871 11 g-index
15 all docs	15 docs citations	15 times ranked	239 citing authors

#	Article	IF	Citations
1	Key Interacting Residues between RBD of SARS-CoV-2 and ACE2 Receptor: Combination of Molecular Dynamics Simulation and Density Functional Calculation. Journal of Chemical Information and Modeling, 2021, 61, 4425-4441.	5.4	100
2	Molecular mechanism and binding free energy of doxorubicin intercalation in DNA. Physical Chemistry Chemical Physics, 2019, 21, 3877-3893.	2.8	70
3	Binding Interactions between Receptor-Binding Domain of Spike Protein and Human Angiotensin Converting Enzyme-2 in Omicron Variant. Journal of Physical Chemistry Letters, 2022, 13, 3915-3921.	4.6	49
4	Thermodynamic Dissection of the Intercalation Binding Process of Doxorubicin to dsDNA with Implications of Ionic and Solvent Effects. Journal of Physical Chemistry B, 2020, 124, 7803-7818.	2.6	24
5	Ultra-large-scale ab initio quantum chemical computation of bio-molecular systems: The case of spike protein of SARS-CoV-2 virus. Computational and Structural Biotechnology Journal, 2021, 19, 1288-1301.	4.1	21
6	Mutations of Omicron Variant at the Interface of the Receptor Domain Motif and Human Angiotensin-Converting Enzyme-2. International Journal of Molecular Sciences, 2022, 23, 2870.	4.1	18
7	First-Principles Simulation of Dielectric Function in Biomolecules. Materials, 2021, 14, 5774.	2.9	15
8	Computational Design of Miniproteins as SARS-CoV-2 Therapeutic Inhibitors. International Journal of Molecular Sciences, 2022, 23, 838.	4.1	15
9	Delta Variant with P681R Critical Mutation Revealed by Ultra-Large Atomic-Scale Ab Initio Simulation: Implications for the Fundamentals of Biomolecular Interactions. Viruses, 2022, 14, 465.	3.3	11
10	Solvent Effect on the Structure and Properties of RGD Peptide (1FUV) at Body Temperature (310 K) Using Ab Initio Molecular Dynamics. Polymers, 2021, 13, 3434.	4.5	10
11	Molecular Dynamic and Free Energy Analysis of Doxorubicin and DNA Complex. Biophysical Journal, 2018, 114, 528a.	0.5	2