

# Bahaa Jawad

## List of Publications by Year in descending order

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Version: 2024-02-01

11  
papers

347  
citations

1163117

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1281871

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docs citations

15  
times ranked

239  
citing authors

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