

Abdulrahim A Alzain

List of Publications by Year in descending order

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13
papers

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1478505

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13
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citing authors

#	ARTICLE	IF	CITATIONS
1	Discovery of novel TMPRSS2 inhibitors for COVID-19 using in silico fragment-based drug design, molecular docking, molecular dynamics, and quantum mechanics studies. Informatics in Medicine Unlocked, 2022, 29, 100870.	3.4	22
2	Identification of novel transmembrane Protease Serine Type 2 drug candidates for COVID-19 using computational studies. Informatics in Medicine Unlocked, 2021, 26, 100725.	3.4	20
3	Drug repurposing for SARS-CoV-2 main protease: Molecular docking and molecular dynamics investigations. Biochemistry and Biophysics Reports, 2022, 29, 101225.	1.3	16
4	Identification of novel TMPRSS2 inhibitors for COVID-19 using e-pharmacophore modelling, molecular docking, molecular dynamics and quantum mechanics studies. Informatics in Medicine Unlocked, 2021, 26, 100758.	3.4	15
5	Design of novel coumarins as potent Mcl-1 inhibitors for cancer treatment guided by 3D-QSAR, molecular docking and molecular dynamics. Informatics in Medicine Unlocked, 2021, 26, 100765.	3.4	10
6	Identification of novel Plasmodium falciparum dihydroorotate dehydrogenase inhibitors for malaria using in silico studies. Scientific African, 2022, 16, e01214.	1.5	6
7	Drug repurposing against main protease and RNA-dependent RNA polymerase of SARS-CoV-2 using molecular docking, MM-GBSA calculations and molecular dynamics. Structural Chemistry, 2022, 33, 1553-1567.	2.0	6
8	Dual targeting inhibitors for HIV-1 capsid and cyclophilin A: molecular docking, molecular dynamics, and quantum mechanics. Molecular Simulation, 2022, 48, 1476-1489.	2.0	6
9	Bioinspired imidazo[1,2-a:4,5-câ€™]dipyridines with dual antiproliferative and anti-migrative properties in human cancer cells: The SAR investigation. European Journal of Medicinal Chemistry, 2021, 218, 113258.	5.5	3
10	Discovery of 5-Chlorobenzimidazole-based as Promising Inhibitors of Chloroquine-Resistant Plasmodium Strains: Synthesis, Biological Evaluation, Molecular Docking and Computational Studies. Journal of Pharmaceutical Research International, 0, , 136-147.	1.0	1
11	De novo design of novel spike glycoprotein inhibitors using e-pharmacophore modeling, molecular hybridization, ADMET, quantum mechanics and molecular dynamics studies for COVID-19.. Pakistan Journal of Pharmaceutical Sciences, 2022, 35, 313-321.	0.2	1
12	Phthalide derivatives as dihydrofolate reductase inhibitors for malaria: molecular docking and molecular dynamics studies. Journal of Biomolecular Structure and Dynamics, 0, , 1-11.	3.5	1
13	Discovery of novel natural products as rhodesain inhibitors for human African trypanosomiasis using in silico techniques. Journal of Biomolecular Structure and Dynamics, 2023, 41, 5672-5684.	3.5	0