Kiran Bharat Lokhande

List of Publications by Year
in descending order

22	411	759055 12	794469 19
papers	citations	h-index	g-index

25	25	25	418
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	High throughput virtual screening and molecular dynamics simulation analysis of phytomolecules against BfmR of Acinetobacter baumannii: anti-virulent drug development campaign. Journal of Biomolecular Structure and Dynamics, 2023, 41, 2698-2712.	2.0	17
2	Probing intermolecular interactions and binding stability of kaempferol, quercetin and resveratrol derivatives with PPAR-Î³: docking, molecular dynamics and MM/GBSA approach to reveal potent PPAR- Î³ agonist against cancer. Journal of Biomolecular Structure and Dynamics, 2022, 40, 971-981.	2.0	24
3	Antioxidant, anti-quorum sensing, biofilm inhibitory activities and chemical composition of Patchouli essential oil: inÂvitro and in silico approach. Journal of Biomolecular Structure and Dynamics, 2022, 40, 154-165.	2.0	21
4	Sensing the interactions between carbohydrate-binding agents and N-linked glycans of SARS-CoV-2 spike glycoprotein using molecular docking and simulation studies. Journal of Biomolecular Structure and Dynamics, 2022, 40, 3880-3898.	2.0	33
5	Biflavonoids from Rhus succedanea as probable natural inhibitors against SARS-CoV-2: a molecular docking and molecular dynamics approach. Journal of Biomolecular Structure and Dynamics, 2022, 40, 4376-4388.	2.0	33
6	An in silico scientific basis for <scp>LL</scp>â€37 as a therapeutic for Covidâ€19. Proteins: Structure, Function and Bioinformatics, 2022, 90, 1029-1043.	1.5	21
7	Novel B, C-ring truncated deguelin derivatives reveals as potential inhibitors of cyclin D1 and cyclin E using molecular docking and molecular dynamic simulation. Molecular Diversity, 2022, 26, 2295-2309.	2.1	18
8	GC-MS profiling of Bauhinia variegata major phytoconstituents with computational identification of potential lead inhibitors of SARS-CoV-2 Mpro. Computers in Biology and Medicine, 2022, 147, 105679.	3.9	12
9	Molecular docking and simulation studies on SARS-CoV-2 M^{pro} reveals Mitoxantrone, Leucovorin, Birinapant, and Dynasore as potent drugs against COVID-19. Journal of Biomolecular Structure and Dynamics, 2021, 39, 7294-7305.	2.0	82
10	In Silico Exploration of Phytoconstituents From Phyllanthus emblica and Aegle marmelos as Potential Therapeutics Against SARS-CoV-2 RdRp. Bioinformatics and Biology Insights, 2021, 15, 117793222110274.	1.0	14
11	An immunoprophylactic evaluation of Ld-ODC derived HLA-A0201 restricted peptides against visceral leishmaniasis. Journal of Biomolecular Structure and Dynamics, 2021, , 1-11.	2.0	2
12	Detection of Nail Oncometabolite SAICAR in Oral Cancer Patients and Its Molecular Interactions with PKM2 Enzyme. International Journal of Environmental Research and Public Health, 2021, 18, 11225.	1.2	4
13	Transferrin binding protein-B from Neisseria meningitidis C as a novel carrier protein in glycoconjugate preparation: an in silico approach. Journal of Biomolecular Structure and Dynamics, 2021, , 1-11.	2.0	1
14	Molecular profiling of multidrug-resistant river water isolates: insights into resistance mechanism and potential inhibitors. Environmental Science and Pollution Research, 2020, 27, 27279-27292.	2.7	11
15	Exploring conformational changes of PPAR-Æ” complexed with novel kaempferol, quercetin, and resveratrol derivatives to understand binding mode assessment: a small-molecule checkmate to cancer therapy. Journal of Molecular Modeling, 2020, 26, 242.	0.8	18
16	Carbohydrate-Binding Agents: Potential of Repurposing for COVID-19 Therapy. Current Protein and Peptide Science, 2020, 21, 1085-1096.	0.7	13
17	Novel nitrogen-containing heterocyclic compounds in GPR109A as an anti-hyperlipidemic: Homology modeling, docking, dynamic simulation studies. Journal of Research in Pharmacy, 2020, 24, 452-463.	0.1	0
18	Computational data of phytoconstituents from Hibiscus rosa-sinensis on various anti-obesity targets. Data in Brief, 2019, 24, 103994.	0.5	16

#	Article	IF	Citations
19	Data on docking of phytoconstituents of Actinidia deliciosa on dengue viral targets. Data in Brief, 2019, 25, 103996.	0.5	1
20	Molecular interaction studies of Deguelin and its derivatives with Cyclin D1 and Cyclin E in cancer cell signaling pathway: The computational approach. Scientific Reports, 2019, 9, 1778.	1.6	31
21	Molecular Modeling, Docking, Dynamics and Simulation of Gefitinib and its Derivatives with EGFR in Non-small Cell Lung Cancer. Current Computer-Aided Drug Design, 2018, 14, 246-252.	0.8	18
22	In vivo and molecular docking studies using whole extract and phytocompounds of Aegle marmelos fruit protective effects against Isoproterenol-induced Myocardial infarction in rats. Biomedicine and Pharmacotherapy, 2017, 91, 880-889.	2.5	17