

Kiran Bharat Lokhande

List of Publications by Year in descending order

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Version: 2024-02-01

22
papers

411
citations

759055

12
h-index

794469

19
g-index

25
all docs

25
docs citations

25
times ranked

418
citing authors

#	ARTICLE	IF	CITATIONS
1	Molecular docking and simulation studies on SARS-CoV-2 M ^{pro} reveals Mitoxantrone, Leucovorin, Birinapant, and Dynasore as potent drugs against COVID-19. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 7294-7305.	2.0	82
2	Sensing the interactions between carbohydrate-binding agents and N-linked glycans of SARS-CoV-2 spike glycoprotein using molecular docking and simulation studies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 3880-3898.	2.0	33
3	Biflavonoids from <i>Rhus succedanea</i> as probable natural inhibitors against SARS-CoV-2: a molecular docking and molecular dynamics approach. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 4376-4388.	2.0	33
4	Molecular interaction studies of Deguelin and its derivatives with Cyclin D1 and Cyclin E in cancer cell signaling pathway: The computational approach. <i>Scientific Reports</i> , 2019, 9, 1778.	1.6	31
5	Probing intermolecular interactions and binding stability of kaempferol, quercetin and resveratrol derivatives with PPAR- β : docking, molecular dynamics and MM/GBSA approach to reveal potent PPAR- β agonist against cancer. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 971-981.	2.0	24
6	Antioxidant, anti-quorum sensing, biofilm inhibitory activities and chemical composition of Patchouli essential oil: <i>in vitro</i> and <i>in silico</i> approach. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 154-165.	2.0	21
7	An <i>in silico</i> scientific basis for β as a therapeutic for Covid-19. <i>Proteins: Structure, Function and Bioinformatics</i> , 2022, 90, 1029-1043.	1.5	21
8	Exploring conformational changes of PPAR- β complexed with novel kaempferol, quercetin, and resveratrol derivatives to understand binding mode assessment: a small-molecule checkmate to cancer therapy. <i>Journal of Molecular Modeling</i> , 2020, 26, 242.	0.8	18
9	Molecular Modeling, Docking, Dynamics and Simulation of Gefitinib and its Derivatives with EGFR in Non-small Cell Lung Cancer. <i>Current Computer-Aided Drug Design</i> , 2018, 14, 246-252.	0.8	18
10	Novel B, C-ring truncated deguelin derivatives reveals as potential inhibitors of cyclin D1 and cyclin E using molecular docking and molecular dynamic simulation. <i>Molecular Diversity</i> , 2022, 26, 2295-2309.	2.1	18
11	<i>In vivo</i> and molecular docking studies using whole extract and phytochemicals of Aegle marmelos fruit protective effects against Isoproterenol-induced Myocardial infarction in rats. <i>Biomedicine and Pharmacotherapy</i> , 2017, 91, 880-889.	2.5	17
12	High throughput virtual screening and molecular dynamics simulation analysis of phytomolecules against BfmR of <i>Acinetobacter baumannii</i> : anti-virulent drug development campaign. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 2698-2712.	2.0	17
13	Computational data of phytoconstituents from <i>Hibiscus rosa-sinensis</i> on various anti-obesity targets. <i>Data in Brief</i> , 2019, 24, 103994.	0.5	16
14	<i>In Silico</i> Exploration of Phytoconstituents From <i>Phyllanthus emblica</i> and <i>Aegle marmelos</i> as Potential Therapeutics Against SARS-CoV-2 RdRp. <i>Bioinformatics and Biology Insights</i> , 2021, 15, 117793222110274.	1.0	14
15	Carbohydrate-Binding Agents: Potential of Repurposing for COVID-19 Therapy. <i>Current Protein and Peptide Science</i> , 2020, 21, 1085-1096.	0.7	13
16	GC-MS profiling of <i>Bauhinia variegata</i> major phytoconstituents with computational identification of potential lead inhibitors of SARS-CoV-2 M ^{pro} . <i>Computers in Biology and Medicine</i> , 2022, 147, 105679.	3.9	12
17	Molecular profiling of multidrug-resistant river water isolates: insights into resistance mechanism and potential inhibitors. <i>Environmental Science and Pollution Research</i> , 2020, 27, 27279-27292.	2.7	11
18	Detection of Nail Oncometabolite SAICAR in Oral Cancer Patients and Its Molecular Interactions with PKM2 Enzyme. <i>International Journal of Environmental Research and Public Health</i> , 2021, 18, 11225.	1.2	4

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19	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
20	Data on docking of phytoconstituents of Actinidia deliciosa on dengue viral targets. Data in Brief, 2019, 25, 103996.	0.5	1
21	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
22	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