

Rohit Shukla

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

44
papers

644
citations

15
h-index

24
g-index

45
ext. papers

790
ext. citations

4.2
avg, IF

4.94
L-index

#	Paper	IF	Citations
44	Systems biology and big data analytics 2022 , 425-442		
43	Topological parameters, patterns, and motifs in biological networks 2022 , 367-380		
42	Unraveling the Structural Basis of Urea-induced Unfolding of <i>Fasciola gigantica</i> Cytosolic Malate Dehydrogenase. <i>Journal of Molecular Liquids</i> , 2021 , 118170	6	0
41	High-throughput screening of natural compounds and inhibition of a major therapeutic target HsGSK-3 β for Alzheimer's disease using computational approaches. <i>Journal of Genetic Engineering and Biotechnology</i> , 2021 , 19, 61	3.1	2
40	Structure-based discovery of phenyl-diketo acids derivatives as malate synthase inhibitors. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021 , 39, 2945-2958	3.6	8
39	Physicochemical characterization of paclitaxel prodrugs with cytochrome 3A4 to correlate solubility and bioavailability implementing molecular docking and simulation studies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021 , 1-13	3.6	0
38	Application of Deep Learning in Biological Big Data Analysis. <i>Advances in Information Security, Privacy, and Ethics Book Series</i> , 2021 , 117-148	0.3	1
37	Molecular Dynamics Simulation in Drug Discovery: Opportunities and Challenges 2021 , 295-316		2
36	A distant angiogenin variant causes amyotrophic lateral sclerosis through loss-of-function mechanisms: Insights from long-timescale atomistic simulations and conformational dynamics. <i>Computers in Biology and Medicine</i> , 2021 , 135, 104602	7	1
35	Machine learning in expert systems for disease diagnostics in human healthcare 2021 , 179-200		5
34	High-throughput rational design of the remdesivir binding site in the RdRp of SARS-CoV-2: implications for potential resistance. <i>iScience</i> , 2021 , 24, 101992	6.1	39
33	Identification of small molecules against cyclin dependent kinase-5 using chemoinformatics approach for Alzheimer's disease and other tauopathies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020 , 1-13	3.6	3
32	Draft Genome of the Liver Fluke. <i>ACS Omega</i> , 2020 , 5, 11084-11091	3.9	14
31	Molecular Dynamics Simulation of Protein and Protein-Ligand Complexes 2020 , 133-161		14
30	Identification and characterization of cytosolic malate dehydrogenase from the liver fluke <i>Fasciola gigantica</i> . <i>Scientific Reports</i> , 2020 , 10, 13372	4.9	3
29	Identification of mimicking molecule(s) triggering von Willebrand factor in human: a molecular drug target for regulating coagulation pathway. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020 , 38, 124-136	3.6	5
28	Virtual screening, pharmacokinetics, molecular dynamics and binding free energy analysis for small natural molecules against cyclin-dependent kinase 5 for Alzheimer's disease. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020 , 38, 248-262	3.6	21

27	nucleoside diphosphate kinase shows interaction with putative ATP binding cassette (ABC) transporter, Rv1273c. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020 , 38, 1083-1093	3.6	1
26	Identification and characterization of glyceraldehyde 3-phosphate dehydrogenase from <i>Fasciola gigantica</i> . <i>Parasitology Research</i> , 2019 , 118, 861-872	2.4	6
25	Identification of novel small molecules against GSK3 β for Alzheimer's disease using chemoinformatics approach. <i>Journal of Molecular Graphics and Modelling</i> , 2019 , 91, 91-104	2.8	17
24	Exploring Medicinal Plant Legacy for Drug Discovery in Post-genomic Era. <i>Proceedings of the National Academy of Sciences India Section B - Biological Sciences</i> , 2019 , 89, 1141-1151	1.4	13
23	Chemometric approach to estimate kinetic properties of paclitaxel prodrugs and their substructures for solubility prediction through molecular modelling and simulation studies. <i>Journal of Chemometrics</i> , 2019 , 33, e3181	1.6	1
22	screening of deleterious single nucleotide polymorphisms (SNPs) and molecular dynamics simulation of disease associated mutations in gene responsible for oculocutaneous albinism type 6 (OCA 6) disorder. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019 , 37, 3513-3523	3.6	12
21	Structural basis of urea-induced unfolding of <i>Fasciola gigantica</i> glutathione S-transferase. <i>Journal of Cellular Physiology</i> , 2019 , 234, 4491-4503	7	14
20	Unfolding of <i>Acinetobacter baumannii</i> MurA proceeds through a metastable intermediate: A combined spectroscopic and computational investigation. <i>International Journal of Biological Macromolecules</i> , 2019 , 126, 941-951	7.9	5
19	Activity loss by H46A mutation in <i>Mycobacterium tuberculosis</i> isocitrate lyase is due to decrease in structural plasticity and collective motions of the active site. <i>Tuberculosis</i> , 2018 , 108, 143-150	2.6	26
18	Biochemical and thermodynamic comparison of the selenocysteine containing and non-containing thioredoxin glutathione reductase of <i>Fasciola gigantica</i> . <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2018 , 1862, 1306-1316	4	11
17	Structure-based screening and molecular dynamics simulations offer novel natural compounds as potential inhibitors of <i>Mycobacterium tuberculosis</i> isocitrate lyase. <i>Journal of Biomolecular Structure and Dynamics</i> , 2018 , 36, 2045-2057	3.6	46
16	Identification of potential inhibitors of <i>Fasciola gigantica</i> thioredoxin1: computational screening, molecular dynamics simulation, and binding free energy studies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2018 , 36, 2147-2162	3.6	37
15	Structural insights into natural compounds as inhibitors of <i>Fasciola gigantica</i> thioredoxin glutathione reductase. <i>Journal of Cellular Biochemistry</i> , 2018 , 119, 3067-3080	4.7	30
14	Identification of novel natural inhibitors of <i>Opisthorchis felinus</i> cytochrome P450 using structure-based screening and molecular dynamic simulation. <i>Journal of Biomolecular Structure and Dynamics</i> , 2018 , 36, 3541-3556	3.6	26
13	Point mutation A394E in the central intrinsic disordered region of Rna14 leads to chromosomal instability in fission yeast. <i>International Journal of Biological Macromolecules</i> , 2018 , 119, 785-791	7.9	
12	Targeting Nucleotide Binding Domain of Multidrug Resistance-associated Protein-1 (MRP1) for the Reversal of Multi Drug Resistance in Cancer. <i>Scientific Reports</i> , 2018 , 8, 11973	4.9	8
11	Alternate pathway to ascorbate induced inhibition of <i>Mycobacterium tuberculosis</i> . <i>Tuberculosis</i> , 2018 , 111, 161-169	2.6	12
10	Structural and energetic understanding of novel natural inhibitors of <i>Mycobacterium tuberculosis</i> malate synthase. <i>Journal of Cellular Biochemistry</i> , 2018 , 120, 2469	4.7	18

9	Structure-function studies of the asparaginyl-tRNA synthetase from understanding the role of catalytic and non-catalytic domains. <i>Biochemical Journal</i> , 2018 , 475, 3377-3391	3.8	5
8	Identification of new drug-like compounds from millets as Xanthine oxidoreductase inhibitors for treatment of Hyperuricemia: A molecular docking and simulation study. <i>Computational Biology and Chemistry</i> , 2018 , 76, 32-41	3.6	27
7	UDP-N-Acetylglucosamine enolpyruvyl transferase (MurA) of <i>Acinetobacter baumannii</i> (AbMurA): Structural and functional properties. <i>International Journal of Biological Macromolecules</i> , 2017 , 97, 106-114	7.9	26
6	Alterations in conformational topology and interaction dynamics caused by L418A mutation leads to activity loss of <i>Mycobacterium tuberculosis</i> isocitrate lyase. <i>Biochemical and Biophysical Research Communications</i> , 2017 , 490, 276-282	3.4	43
5	Distant Phe345 mutation compromises the stability and activity of <i>Mycobacterium tuberculosis</i> isocitrate lyase by modulating its structural flexibility. <i>Scientific Reports</i> , 2017 , 7, 1058	4.9	53
4	Comprehensive analysis of the catalytic and structural properties of a mu-class glutathione s-transferase from <i>Fasciola gigantica</i> . <i>Scientific Reports</i> , 2017 , 7, 17547	4.9	15
3	A combined biochemical and computational studies of the rho-class glutathione s-transferase sll1545 of <i>Synechocystis</i> PCC 6803. <i>International Journal of Biological Macromolecules</i> , 2017 , 94, 378-385	7.9	31
2	Identification of Mimicking Molecules as Defense Inducers Triggering Jasmonic Acid Mediated Immunity against Blight Disease in Species. <i>Frontiers in Plant Science</i> , 2017 , 8, 609	6.2	31
1	A comprehensive metabolic modeling of thyroid pathway in relation to thyroid pathophysiology and therapeutics. <i>OMICS A Journal of Integrative Biology</i> , 2013 , 17, 584-93	3.8	12