Rohit Shukla

List of Publications by Citations

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	Distant Phe345 mutation compromises the stability and activity of Mycobacterium tuberculosis isocitrate lyase by modulating its structural flexibility. *Scientific Reports*, **2017**, 7, 1058	4.9	53
43	Structure-based screening and molecular dynamics simulations offer novel natural compounds as potential inhibitors of Mycobacterium tuberculosis isocitrate lyase. *Journal of Biomolecular Structure and Dynamics*, **2018**, 36, 2045-2057	3.6	46
42	Alterations in conformational topology and interaction dynamics caused by L418A mutation leads to activity loss of Mycobacterium tuberculosis isocitrate lyase. *Biochemical and Biophysical Research Communications*, **2017**, 490, 276-282	3.4	43
41	High-throughput rational design of the remdesivir binding site in the RdRp of SARS-CoV-2: implications for potential resistance. *IScience*, **2021**, 24, 101992	6.1	39
40	Identification of potential inhibitors of Fasciola gigantica thioredoxin1: computational screening, molecular dynamics simulation, and binding free energy studies. *Journal of Biomolecular Structure and Dynamics*, **2018**, 36, 2147-2162	3.6	37
39	A combined biochemical and computational studies of the rho-class glutathione s-transferase sll1545 of Synechocystis PCC 6803. *International Journal of Biological Macromolecules*, **2017**, 94, 378-385	7.9	31
38	Identification of Mimicking Molecules as Defense Inducers Triggering Jasmonic Acid Mediated Immunity against Blight Disease in Species. *Frontiers in Plant Science*, **2017**, 8, 609	6.2	31
37	Structural insights into natural compounds as inhibitors of Fasciola gigantica thioredoxin glutathione reductase. *Journal of Cellular Biochemistry*, **2018**, 119, 3067-3080	4.7	30
36	Identification of new drug-like compounds from millets as Xanthine oxidoreductase inhibitors for treatment of Hyperuricemia: A molecular docking and simulation study. *Computational Biology and Chemistry*, **2018**, 76, 32-41	3.6	27
35	UDP-N-Acetylglucosamine enolpyruvyl transferase (MurA) of Acinetobacter baumannii (AbMurA): Structural and functional properties. *International Journal of Biological Macromolecules*, **2017**, 97, 106-114	7.9	26
34	Activity loss by H46A mutation in Mycobacterium tuberculosis isocitrate lyase is due to decrease in structural plasticity and collective motions of the active site. *Tuberculosis*, **2018**, 108, 143-150	2.6	26
33	Identification of novel natural inhibitors of Opisthorchis felineus cytochrome P450 using structure-based screening and molecular dynamic simulation. *Journal of Biomolecular Structure and Dynamics*, **2018**, 36, 3541-3556	3.6	26
32	Virtual screening, pharmacokinetics, molecular dynamics and binding free energy analysis for small natural molecules against cyclin-dependent kinase 5 for Alzheimer's disease. *Journal of Biomolecular Structure and Dynamics*, **2020**, 38, 248-262	3.6	21
31	Structural and energetic understanding of novel natural inhibitors of Mycobacterium tuberculosis malate synthase. *Journal of Cellular Biochemistry*, **2018**, 120, 2469	4.7	18
30	Identification of novel small molecules against GSK3β for Alzheimer's disease using chemoinformatics approach. *Journal of Molecular Graphics and Modelling*, **2019**, 91, 91-104	2.8	17
29	Comprehensive analysis of the catalytic and structural properties of a mu-class glutathione s-transferase from Fasciola gigantica. *Scientific Reports*, **2017**, 7, 17547	4.9	15
28	Draft Genome of the Liver Fluke. *ACS Omega*, **2020**, 5, 11084-11091	3.9	14

27	Molecular Dynamics Simulation of Protein and Protein□ligand Complexes **2020**, 133-161		14
26	Structural basis of urea-induced unfolding of Fasciola gigantica glutathione S-transferase. *Journal of Cellular Physiology*, **2019**, 234, 4491-4503	7	14
25	Exploring Medicinal Plant Legacy for Drug Discovery in Post-genomic Era. *Proceedings of the National Academy of Sciences India Section B - Biological Sciences*, **2019**, 89, 1141-1151	1.4	13
24	Alternate pathway to ascorbate induced inhibition of Mycobacterium tuberculosis. *Tuberculosis*, **2018**, 111, 161-169	2.6	12
23	A comprehensive metabolic modeling of thyroid pathway in relation to thyroid pathophysiology and therapeutics. *OMICS A Journal of Integrative Biology*, **2013**, 17, 584-93	3.8	12
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. *Journal of Biomolecular Structure and Dynamics*, **2019**, 37, 3513-3523	3.6	12
21	Biochemical and thermodynamic comparison of the selenocysteine containing and non-containing thioredoxin glutathione reductase of Fasciola gigantica. *Biochimica Et Biophysica Acta - General Subjects*, **2018**, 1862, 1306-1316	4	11
20	Targeting Nucleotide Binding Domain of Multidrug Resistance-associated Protein-1 (MRP1) for the Reversal of Multi Drug Resistance in Cancer. *Scientific Reports*, **2018**, 8, 11973	4.9	8
19	Structure-based discovery of phenyl-diketo acids derivatives as malate synthase inhibitors. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 2945-2958	3.6	8
18	Identification and characterization of glyceraldehyde 3-phosphate dehydrogenase from Fasciola gigantica. *Parasitology Research*, **2019**, 118, 861-872	2.4	6
17	Unfolding of Acinetobacter baumannii MurA proceeds through a metastable intermediate: A combined spectroscopic and computational investigation. *International Journal of Biological Macromolecules*, **2019**, 126, 941-951	7.9	5
16	identification of mimicking molecule(s) triggering von Willebrand factor in human: a molecular drug target for regulating coagulation pathway. *Journal of Biomolecular Structure and Dynamics*, **2020**, 38, 124-136	3.6	5
15	Structure-function studies of the asparaginyl-tRNA synthetase from understanding the role of catalytic and non-catalytic domains. *Biochemical Journal*, **2018**, 475, 3377-3391	3.8	5
14	Machine learning in expert systems for disease diagnostics in human healthcare **2021**, 179-200		5
13	Identification of small molecules against cyclin dependent kinase-5 using chemoinformatics approach for Alzheimer\ disease and other tauopathies. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-13	3.6	3
12	Identification and characterization of cytosolic malate dehydrogenase from the liver fluke Fasciola gigantica. *Scientific Reports*, **2020**, 10, 13372	4.9	3
11	High-throughput screening of natural compounds and inhibition of a major therapeutic target HsGSK-3□for Alzheimer\ disease using computational approaches. *Journal of Genetic Engineering and Biotechnology*, **2021**, 19, 61	3.1	2
10	Molecular Dynamics Simulation in Drug Discovery: Opportunities and Challenges **2021**, 295-316		2

9	Chemometric approach to estimate kinetic properties of paclitaxel prodrugs and their substructures for solubility prediction through molecular modelling and simulation studies. *Journal of Chemometrics*, **2019**, 33, e3181	1.6	1
8	nucleoside diphosphate kinase shows interaction with putative ATP binding cassette (ABC) transporter, Rv1273c. *Journal of Biomolecular Structure and Dynamics*, **2020**, 38, 1083-1093	3.6	1
7	Application of Deep Learning in Biological Big Data Analysis. *Advances in Information Security, Privacy, and Ethics Book Series*, **2021**, 117-148	0.3	1
6	A distant angiogenin variant causes amyotrophic lateral sclerosis through loss-of-function mechanisms: Insights from long-timescale atomistic simulations and conformational dynamics. *Computers in Biology and Medicine*, **2021**, 135, 104602	7	1
5	Unraveling the Structural Basis of Urea-induced Unfolding of Fasciola gigantica Cytosolic Malate Dehydrogenase. *Journal of Molecular Liquids*, **2021**, 118170	6	0
4	Physicochemical characterization of paclitaxel prodrugs with cytochrome 3A4 to correlate solubility and bioavailability implementing molecular docking and simulation studies. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-13	3.6	0
3	Point mutation A394E in the central intrinsic disordered region of Rna14 leads to chromosomal instability in fission yeast. *International Journal of Biological Macromolecules*, **2018**, 119, 785-791	7.9	
2	Systems biology and big data analytics **2022**, 425-442		
1	Topological parameters, patterns, and motifs in biological networks **2022**, 367-380		