

Mohd Shahbaaz

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.

51
papers

645
citations

16
h-index

24
g-index

54
ext. papers

853
ext. citations

4
avg, IF

4.26
L-index

#	Paper	IF	Citations
51	Drug repurposing through virtual screening and in vitro validation identifies tigecycline as a novel putative HCV polymerase inhibitor.. <i>Virology</i> , 2022 , 570, 9-17	3.6	0
50	In silico repurposing of a Novobiocin derivative for activity against latency associated Mycobacterium tuberculosis drug target nicotinate-nucleotide adenylyl transferase (Rv2421c). <i>PLoS ONE</i> , 2021 , 16, e0259348	3.7	0
49	Computational Approaches for the Design of Novel Anticancer Compounds Based on Pyrazolo[3,4-d]pyrimidine Derivatives as TRAP1 Inhibitor. <i>Molecules</i> , 2021 , 26,	4.8	1
48	Peptides-based therapeutics: Emerging potential therapeutic agents for COVID-19. <i>Therapie</i> , 2021 ,	3.8	2
47	Unravelling the unfolding pathway of human Fas-activated serine/threonine kinase induced by urea. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021 , 39, 5516-5525	3.6	0
46	A computational study on active constituents of and as inhibitors of SARS-CoV-2 main protease. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021 , 1-12	3.6	1
45	Antennal Enriched Odorant Binding Proteins Are Required for Odor Communication in. <i>Biomolecules</i> , 2021 , 11,	5.9	4
44	Targeting cyclin-dependent kinase 6 by vanillin inhibits proliferation of breast and lung cancer cells: Combined computational and biochemical studies. <i>Journal of Cellular Biochemistry</i> , 2021 , 122, 897-910	4.7	10
43	Synthesis and Cytotoxic Activity of Novel Indole Derivatives and Their Screening on Spike Glycoprotein of SARS-CoV-2. <i>Frontiers in Molecular Biosciences</i> , 2021 , 8, 637989	5.6	3
42	Sensitivity Enhancement of Pre-Capillary Chelation Method for the Separation of Metal Ions: Experimental and DFT Study. <i>Current Analytical Chemistry</i> , 2021 , 17, 839-848	1.7	0
41	Synthesis of Oxygen Deficient TiO ₂ for Improved Photocatalytic Efficiency in Solar Radiation. <i>Catalysts</i> , 2021 , 11, 904	4	1
40	Current Perspectives in the Discovery of Newer Medications Against the Outbreak of COVID-19. <i>Frontiers in Molecular Biosciences</i> , 2021 , 8, 648232	5.6	1
39	Transcriptomic Profile of in Response to an Imidazo[1,2-][1,2,4,5]tetrazine Reveals Its Possible Impact on Iron Metabolism. <i>Frontiers in Microbiology</i> , 2021 , 12, 724042	5.7	0
38	A novel nano therapeutic using convalescent plasma derived exosomal (CP) for COVID-19: A combined hyperactive immune modulation and diagnostics. <i>Chemico-Biological Interactions</i> , 2021 , 344, 109497	5	6
37	Oxazinethione Derivatives as a Precursor to Pyrazolone and Pyrimidine Derivatives: Synthesis, Biological Activities, Molecular Modeling, ADME, and Molecular Dynamics Studies. <i>Molecules</i> , 2021 , 26,	4.8	1
36	Ellagic Acid Controls Cell Proliferation and Induces Apoptosis in Breast Cancer Cells via Inhibition of Cyclin-Dependent Kinase 6. <i>International Journal of Molecular Sciences</i> , 2020 , 21,	6.3	36
35	Classification and functional analyses of putative virulence factors of Mycobacterium tuberculosis: A combined sequence and structure based study. <i>Computational Biology and Chemistry</i> , 2020 , 87, 107270 ^{3.6}	3.6	0

34	Cellular and Molecular Targets of Waterbuck Repellent Blend Odors in Antennae of Newstead, 1910. <i>Frontiers in Cellular Neuroscience</i> , 2020 , 14, 137	6.1	5
33	Rosmarinic Acid Exhibits Anticancer Effects via MARK4 Inhibition. <i>Scientific Reports</i> , 2020 , 10, 10300	4.9	51
32	Electronic properties investigation of human dihydrofolate reductase complexes with ligands. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020 , 1-16	3.6	1
31	Functional and Structural Analysis of Predicted Proteins Obtained from Minisatellite 33.15-Tagged Transcript pAKT-45 Variants. <i>BioMed Research International</i> , 2020 , 2020, 2562950	3	1
30	Multistage antiplasmodial activity of hydroxyethylamine compounds, in vitro and in vivo evaluations. <i>RSC Advances</i> , 2020 , 10, 35516-35530	3.7	4
29	Inhibiting CDK6 Activity by Quercetin Is an Attractive Strategy for Cancer Therapy. <i>ACS Omega</i> , 2020 , 5, 27480-27491	3.9	22
28	Evaluation of Binding of Rosmarinic Acid with Human Transferrin and Its Impact on the Protein Structure: Targeting Polyphenolic Acid-Induced Protection of Neurodegenerative Disorders. <i>Oxidative Medicine and Cellular Longevity</i> , 2020 , 2020, 1245875	6.7	10
27	Structural analyses and classification of novel isoniazid resistance coupled mutational landscapes in : a combined molecular docking and MD simulation study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020 , 1-10	3.6	
26	The structural basis of acid resistance in : insights from multiple pH regime molecular dynamics simulations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020 , 38, 4483-4492	3.6	2
25	Structure based identification of novel inhibitors against ATP synthase of Mycobacterium tuberculosis: A combined in silico and in vitro study. <i>International Journal of Biological Macromolecules</i> , 2019 , 135, 582-590	7.9	4
24	Designing novel possible kinase inhibitor derivatives as therapeutics against Mycobacterium tuberculosis: An in silico study. <i>Scientific Reports</i> , 2019 , 9, 4405	4.9	22
23	Estimation of pH effect on the structure and stability of kinase domain of human integrin-linked kinase. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019 , 37, 156-165	3.6	10
22	Selectivity and sensitivity enhanced green energy waste based indirect-solid phase extraction of carbaryl supported by DFT and molecular docking studies. <i>Journal of Molecular Liquids</i> , 2018 , 257, 112-120	6	8
21	One-pot biosynthesis of silver nanoparticles using Iboza Riparia and Ilex Mitis for cytotoxicity on human embryonic kidney cells. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2018 , 178, 560-567	6.7	17
20	Structural basis of pesticide detection by enzymatic biosensing: a molecular docking and MD simulation study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2018 , 36, 1402-1416	3.6	13
19	Structural insights into Rab21 GTPase activation mechanism by molecular dynamics simulations. <i>Molecular Simulation</i> , 2018 , 44, 179-189	2	12
18	Carbonic Anhydrase II Based Biosensing of Carbon Dioxide at High Temperature: An Analytical and MD Simulation Study. <i>Journal of Bioremediation & Biodegradation</i> , 2018 , 09,	0.5	2
17	Classification and Functional Analyses of Putative Conserved Proteins from Chlamydomonas reinhardtii CWL029. <i>Interdisciplinary Sciences, Computational Life Sciences</i> , 2017 , 9, 96-106	3.5	1

16	Effect of pH on structure, function, and stability of mitochondrial carbonic anhydrase VA. <i>Journal of Biomolecular Structure and Dynamics</i> , 2017 , 35, 449-461	3.6	21
15	Urea-induced denaturation of human calcium/calmodulin-dependent protein kinase IV: a combined spectroscopic and MD simulation studies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2017 , 35, 463-475	3.6	24
14	Classification and structural analyses of mutational landscapes in hemochromatosis factor E protein: A protein defective in the hereditary hemochromatosis. <i>Gene Reports</i> , 2017 , 6, 93-102	1.4	3
13	Estimation of thermodynamic stability of human carbonic anhydrase IX from urea-induced denaturation and MD simulation studies. <i>International Journal of Biological Macromolecules</i> , 2017 , 105, 183-189	7.9	13
12	Effect of pH on the structure, function, and stability of human calcium/calmodulin-dependent protein kinase IV: combined spectroscopic and MD simulation studies. <i>Biochemistry and Cell Biology</i> , 2016 , 94, 221-8	3.6	28
11	Large scale analysis of the mutational landscape in β -glucuronidase: A major player of mucopolysaccharidosis type VII. <i>Gene</i> , 2016 , 576, 36-44	3.8	67
10	Current Advances in the Identification and Characterization of Putative Drug and Vaccine Targets in the Bacterial Genomes. <i>Current Topics in Medicinal Chemistry</i> , 2016 , 16, 1040-69	3	18
9	Towards New Drug Targets? Function Prediction of Putative Proteins of <i>Neisseria meningitidis</i> MC58 and Their Virulence Characterization. <i>OMICS A Journal of Integrative Biology</i> , 2015 , 19, 416-34	3.8	17
8	Structure-based function analysis of putative conserved proteins with isomerase activity from <i>Haemophilus influenzae</i> . <i>3 Biotech</i> , 2015 , 5, 741-763	2.8	11
7	In silico approaches for the identification of virulence candidates amongst hypothetical proteins of <i>Mycoplasma pneumoniae</i> 309. <i>Computational Biology and Chemistry</i> , 2015 , 59 Pt A, 67-80	3.6	22
6	PKR-inhibitor binds efficiently with human microtubule affinity-regulating kinase 4. <i>Journal of Molecular Graphics and Modelling</i> , 2015 , 62, 245-252	2.8	25
5	Structure-based functional annotation of putative conserved proteins having lyase activity from <i>Haemophilus influenzae</i> . <i>3 Biotech</i> , 2015 , 5, 317-336	2.8	11
4	Identification of functional candidates amongst hypothetical proteins of <i>Treponema pallidum</i> ssp. <i>pallidum</i> . <i>PLoS ONE</i> , 2015 , 10, e0124177	3.7	31
3	Designing New Kinase Inhibitor Derivatives as Therapeutics Against Common Complex Diseases: Structural Basis of Microtubule Affinity-Regulating Kinase 4 (MARK4) Inhibition. <i>OMICS A Journal of Integrative Biology</i> , 2015 , 19, 700-11	3.8	39
2	Functional Insight into Putative Conserved Proteins of <i>Rickettsia rickettsii</i> and their Virulence Characterization. <i>Current Proteomics</i> , 2015 , 12, 101-116	0.7	5
1	Functional annotation of conserved hypothetical proteins from <i>Haemophilus influenzae</i> Rd KW20. <i>PLoS ONE</i> , 2013 , 8, e84263	3.7	59