## Mohd Shahbaaz

## List of Publications by Citations

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51 645 16 24 g-index

54 853 4 4.26 ext. papers ext. citations avg, IF L-index

#	Paper	IF	Citations
51	Large scale analysis of the mutational landscape in Eglucuronidase: A major player of mucopolysaccharidosis type VII. <i>Gene</i> , <b>2016</b> , 576, 36-44	3.8	67
50	Functional annotation of conserved hypothetical proteins from Haemophilus influenzae Rd KW20. <i>PLoS ONE</i> , <b>2013</b> , 8, e84263	3.7	59
49	Rosmarinic Acid Exhibits Anticancer Effects via MARK4 Inhibition. <i>Scientific Reports</i> , <b>2020</b> , 10, 10300	4.9	51
48	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> , <b>2015</b> , 19, 700-11	3.8	39
47	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> , <b>2020</b> , 21,	6.3	36
46	Identification of functional candidates amongst hypothetical proteins of Treponema pallidum ssp. pallidum. <i>PLoS ONE</i> , <b>2015</b> , 10, e0124177	3.7	31
45	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> , <b>2016</b> , 94, 221-8	3.6	28
44	PKR-inhibitor binds efficiently with human microtubule affinity-regulating kinase 4. <i>Journal of Molecular Graphics and Modelling</i> , <b>2015</b> , 62, 245-252	2.8	25
43	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> , <b>2017</b> , 35, 463	- <del>4</del> 75	24
42	Designing novel possible kinase inhibitor derivatives as therapeutics against Mycobacterium tuberculosis: An in silico study. <i>Scientific Reports</i> , <b>2019</b> , 9, 4405	4.9	22
41	In silico approaches for the identification of virulence candidates amongst hypothetical proteins of Mycoplasma pneumoniae 309. <i>Computational Biology and Chemistry</i> , <b>2015</b> , 59 Pt A, 67-80	3.6	22
40	Inhibiting CDK6 Activity by Quercetin Is an Attractive Strategy for Cancer Therapy. <i>ACS Omega</i> , <b>2020</b> , 5, 27480-27491	3.9	22
39	Effect of pH on structure, function, and stability of mitochondrial carbonic anhydrase VA. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2017</b> , 35, 449-461	3.6	21
38	Current Advances in the Identification and Characterization of Putative Drug and Vaccine Targets in the Bacterial Genomes. <i>Current Topics in Medicinal Chemistry</i> , <b>2016</b> , 16, 1040-69	3	18
37	Towards New Drug Targets? Function Prediction of Putative Proteins of Neisseria meningitidis MC58 and Their Virulence Characterization. <i>OMICS A Journal of Integrative Biology</i> , <b>2015</b> , 19, 416-34	3.8	17
36	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> , <b>2018</b> , 178, 560-56	5 <del>6</del> .7	17
35	Structural basis of pesticide detection by enzymatic biosensing: a molecular docking and MD simulation study. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2018</b> , 36, 1402-1416	3.6	13

## (2020-2017)

34	denaturation of thermodynamic stability of human carbonic anhydrase IX from urea-induced denaturation and MD simulation studies. <i>International Journal of Biological Macromolecules</i> , <b>2017</b> , 105, 183-189	7.9	13	
33	Structural insights into Rab21 GTPase activation mechanism by molecular dynamics simulations. <i>Molecular Simulation</i> , <b>2018</b> , 44, 179-189	2	12	
32	Structure-based function analysis of putative conserved proteins with isomerase activity from Haemophilus influenzae. <i>3 Biotech</i> , <b>2015</b> , 5, 741-763	2.8	11	
31	Structure-based functional annotation of putative conserved proteins having lyase activity from Haemophilus influenzae. <i>3 Biotech</i> , <b>2015</b> , 5, 317-336	2.8	11	
30	Evaluation of Binding of Rosmarinic Acid with Human Transferrin and Its Impact on the Protein Structure: Targeting Polyphenolic Acid-Induced Protection of Neurodegenerative Disorders.  Oxidative Medicine and Cellular Longevity, 2020, 2020, 1245875	6.7	10	
29	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> , <b>2021</b> , 122, 897-910	4.7	10	
28	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> , <b>2019</b> , 37, 156-165	3.6	10	
27	Selectivity and sensitivity enhanced green energy waste based indirect-Esolid phase extraction of carbaryl supported by DFT and molecular docking studies. <i>Journal of Molecular Liquids</i> , <b>2018</b> , 257, 112-1	120	8	
26	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> , <b>2021</b> , 344, 109497	5	6	
25	Cellular and Molecular Targets of Waterbuck Repellent Blend Odors in Antennae of Newstead, 1910. <i>Frontiers in Cellular Neuroscience</i> , <b>2020</b> , 14, 137	6.1	5	
24	Functional Insight into Putative Conserved Proteins of Rickettsia rickettsii and their Virulence Characterization. <i>Current Proteomics</i> , <b>2015</b> , 12, 101-116	0.7	5	
23	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> , <b>2019</b> , 135, 582-590	7.9	4	
22	Multistage antiplasmodial activity of hydroxyethylamine compounds, in vitro and in vivo evaluations. <i>RSC Advances</i> , <b>2020</b> , 10, 35516-35530	3.7	4	
21	Antennal Enriched Odorant Binding Proteins Are Required for Odor Communication in. <i>Biomolecules</i> , <b>2021</b> , 11,	5.9	4	
20	Classification and structural analyses of mutational landscapes in hemochromatosis factor E protein: A protein defective in the hereditary hemochromatosis. <i>Gene Reports</i> , <b>2017</b> , 6, 93-102	1.4	3	
19	Synthesis and Cytotoxic Activity of Novel Indole Derivatives and Their Screening on Spike Glycoprotein of SARS-CoV-2. <i>Frontiers in Molecular Biosciences</i> , <b>2021</b> , 8, 637989	5.6	3	
18	Peptides-based therapeutics: Emerging potential therapeutic agents for COVID-19. <i>Therapie</i> , <b>2021</b> ,	3.8	2	
17	The structural basis of acid resistance in : insights from multiple pH regime molecular dynamics simulations. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2020</b> , 38, 4483-4492	3.6	2	

16	Carbonic Anhydrase II Based Biosensing of Carbon Dioxide at High Temperature: An Analytical and MD Simulation Study. <i>Journal of Bioremediation &amp; Biodegradation</i> , <b>2018</b> , 09,	0.5	2
15	Classification and Functional Analyses of Putative Conserved Proteins from Chlamydophila pneumoniae CWL029. <i>Interdisciplinary Sciences, Computational Life Sciences</i> , <b>2017</b> , 9, 96-106	3.5	1
14	Computational Approaches for the Design of Novel Anticancer Compounds Based on Pyrazolo[3,4-d]pyrimidine Derivatives as TRAP1 Inhibitor. <i>Molecules</i> , <b>2021</b> , 26,	4.8	1
13	Electronic properties investigation of human dihydrofolate reductase complexes with ligands. Journal of Biomolecular Structure and Dynamics, 2020, 1-16	3.6	1
12	Functional and Structural Analysis of Predicted Proteins Obtained from Minisatellite 33.15-Tagged Transcript pAKT-45 Variants. <i>BioMed Research International</i> , <b>2020</b> , 2020, 2562950	3	1
11	A computational study on active constituents of and as inhibitors of SARS-CoV-2 main protease. Journal of Biomolecular Structure and Dynamics, <b>2021</b> , 1-12	3.6	1
10	Synthesis of Oxygen Deficient TiO2 for Improved Photocatalytic Efficiency in Solar Radiation. <i>Catalysts</i> , <b>2021</b> , 11, 904	4	1
9	Current Perspectives in the Discovery of Newer Medications Against the Outbreak of COVID-19. <i>Frontiers in Molecular Biosciences</i> , <b>2021</b> , 8, 648232	5.6	1
8	Oxazinethione Derivatives as a Precursor to Pyrazolone and Pyrimidine Derivatives: Synthesis, Biological Activities, Molecular Modeling, ADME, and Molecular Dynamics Studies. <i>Molecules</i> , <b>2021</b> , 26,	4.8	1
7	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> , <b>2021</b> , 16, e0259348	3.7	O
6	Unravelling the unfolding pathway of human Fas-activated serine/threonine kinase induced by urea. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2021</b> , 39, 5516-5525	3.6	О
5	Classification and functional analyses of putative virulence factors of Mycobacterium tuberculosis: A combined sequence and structure based study. <i>Computational Biology and Chemistry</i> , <b>2020</b> , 87, 10727	д.6	
4	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> , <b>2020</b> , 1-10	3.6	
3	Sensitivity Enhancement of Pre-Capillary Chelation Method for the Separation of Metal Ions: Experimental and DFT Study. <i>Current Analytical Chemistry</i> , <b>2021</b> , 17, 839-848	1.7	
2	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> , <b>2021</b> , 12, 724042	5.7	
1	Drug repurposing through virtual screening and in vitro validation identifies tigecycline as a novel putative HCV polymerase inhibitor <i>Virology</i> , <b>2022</b> , 570, 9-17	3.6	