Muhammad Usman Mirza

List of Publications by Year
in descending order

50 papers	1,665 citations	304743 22 h-index	315739 38 g-index
57 all docs	57 docs citations	57 times ranked	2269 citing authors

#	Article	IF	Citations
1	Engineering processive cellulase of Clostridium thermocellum to divulge the role of the carbohydrateâ€binding module. Biotechnology and Applied Biochemistry, 2023, 70, 290-305.	3.1	2
2	Folate Conjugated Polyethylene Glycol Probe for Tumor-Targeted Drug Delivery of 5-Fluorouracil. Molecules, 2022, 27, 1780.	3.8	7
3	Structural Elucidation of Rift Valley Fever Virus L Protein towards the Discovery of Its Potential Inhibitors. Pharmaceuticals, 2022, 15, 659.	3.8	13
4	The discovery of Zika virus NS2B-NS3 inhibitors with antiviral activity via an integrated virtual screening approach. European Journal of Pharmaceutical Sciences, 2022, 175, 106220.	4.0	7
5	Discovery of Rift Valley fever virus natural pan-inhibitors by targeting its multiple key proteins through computational approaches. Scientific Reports, 2022, 12, .	3.3	13
6	Pharmacoinformatics and molecular dynamics simulation studies reveal potential covalent and FDA-approved inhibitors of SARS-CoV-2 main protease 3CL^{pro}. Journal of Biomolecular Structure and Dynamics, 2021, 39, 4936-4948.	3.5	103
7	Impact of IL-17F 7488T/C Functional Polymorphism on Progressive Rheumatoid Arthritis: Novel Insight from the Molecular Dynamic Simulations. Immunological Investigations, 2021, 50, 416-426.	2.0	11
8	Effect of Berberis vulgaris L. root extract on ifosfamide-induced in vivo toxicity and in vitro cytotoxicity. Scientific Reports, 2021, 11, 1708.	3.3	16
9	Toxicological Screening of 4-Phenyl-3,4-dihydrobenzo[h]quinolin-2(1H)-one: A New Potential Candidate for Alzheimerâ€™s Treatment. ACS Omega, 2021, 6, 10897-10909.	3.5	4
10	Designing multi-epitope vaccine against Staphylococcus aureus by employing subtractive proteomics, reverse vaccinology and immuno-informatics approaches. Computers in Biology and Medicine, 2021, 132, 104389.	7.0	73
11	Toxicity Evaluation of the Naphthalen-2-yl 3,5-Dinitrobenzoate: A Drug Candidate for Alzheimer Disease. Frontiers in Pharmacology, 2021, 12, 607026.	3.5	9
12	New isolate from <scp>Salvinia molesta</scp> with antioxidant and urease inhibitory activity. Drug Development Research, 2021, 82, 1169-1181.	2.9	12
13	Development of a Novel Multi-Epitope Vaccine Against Crimean-Congo Hemorrhagic Fever Virus: An Integrated Reverse Vaccinology, Vaccine Informatics and Biophysics Approach. Frontiers in Immunology, 2021, 12, 669812.	4.8	34
14	Fragmentâ€based in silico design of SARSâ€CoVâ€2 main protease inhibitors. Chemical Biology and Drug Design, 2021, 98, 604-619.	3.2	10
15	Probing the structural basis of Citrus phytochrome B using computational modelling and molecular dynamics simulation approaches. Journal of Molecular Liquids, 2021, 340, 116895.	4.9	11
16	Molecular Dynamics Simulations in Drug Discovery and Pharmaceutical Development. Processes, 2021, 9, 71.	2.8	162
17	Structural probing of HapR to identify potent phytochemicals to control Vibrio cholera through integrated computational approaches. Computers in Biology and Medicine, 2021, 138, 104929.	7.0	17
18	Acute Oral, Subacute, and Developmental Toxicity Profiling of Naphthalene 2-Yl, 2-Chloro, 5-Nitrobenzoate: Assessment Based on Stress Response, Toxicity, and Adverse Outcome Pathways. Frontiers in Pharmacology, 2021, 12, 810704.	3.5	6

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19	A Putative Prophylactic Solution for COVID-19: Development of Novel Multiepitope Vaccine Candidate against SARS-COV-2 by Comprehensive Immunoinformatic and Molecular Modelling Approach. Biology, 2020, 9, 296.	2.8	17
20	Identification of novel human USP2 inhibitor and its putative role in treatment of COVID-19 by inhibiting SARS-CoV-2 papain-like (PLpro) protease. Computational Biology and Chemistry, 2020, 89, 107376.	2.3	31
21	Discovery of HIV entry inhibitors via a hybrid CXCR4 and CCR5 receptor pharmacophoreâ€based virtual screening approach. European Journal of Pharmaceutical Sciences, 2020, 155, 105537.	4.0	22
22	Discovery of human coronaviruses pan-papain-like protease inhibitors using computational approaches. Journal of Pharmaceutical Analysis, 2020, 10, 546-559.	5.3	67
23	Enhanced Thermostability and Enzymatic Activity of cel6A Variants from Thermobifida fusca by Empirical Domain Engineering. Biology, 2020, 9, 214.	2.8	6
24	Isolation of Antidiabetic Withanolides from Withania coagulans Dunal and Their In Vitro and In Silico Validation. Biology, 2020, 9, 197.	2.8	16
25	New naphthalene derivative for cost-effective AChE inhibitors for Alzheimerâ€™s treatment: In silico identification, in vitro and in vivo validation. Computational Biology and Chemistry, 2020, 89, 107378.	2.3	20
26	Discovery of novel Hepatitis C virus inhibitor targeting multiple allosteric sites of NS5B polymerase. Infection, Genetics and Evolution, 2020, 84, 104371.	2.3	13
27	Structural elucidation of SARS-CoV-2 vital proteins: Computational methods reveal potential drug candidates against main protease, Nsp12 polymerase and Nsp13 helicase. Journal of Pharmaceutical Analysis, 2020, 10, 320-328.	5.3	207
28	Rational design of an XNA ligase through docking of unbound nucleic acids to toroidal proteins. Nucleic Acids Research, 2019, 47, 7130-7142.	14.5	23
29	Bioassay Directed Isolation, Biological Evaluation and in Silico Studies of New Isolates from Pteris cretica L.. Antioxidants, 2019, 8, 231.	5.1	5
30	A novel pathogenic missense variant in CNNM4 underlying Jalili syndrome: Insights from molecular dynamics simulations. Molecular Genetics & Genomic Medicine, 2019, 7, e902.	1.2	11
31	Quantification of Berberine in Berberis vulgaris L. Root Extract and Its Curative and Prophylactic Role in Cisplatin-Induced In Vivo Toxicity and In Vitro Cytotoxicity. Antioxidants, 2019, 8, 185.	5.1	29
32	Deleterious Variants in WNT10A, EDAR, and EDA Causing Isolated and Syndromic Tooth Agenesis: A Structural Perspective from Molecular Dynamics Simulations. International Journal of Molecular Sciences, 2019, 20, 5282.	4.1	19
33	Mutagenesis of DsbAss is Crucial for the Signal Recognition Particle Mechanism in Escherichia coli: Insights from Molecular Dynamics Simulations. Biomolecules, 2019, 9, 133.	4.0	12
34	In silico structural elucidation of RNA-dependent RNA polymerase towards the identification of potential Crimean-Congo Hemorrhagic Fever Virus inhibitors. Scientific Reports, 2019, 9, 6809.	3.3	26
35	Inhibition of Oncogenic Kinases: An In Vitro Validated Computational Approach Identified Potential Multi-Target Anticancer Compounds. Biomolecules, 2019, 9, 124.	4.0	26
36	In Vitro Antidiabetic, Anti-Obesity and Antioxidant Analysis of Ocimum basilicum Aerial Biomass and in Silico Molecular Docking Simulations with Alpha-Amylase and Lipase Enzymes. Biology, 2019, 8, 92.	2.8	32

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37	Perspectives towards antiviral drug discovery against Ebola virus. Journal of Medical Virology, 2019, 91, 2029-2048.	5.0	35
38	Loss-of-function mutations in ADCY3 cause monogenic severe obesity. Nature Genetics, 2018, 50, 175-179.	21.4	122
39	Small Ubiquitin-Like Modifier Protein 3 Enhances the Solubilization of Human Bone Morphogenetic Protein 2 in E. coli. Applied Biochemistry and Biotechnology, 2018, 186, 256-270.	2.9	4
40	Medicinal plant phytochemicals and their inhibitory activities against pancreatic lipase: molecular docking combined with molecular dynamics simulation approach. Natural Product Research, 2018, 32, 1123-1129.	1.8	36
41	Antigenic Peptide Prediction From E6 and E7 Oncoproteins of HPV Types 16 and 18 for Therapeutic Vaccine Design Using Immunoinformatics and MD Simulation Analysis. Frontiers in Immunology, 2018, 9, 3000.	4.8	44
42	In silico Structure-based Identification of Novel Acetylcholinesterase Inhibitors Against Alzheimerâ€™s Disease. CNS and Neurological Disorders - Drug Targets, 2018, 17, 54-68.	1.4	24
43	In silico and in vivo characterization of cabralealactone, solasodin and salvadorin in a rat model: potential anti-inflammatory agents. Drug Design, Development and Therapy, 2018, Volume 12, 1431-1443.	4.3	11
44	Molecular docking and in silico ADMET studies of silibinin and glycyrrhetic acid anti-inflammatory activity. Tropical Journal of Pharmaceutical Research, 2017, 16, 67.	0.3	13
45	Structure-based virtual screening and molecular docking for the identification of potential multi-targeted inhibitors against breast cancer. Breast Cancer: Targets and Therapy, 2017, Volume 9, 447-459.	1.8	30
46	Integrated Computational Approach for Virtual Hit Identification against Ebola Viral Proteins VP35 and VP40. International Journal of Molecular Sciences, 2016, 17, 1748.	4.1	37
47	Towards peptide vaccines against Zika virus: Immunoinformatics combined with molecular dynamics simulations to predict antigenic epitopes of Zika viral proteins. Scientific Reports, 2016, 6, 37313.	3.3	98
48	Glycyrrhetinic acid and E.resveratroloside act as potential plant derived compounds against dopamine receptor D3 for Parkinson’s disease: a pharmacoinformatics study. Drug Design, Development and Therapy, 2015, 9, 187.	4.3	23
49	Pharmacoinformatics approach for investigation of alternative potential hepatitis C virus nonstructural protein 5B inhibitors. Drug Design, Development and Therapy, 2015, 9, 1825.	4.3	23
50	Docking Studies reveal Phytochemicals as the long searched Anticancer Drugs for Breast Cancer. International Journal of Computer Applications, 2013, 67, 1-5.	0.2	14