Muhammad Usman Mirza

List of Publications by Year
in descending order

50	1,665	304368 22	315357 38
papers	citations	h-index	g-index

57	57	57	2269
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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.	2.4	207
2	Molecular Dynamics Simulations in Drug Discovery and Pharmaceutical Development. Processes, 2021, 9, 71.	1.3	162
3	Loss-of-function mutations in ADCY3 cause monogenic severe obesity. Nature Genetics, 2018, 50, 175-179.	9.4	122
4	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.	2.0	103
5	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.	1.6	98
6	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.	3.9	73
7	Discovery of human coronaviruses pan-papain-like protease inhibitors using computational approaches. Journal of Pharmaceutical Analysis, 2020, 10, 546-559.	2.4	67
8	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.	2.2	44
9	Integrated Computational Approach for Virtual Hit Identification against Ebola Viral Proteins VP35 and VP40. International Journal of Molecular Sciences, 2016, 17, 1748.	1.8	37
10	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.	1.0	36
11	Perspectives towards antiviral drug discovery against Ebola virus. Journal of Medical Virology, 2019, 91, 2029-2048.	2.5	35
12	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.	2.2	34
13	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.	1.3	32
14	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.	1.1	31
15	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.	1.0	30
16	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.	2.2	29
17	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.	1.6	26
18	Inhibition of Oncogenic Kinases: An In Vitro Validated Computational Approach Identified Potential Multi-Target Anticancer Compounds. Biomolecules, 2019, 9, 124.	1.8	26

#	Article	IF	Citations
19	In silico Structure-based Identification of Novel Acetylcholinesterase Inhibitors Against Alzheimerâ€™s Disease. CNS and Neurological Disorders - Drug Targets, 2018, 17, 54-68.	0.8	24
20	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.	2.0	23
21	Pharmacoinformatics approach for investigation of alternative potential hepatitis C virus nonstructural protein 5B inhibitors. Drug Design, Development and Therapy, 2015, 9, 1825.	2.0	23
22	Rational design of an XNA ligase through docking of unbound nucleic acids to toroidal proteins. Nucleic Acids Research, 2019, 47, 7130-7142.	6.5	23
23	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.	1.9	22
24	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.	1.1	20
25	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.	1.8	19
26	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.	1.3	17
27	Structural probing of HapR to identify potent phytochemicals to control Vibrio cholera through integrated computational approaches. Computers in Biology and Medicine, 2021, 138, 104929.	3.9	17
28	Isolation of Antidiabetic Withanolides from Withania coagulans Dunal and Their In Vitro and In Silico Validation. Biology, 2020, 9, 197.	1.3	16
29	Effect of Berberis vulgaris L. root extract on ifosfamide-induced in vivo toxicity and in vitro cytotoxicity. Scientific Reports, 2021, 11, 1708.	1.6	16
30	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
31	Molecular docking and in silico ADMET studies of silibinin and glycyrrhetic acid anti-inflammatory activity. Tropical Journal of Pharmaceutical Research, 2017, 16, 67.	0.2	13
32	Discovery of novel Hepatitis C virus inhibitor targeting multiple allosteric sites of NS5B polymerase. Infection, Genetics and Evolution, 2020, 84, 104371.	1.0	13
33	Structural Elucidation of Rift Valley Fever Virus L Protein towards the Discovery of Its Potential Inhibitors. Pharmaceuticals, 2022, 15, 659.	1.7	13
34	Discovery of Rift Valley fever virus natural pan-inhibitors by targeting its multiple key proteins through computational approaches. Scientific Reports, 2022, 12, .	1.6	13
35	Mutagenesis of DsbAss is Crucial for the Signal Recognition Particle Mechanism in Escherichia coli: Insights from Molecular Dynamics Simulations. Biomolecules, 2019, 9, 133.	1.8	12
36	New isolate from <scp>Salvinia molesta</scp> with antioxidant and urease inhibitory activity. Drug Development Research, 2021, 82, 1169-1181.	1.4	12

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37	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.	2.0	11
38	A novel pathogenic missense variant in CNNM4 underlying Jalili syndrome: Insights from molecular dynamics simulations. Molecular Genetics & Genomic Medicine, 2019, 7, e902.	0.6	11
39	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.	1.0	11
40	Probing the structural basis of Citrus phytochrome B using computational modelling and molecular dynamics simulation approaches. Journal of Molecular Liquids, 2021, 340, 116895.	2.3	11
41	Fragmentâ€based in silico design of SARSâ€CoVâ€2 main protease inhibitors. Chemical Biology and Drug Design, 2021, 98, 604-619.	1.5	10
42	Toxicity Evaluation of the Naphthalen-2-yl 3,5-Dinitrobenzoate: A Drug Candidate for Alzheimer Disease. Frontiers in Pharmacology, 2021, 12, 607026.	1.6	9
43	Folate Conjugated Polyethylene Glycol Probe for Tumor-Targeted Drug Delivery of 5-Fluorouracil. Molecules, 2022, 27, 1780.	1.7	7
44	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.	1.9	7
45	Enhanced Thermostability and Enzymatic Activity of cel6A Variants from Thermobifida fusca by Empirical Domain Engineering. Biology, 2020, 9, 214.	1.3	6
46	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.	1.6	6
47	Bioassay Directed Isolation, Biological Evaluation and in Silico Studies of New Isolates from Pteris cretica L.. Antioxidants, 2019, 8, 231.	2.2	5
48	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.	1.4	4
49	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.	1.6	4
50	Engineering processive cellulase of Clostridium thermocellum to divulge the role of the carbohydrateâ€binding module. Biotechnology and Applied Biochemistry, 2023, 70, 290-305.	1.4	2