Sajjad Ahmad

List of Publications by Year
in descending order

88	2,806	279798 23	233421 45
papers	citations	h-index	g-index

89	89	89	1903
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Abrogation of SARS-CoV-2 interaction with host (NRP1) neuropilin-1 receptor through high-affinity marine natural compounds to curtail the infectivity: A structural-dynamics data. Computers in Biology and Medicine, 2022, 141, 104714.	7.0	14
2	Bacillusspecies; a potential source of anti-SARS-CoV-2 main protease inhibitors. Journal of Biomolecular Structure and Dynamics, 2022, 40, 5748-5758.	3.5	7
3	Designing of a multi-epitopes-based peptide vaccine against rift valley fever virus and its validation through integrated computational approaches. Computers in Biology and Medicine, 2022, 141, 105151.	7.0	16
4	Designing a Recombinant Vaccine against Providencia rettgeri Using Immunoinformatics Approach. Vaccines, 2022, 10, 189.	4.4	32
5	Discovery of Potential Antiviral Compounds against Hendra Virus by Targeting Its Receptor-Binding Protein (G) Using Computational Approaches. Molecules, 2022, 27, 554.	3.8	15
6	An in silico study to unveil potential drugs and vaccine chimera for HBV capsid assembly protein: combined molecular docking and dynamics simulation approach. Journal of Molecular Modeling, 2022, 28, 51.	1.8	1
7	Cancer Incidence, Mortality, Years of Life Lost, Years Lived With Disability, and Disability-Adjusted Life Years for 29 Cancer Groups From 2010 to 2019. JAMA Oncology, 2022, 8, 420.	7.1	719
8	Computational Design of a Multi-Epitope Vaccine Against Porphyromonas gingivalis. Frontiers in Immunology, 2022, 13, 806825.	4.8	9
9	Design of a Multi-Epitopes Vaccine against Hantaviruses: An Immunoinformatics and Molecular Modelling Approach. Vaccines, 2022, 10, 378.	4.4	10
10	Designing of a Recombinant Multi-Epitopes Based Vaccine against Enterococcus mundtii Using Bioinformatics and Immunoinformatics Approaches. International Journal of Environmental Research and Public Health, 2022, 19, 3729.	2.6	24
11	Whole Proteome-Based Therapeutic Targets Annotation and Designing of Multi-Epitope-Based Vaccines against the Gram-Negative XDR-Alcaligenes faecalis Bacterium. Vaccines, 2022, 10, 462.	4.4	12
12	Designing a multi-epitope vaccine against Chlamydia pneumoniae by integrating the core proteomics, subtractive proteomics and reverse vaccinology-based immunoinformatics approaches. Computers in Biology and Medicine, 2022, 145, 105507.	7.0	12
13	Novel 3-chloro-6-nitro-1H-indazole derivatives as promising antileishmanial candidates: synthesis, biological activity, and molecular modelling studies. Journal of Enzyme Inhibition and Medicinal Chemistry, 2022, 37, 151-167.	5.2	4
14	Designing of a Novel Multi-Antigenic Epitope-Based Vaccine against E. hormaechei: An Intergraded Reverse Vaccinology and Immunoinformatics Approach. Vaccines, 2022, 10, 665.	4.4	19
15	Design of a Multi-Epitope Vaccine against Tropheryma whipplei Using Immunoinformatics and Molecular Dynamics Simulation Techniques. Vaccines, 2022, 10, 691.	4.4	13
16	Vaccinomics to Design a Multi-Epitopes Vaccine for Acinetobacter baumannii. International Journal of Environmental Research and Public Health, 2022, 19, 5568.	2.6	24
17	Structural Elucidation of Rift Valley Fever Virus L Protein towards the Discovery of Its Potential Inhibitors. Pharmaceuticals, 2022, 15, 659.	3.8	13
18	Growth, single crystal investigations, Hirshfeld surface analysis, DFT studies, molecular dynamics simulations, molecular docking, physico-chemical characterization and biological activity of novel thiocyanic complex with zinc transition metal precursor. Polyhedron, 2022, 222, 115937.	2.2	8

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19	Synthesis, crystal structure, and a molecular modeling approach to identify effective antiviral hydrazide derivative against the main protease of SARS-CoV-2. Journal of Molecular Structure, 2022, 1265, 133391.	3.6	6
20	Deciphering the dynamics of cathepsin D as a potential drug target to enhance anticancer drug-induced apoptosis. Journal of Molecular Liquids, 2022, 361, 119677.	4.9	2
21	Computer-Aided Multi-Epitope Vaccine Design against Enterobacter xiangfangensis. International Journal of Environmental Research and Public Health, 2022, 19, 7723.	2.6	14
22	Pan-Genome Analysis of Oral Bacterial Pathogens to Predict a Potential Novel Multi-Epitopes Vaccine Candidate. International Journal of Environmental Research and Public Health, 2022, 19, 8408.	2.6	16
23	Molecular docking, simulation and MM-PBSA studies of nigella sativa compounds: a computational quest to identify potential natural antiviral for COVID-19 treatment. Journal of Biomolecular Structure and Dynamics, 2021, 39, 4225-4233.	3.5	89
24	Stilbene-based natural compounds as promising drug candidates against COVID-19. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1-10.	3.5	213
25	A computational study to disclose potential drugs and vaccine ensemble for COVID-19 conundrum. Journal of Molecular Liquids, 2021, 324, 114734.	4.9	15
26	Towards a novel peptide vaccine for Middle East respiratory syndrome coronavirus and its possible use against pandemic COVID-19. Journal of Molecular Liquids, 2021, 324, 114706.	4.9	10
27	Inhibitory Potential of Phytochemicals on Interleukin-6-Mediated T-Cell Reduction in COVID-19 Patients: A Computational Approach. Bioinformatics and Biology Insights, 2021, 15, 117793222110214.	2.0	10
28	Computational Determination of Potential Multiprotein Targeting Natural Compounds for Rational Drug Design Against SARS-COV-2. Molecules, 2021, 26, 674.	3.8	27
29	SARS-CoV-2: An Update on Genomics, Risk Assessment, Potential Therapeutics and Vaccine Development. International Journal of Environmental Research and Public Health, 2021, 18, 1626.	2.6	17
30	Proteome wide vaccine targets prioritization and designing of antigenic vaccine candidate to trigger the host immune response against the Mycoplasma genitalium infection. Microbial Pathogenesis, 2021, 152, 104771.	2.9	9
31	Structure-Based Virtual Screening Identifies Multiple Stable Binding Sites at the RecA Domains of SARS-CoV-2 Helicase Enzyme. Molecules, 2021, 26, 1446.	3.8	18
32	Immuno-Informatics Analysis of Pakistan-Based HCV Subtype-3a for Chimeric Polypeptide Vaccine Design. Vaccines, 2021, 9, 293.	4.4	26
33	Rational design of potent anti-COVID-19 main protease drugs: An extensive multi-spectrum in silico approach. Journal of Molecular Liquids, 2021, 330, 115636.	4.9	10
34	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
35	Designing a multi-epitope vaccine against Mycobacteroides abscessus by pangenome-reverse vaccinology. Scientific Reports, 2021, 11, 11197.	3.3	25
36	Immunogenomics guided design of immunomodulatory multi-epitope subunit vaccine against the SARS-CoV-2 new variants, and its validation through in silico cloning and immune simulation. Computers in Biology and Medicine, 2021, 133, 104420.	7.0	59

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37	Integrated Core Proteomics, Subtractive Proteomics, and Immunoinformatics Investigation to Unveil a Potential Multi-Epitope Vaccine against Schistosomiasis. Vaccines, 2021, 9, 658.	4.4	30
38	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
39	Mechanistic evaluation of a novel cyclohexenone derivativeâ€™s functionality against nociception and inflammation: An in-vitro, in-vivo and in-silico approach. European Journal of Pharmacology, 2021, 902, 174091.	3.5	18
40	Natural products for treatment of Plasmodium falciparum malaria: An integrated computational approach. Computers in Biology and Medicine, 2021, 134, 104415.	7.0	5
41	Synthesis and Identification of Novel Potential Molecules Against COVID-19 Main Protease Through Structure-Guided Virtual Screening Approach. Applied Biochemistry and Biotechnology, 2021, 193, 3602-3623.	2.9	9
42	CytomegaloVirusDb: Multi-omics knowledge database for cytomegaloviruses. Computers in Biology and Medicine, 2021, 135, 104563.	7.0	9
43	Structural basis of UDP-N-acetylglucosamine pyrophosphorylase and identification of promising terpenes to control Aedes aegypti. Colloids and Surfaces B: Biointerfaces, 2021, 204, 111820.	5.0	4
44	Synthesis, Crystal structure, Hirshfeld surface Analysis and computational approach of new 2-methylbenzimidazo[1,2-a]pyrimidin-4(1H)-one. Journal of Molecular Structure, 2021, 1239, 130497.	3.6	10
45	Pan-vaccinomics approach towards a universal vaccine candidate against WHO priority pathogens to address growing global antibiotic resistance. Computers in Biology and Medicine, 2021, 136, 104705.	7.0	35
46	Cyclopentanone Derivative Attenuates Memory Impairment by Inhibiting Amyloid Plaques Formation in the 5xFAD Mice. International Journal of Molecular Sciences, 2021, 22, 9559.	4.1	5
47	In silico methods and tools for drug discovery. Computers in Biology and Medicine, 2021, 137, 104851.	7.0	155
48	Designing a Multi-Epitope Vaccine against Chlamydia trachomatis by Employing Integrated Core Proteomics, Immuno-Informatics and In Silico Approaches. Biology, 2021, 10, 997.	2.8	30
49	Discovery of Novel Inhibitors From Medicinal Plants for V-Domain Ig Suppressor of T-Cell Activation. Frontiers in Molecular Biosciences, 2021, 8, 716735.	3.5	15
50	Towards A Novel Multi-Epitopes Chimeric Vaccine for Simulating Strong Immune Responses and Protection against Morganella morganii. International Journal of Environmental Research and Public Health, 2021, 18, 10961.	2.6	28
51	Immunoinformatics and Immunogenetics-Based Design of Immunogenic Peptides Vaccine against the Emerging Tick-Borne Encephalitis Virus (TBEV) and Its Validation through In Silico Cloning and Immune Simulation. Vaccines, 2021, 9, 1210.	4.4	12
52	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
53	Identification of immunodominant epitopes in allelic variants VK210 and VK247 of Plasmodium Vivax Circumsporozoite immunogen. Infection, Genetics and Evolution, 2021, 96, 105120.	2.3	12
54	In Silico Core Proteomics and Molecular Docking Approaches for the Identification of Novel Inhibitors against Streptococcus pyogenes. International Journal of Environmental Research and Public Health, 2021, 18, 11355.	2.6	6

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55	In silico screening of antigenic B-cell derived T-cell epitopes and designing of a multi-epitope peptide vaccine for Acinetobacter nosocomialis. Journal of Molecular Graphics and Modelling, 2020, 94, 107477.	2.4	20
56	Immunoinformatics design of a novel multi-epitope peptide vaccine to combat multi-drug resistant infections caused by Vibrio vulnificus. European Journal of Pharmaceutical Sciences, 2020, 142, 105160.	4.0	28
57	Multi-epitope based vaccine design against Sarcoptes scabiei paramyosin using immunoinformatics approach. Journal of Molecular Liquids, 2020, 319, 114105.	4.9	9
58	A combine approach of chemical synthesis, biological evaluation and structural dynamics studies revealed thiazole substituted arylamine derivatives as potent FabH enzyme inhibitors. Bioorganic Chemistry, 2020, 105, 104426.	4.1	7
59	Rational Drug Design for Pseudomonas aeruginosa PqsA Enzyme: An in silico Guided Study to Block Biofilm Formation. Frontiers in Molecular Biosciences, 2020, 7, 577316.	3.5	16
60	Conformational transition of Acinetobacter baumannii KdsC enzyme and the role of magnesium in binding: An insight from comparative molecular dynamics simulation and its implications in novel antibiotics design. Journal of Molecular Graphics and Modelling, 2020, 99, 107625.	2.4	1
61	Design of a Novel Multi Epitope-Based Vaccine for Pandemic Coronavirus Disease (COVID-19) by Vaccinomics and Probable Prevention Strategy against Avenging Zoonotics. European Journal of Pharmaceutical Sciences, 2020, 151, 105387.	4.0	33
62	Immunoinformatics characterization of SARS-CoV-2 spike glycoprotein for prioritization of epitope based multivalent peptide vaccine. Journal of Molecular Liquids, 2020, 314, 113612.	4.9	50
63	Vaccinomics to design a novel single chimeric subunit vaccine for broad-spectrum immunological applications targeting nosocomial Enterobacteriaceae pathogens. European Journal of Pharmaceutical Sciences, 2020, 146, 105258.	4.0	44
64	Moleculer dynamics simulaiton revealed reciever domain of Acinetobacter baumannii BfmR enzyme as the hot spot for future antibiotics designing. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2897-2912.	3.5	6
65	Bioactive Heteroleptic Bismuth(V) Complexes: Synthesis, Structural Analysis and Binding Pattern Validation. Applied Organometallic Chemistry, 2019, 33, e5061.	3.5	14
66	Combating tigecycline resistant Acinetobacter baumannii: A leap forward towards multi-epitope based vaccine discovery. European Journal of Pharmaceutical Sciences, 2019, 132, 1-17.	4.0	54
67	Blocking the catalytic mechanism of MurC ligase enzyme from Acinetobacter baumannii: An in Silico guided study towards the discovery of natural antibiotics. Journal of Molecular Liquids, 2019, 281, 117-133.	4.9	5
68	Heteroleptic copper(<scp>i</scp>) halides with triphenylphosphine and acetylthiourea: synthesis, characterization and biological studies (experimental and molecular docking). New Journal of Chemistry, 2019, 43, 19318-19330.	2.8	7
69	Toward novel inhibitors against KdsB: a highly specific and selective broad-spectrum bacterial enzyme. Journal of Biomolecular Structure and Dynamics, 2019, 37, 1326-1345.	3.5	30
70	Subtractive Genomics, Molecular Docking and Molecular Dynamics Simulation Revealed LpxC as a Potential Drug Target Against Multi-Drug Resistant Klebsiella pneumoniae. Interdisciplinary Sciences, Computational Life Sciences, 2019, 11, 508-526.	3.6	26
71	Comparative subtractive proteomics based ranking for antibiotic targets against the dirtiest superbug: Acinetobacter baumannii. Journal of Molecular Graphics and Modelling, 2018, 82, 74-92.	2.4	39
72	Subtractive proteomics revealed plausible drug candidates in the proteome of multi-drug resistant Corynebacterium diphtheriae. Meta Gene, 2018, 17, 34-42.	0.6	8

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73	Structural investigations, anti-leishmanial, antibacterial and docking studies of new pentavalent antimony carboxylates. Inorganica Chimica Acta, 2018, 474, 148-155.	2.4	22
74	Immuno-informatics driven proteome-wide investigation revealed novel peptide-based vaccine targets against emerging multiple drug resistant Providencia stuartii. Journal of Molecular Graphics and Modelling, 2018, 80, 238-250.	2.4	32
75	An integrated computational hierarchy for identification of potent inhibitors against Shikimate Kinase enzyme from Shigella sonnei , a major cause of global dysentery. Gene Reports, 2018, 11, 283-293.	0.8	2
76	A novel approach of virulome based reverse vaccinology for exploring and validating peptide-based vaccine candidates against the most troublesome nosocomial pathogen: Acinetobacter baumannii. Journal of Molecular Graphics and Modelling, 2018, 83, 1-11.	2.4	21
77	Identification of natural inhibitors against Acinetobacter baumannii d-alanine-d-alanine ligase enzyme: A multi-spectrum in silico approach. Journal of Molecular Liquids, 2018, 262, 460-475.	4.9	12
78	Subtractive proteomics and immunoinformatics revealed novel B-cell derived T-cell epitopes against Yersinia enterocolitica: An etiological agent of Yersiniosis. Microbial Pathogenesis, 2018, 125, 336-348.	2.9	22
79	Antiproliferative, antioxidant and binding mechanism analysis of prodigiosin from newly isolated radio-resistant Streptomyces sp. strain WMA-LM31. Molecular Biology Reports, 2018, 45, 1787-1798.	2.3	24
80	Identification of potential antibiotic targets in the proteome of multi-drug resistant Proteus mirabilis. Meta Gene, 2018, 18, 167-173.	0.6	11
81	Implications of sequence conservation patterns of serpin B family leading to structural and functional importance. Gene Reports, 2018, 12, 30-38.	0.8	0
82	Proteome-wide identification of epitope-based vaccine candidates against multi-drug resistant Proteus mirabilis. Biologicals, 2018, 55, 27-37.	1.4	12
83	From phylogeny to protein dynamics: A computational hierarchical quest for potent drug identification against an emerging enteropathogen â€œYersinia enterocoliticaâ€• Journal of Molecular Liquids, 2018, 265, 372-389.	4.9	10
84	Identification of plausible drug targets by investigating the druggable genome of MDR Staphylococcus epidermidis. Gene Reports, 2017, 7, 147-153.	0.8	53
85	Towards a peptide-based vaccine against Shigella sonnei : A subtractive reverse vaccinology based approach. Biologicals, 2017, 50, 87-99.	1.4	71
86	Binding mode analysis, dynamic simulation and binding free energy calculations of the MurF ligase from Acinetobacter baumannii. Journal of Molecular Graphics and Modelling, 2017, 77, 72-85.	2.4	84
87	An overview on phase variation, mechanisms and roles in bacterial adaptation. JPMA the Journal of the Pakistan Medical Association, 2017, 67, 285-291.	0.2	2
88	PCR Based Detection of Phase Variable Genes in Pakistani Based Clinical Helicobacter pylori Strains. Jundishapur Journal of Microbiology, 2016, 9, e31824.	0.5	2