Shafi Mahmud

List of Publications by Year
in descending order

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79 papers	1,789 citations	257101 24 h-index	344852 36 g-index
82 all docs	82 docs citations	82 times ranked	1095 citing authors

#	Article	IF	Citations
1	Phenolic compounds as Î±-glucosidase inhibitors: a docking and molecular dynamics simulation study. Journal of Biomolecular Structure and Dynamics, 2023, 41, 3862-3871.	2.0	10
2	Natural flavonoids effectively block the CD81 receptor of hepatocytes and inhibit HCV infection: a computational drug development approach. Molecular Diversity, 2023, 27, 1309-1322.	2.1	15
3	Screening of phytochemicals as potent inhibitor of 3-chymotrypsin and papain-like proteases of SARS-CoV2: an in silico approach to combat COVID-19. Journal of Biomolecular Structure and Dynamics, 2022, 40, 2067-2081.	2.0	64
4	Designing potent inhibitors against the multidrug resistance P-glycoprotein. Journal of Biomolecular Structure and Dynamics, 2022, 40, 9403-9415.	2.0	3
5	Identification of potential phytochemicals from Citrus Limon against main protease of SARS-CoV-2: molecular docking, molecular dynamic simulations and quantum computations. Journal of Biomolecular Structure and Dynamics, 2022, 40, 10741-10752.	2.0	29
6	Dominant cladeâ€featured SARSâ€CoVâ€2 coâ€occurring mutations reveal plausible epistasis: An in silico based hypothetical model. Journal of Medical Virology, 2022, 94, 1035-1049.	2.5	16
7	Computational screening and biochemical analysis of Pistacia integerrima and Pandanus odorifer plants to find effective inhibitors against Receptor-Binding domain (RBD) of the spike protein of SARS-Cov-2. Arabian Journal of Chemistry, 2022, 15, 103600.	2.3	11
8	Phytochemical Compound Screening to Identify Novel Small Molecules against Dengue Virus: A Docking and Dynamics Study. Molecules, 2022, 27, 653.	1.7	10
9	Methyl Î²-D-galactopyranoside esters as potential inhibitors for SARS-CoV-2 protease enzyme: synthesis, antimicrobial, PASS, molecular docking, molecular dynamics simulations and quantum computations. Glycoconjugate Journal, 2022, 39, 261-290.	1.4	16
10	Potent In Vitro Phosphodiesterase 1 Inhibition of Flavone Isolated from Pistacia integerrima Galls. BioMed Research International, 2022, 2022, 1-6.	0.9	3
11	phytochemdb: a platform for virtual screening and computer-aided drug designing. Database: the Journal of Biological Databases and Curation, 2022, 2022, .	1.4	13
12	Biochemical and Molecular Dynamics Study of a Novel GH 43 Î±-l-Arabinofuranosidase/Î²-Xylosidase From Caldicellulosiruptor saccharolyticus DSM8903. Frontiers in Bioengineering and Biotechnology, 2022, 10, 810542.	2.0	6
13	Use of Next-Generation Sequencing for Identifying Mitochondrial Disorders. Current Issues in Molecular Biology, 2022, 44, 1127-1148.	1.0	6
14	Integrated Machine Learning and Chemoinformatics-Based Screening of Mycotic Compounds against Kinesin Spindle ProteinEg5 for Lung Cancer Therapy. Molecules, 2022, 27, 1639.	1.7	7
15	Can the SARS-CoV-2 Omicron Variant Confer Natural Immunity against COVID-19?. Molecules, 2022, 27, 2221.	1.7	12
16	Identification of Zinc-Binding Inhibitors of Matrix Metalloproteinase-9 to Prevent Cancer Through Deep Learning and Molecular Dynamics Simulation Approach. Frontiers in Molecular Biosciences, 2022, 9, 857430.	1.6	5
17	Pathogenicity and virulence of Marburg virus. Virulence, 2022, 13, 609-633.	1.8	46
18	In search of novel inhibitors of anti-cancer drug target fibroblast growth factor receptors: Insights from virtual screening, molecular docking, and molecular dynamics. Arabian Journal of Chemistry, 2022, 15, 103882.	2.3	15

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19	Curcumin Analogues as a Potential Drug against Antibiotic Resistant Protein, Î²-Lactamases and L, D-Transpeptidases Involved in Toxin Secretion in Salmonella typhi: A Computational Approach. BioMedInformatics, 2022, 2, 77-100.	1.0	3
20	Catabolic profiling of selective enzymes in the saccharification of non-food lignocellulose parts of biomass into functional edible sugars and bioenergy: An in silico bioprospecting. Journal of Advanced Veterinary and Animal Research, 2022, 9, 19.	0.5	21
21	Impacts of nutritive and bioactive compounds on cancer development and therapy. Critical Reviews in Food Science and Nutrition, 2022, , 1-30.	5.4	3
22	Triazoles and Their Derivatives: Chemistry, Synthesis, and Therapeutic Applications. Frontiers in Molecular Biosciences, 2022, 9, 864286.	1.6	67
23	The Emergence of SARS-CoV-2 Variants With a Lower Antibody Response: A Genomic and Clinical Perspective. Frontiers in Medicine, 2022, 9, .	1.2	4
24	Synthesis, antimicrobial, molecular docking and molecular dynamics studies of lauroyl thymidine analogs against SARS-CoV-2: POM study and identification of the pharmacophore sites. Bioorganic Chemistry, 2022, 125, 105850.	2.0	13
25	In vitro antioxidant and cytotoxicity activities and in silico anticancer property of methanolic leaf extract of Leucas indica. Informatics in Medicine Unlocked, 2022, 31, 100963.	1.9	6
26	UHPLC-Q/Orbitrap/MS based chemical fingerprinting and hepatoprotective potential of a medicinal plant, Morinda angustifolia Roxb.. South African Journal of Botany, 2022, 148, 561-572.	1.2	12
27	A conserved subunit vaccine designed against SARS-CoV-2 variants showed evidence in neutralizing the virus. Applied Microbiology and Biotechnology, 2022, 106, 4091-4114.	1.7	6
28	Chemical Characterization, Antioxidant, and Antihyperglycemic Capacity of Ferulated Arabinoxylan Extracted from â€œChicha de Joraâ€•Bagasse: An Ancestral Fermented Beverage from Zea mays L.. Journal of Food Quality, 2022, 2022, 1-16.	1.4	1
29	Determination of Volatile Compounds of Mentha piperita and Lavandula multifida and Investigation of Their Antibacterial, Antioxidant, and Antidiabetic Properties. Evidence-based Complementary and Alternative Medicine, 2022, 2022, 1-9.	0.5	12
30	Synthesis, antimicrobial, SAR, PASS, molecular docking, molecular dynamics and pharmacokinetics studies of 5â€²-O-uridine derivatives bearing acyl moieties: POM study and identification of the pharmacophore sites. Nucleosides, Nucleotides and Nucleic Acids, 2022, 41, 1036-1083.	0.4	11
31	Mixed dye degradation by Bacillus pseudomycoides and Acinetobacter haemolyticus isolated from industrial effluents: A combined affirmation with wetlab and in silico studies. Arabian Journal of Chemistry, 2022, 15, 104078.	2.3	8
32	Molecular docking and dynamics study of natural compound for potential inhibition of main protease of SARS-CoV-2. Journal of Biomolecular Structure and Dynamics, 2021, 39, 6281-6289.	2.0	40
33	Computational discovery of plant-based inhibitors against human carbonic anhydrase IX and molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2021, 39, 2754-2770.	2.0	18
34	Extensive immunoinformatics study for the prediction of novel peptide-based epitope vaccine with docking confirmation against envelope protein of Chikungunya virus: a computational biology approach. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1139-1154.	2.0	30
35	Fermentation optimization of cellulase production from sugarcane bagasse by Bacillus pseudomycoides and molecular modeling study of cellulase. Current Research in Microbial Sciences, 2021, 2, 100013.	1.4	30
36	A molecular phylogeny of Taeniophyllum THRJ inferred from DNA barcode regions. Journal of Advanced Biotechnology and Experimental Therapeutics, 2021, 4, 171.	0.4	0

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37	In silico prediction of a highly immunogenic and conserved epitope against Zika Virus. Informatics in Medicine Unlocked, 2021, 24, 100613.	1.9	5
38	Structure-based design of new diclofenac: Physicochemical, spectral, molecular docking, dynamics simulation and ADMET studies. Informatics in Medicine Unlocked, 2021, 25, 100677.	1.9	23
39	Physicochemical, spectral, molecular docking and ADMET studies of Bisphenol analogues; A computational approach. Informatics in Medicine Unlocked, 2021, 25, 100706.	1.9	19
40	In silico design of an epitope-based vaccine against choline binding protein A of Streptococcus pneumoniae. Informatics in Medicine Unlocked, 2021, 23, 100546.	1.9	16
41	Immunoinformatics-guided design of a multi-epitope vaccine based on the structural proteins of severe acute respiratory syndrome coronavirus 2. RSC Advances, 2021, 11, 18103-18121.	1.7	25
42	A molecular modelling approach for identifying antiviral selenium-containing heterocyclic compounds that inhibit the main protease of SARS-CoV-2: an in silico investigation. Briefings in Bioinformatics, 2021, 22, 1476-1498.	3.2	58
43	Chemical Profiles and Pharmacological Properties with in Silico Studies on Elatostema papillosum Wedd. Molecules, 2021, 26, 809.	1.7	22
44	Virtual screening and molecular dynamics simulation study of plant-derived compounds to identify potential inhibitors of main protease from SARS-CoV-2. Briefings in Bioinformatics, 2021, 22, 1402-1414.	3.2	75
45	Efficacy of Phytochemicals Derived from Avicennia officinalis for the Management of COVID-19: A Combined In Silico and Biochemical Study. Molecules, 2021, 26, 2210.	1.7	68
46	Prospective Role of Peptide-Based Antiviral Therapy Against the Main Protease of SARS-CoV-2. Frontiers in Molecular Biosciences, 2021, 8, 628585.	1.6	31
47	Plant-Based Phytochemical Screening by Targeting Main Protease of SARS-CoV-2 to Design Effective Potent Inhibitors. Biology, 2021, 10, 589.	1.3	46
48	Targeting SARS-CoV-2 nonstructural proteinÂ15 endoribonuclease: anin silicoperspective. Future Virology, 2021, 16, 467-474.	0.9	8
49	Designing a multi-epitope vaccine candidate to combat MERS-CoV by employing an immunoinformatics approach. Scientific Reports, 2021, 11, 15431.	1.6	43
50	Biochemical and in silico study of leaf and bark extracts from Aphanamixis polystachya against common pathogenic bacteria. Saudi Journal of Biological Sciences, 2021, 28, 6592-6605.	1.8	5
51	Phytochemicals from Leucas zeylanica Targeting Main Protease of SARS-CoV-2: Chemical Profiles, Molecular Docking, and Molecular Dynamics Simulations. Biology, 2021, 10, 789.	1.3	30
52	An Analysis Based on Molecular Docking and Molecular Dynamics Simulation Study of Bromelain as Anti-SARS-CoV-2 Variants. Frontiers in Pharmacology, 2021, 12, 717757.	1.6	28
53	Molecular docking and dynamics study to explore phytochemical ligand molecules against the main protease of SARS-CoV-2 from extensive phytochemical datasets. Expert Review of Clinical Pharmacology, 2021, 14, 1305-1315.	1.3	34
54	In vitro and in silico approach of fungal growth inhibition by Trichoderma asperellum HbGT6-07 derived volatile organic compounds. Arabian Journal of Chemistry, 2021, 14, 103290.	2.3	11

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55	Antiviral peptides against the main protease of SARS-CoV-2: A molecular docking and dynamics study. Arabian Journal of Chemistry, 2021, 14, 103315.	2.3	48
56	Analysis of SYK Gene as a Prognostic Biomarker and Suggested Potential Bioactive Phytochemicals as an Alternative Therapeutic Option for Colorectal Cancer: An In-Silico Pharmaco-Informatics Investigation. Journal of Personalized Medicine, 2021, 11, 888.	1.1	13
57	In Silico Evaluation of Iranian Medicinal Plant Phytoconstituents as Inhibitors against Main Protease and the Receptor-Binding Domain of SARS-CoV-2. Molecules, 2021, 26, 5724.	1.7	39
58	In silico analysis of ciprofloxacin analogs as inhibitors of DNA gyrase of Staphylococcus aureus. Informatics in Medicine Unlocked, 2021, 26, 100748.	1.9	10
59	Designing an epitope vaccine against Dermatophagoides pteronyssinus: An in silico study. Acta Tropica, 2021, 222, 106028.	0.9	11
60	Drug Repurposing Approach against Novel Coronavirus Disease (COVID-19) through Virtual Screening Targeting SARS-CoV-2 Main Protease. Biology, 2021, 10, 2.	1.3	67
61	Screening of Potent Phytochemical Inhibitors Against SARS-CoV-2 Main Protease: An Integrative Computational Approach. Frontiers in Bioinformatics, 2021, 1, .	1.0	14
62	Synthesis, Antimicrobial, Anticancer, PASS, Molecular Docking, Molecular Dynamic Simulations & Pharmacokinetic Predictions of Some Methyl Î²-D-Galactopyranoside Analogs. Molecules, 2021, 26, 7016.	1.7	12
63	Designing of a Multi-epitope Vaccine against the Structural Proteins of Marburg Virus Exploiting the Immunoinformatics Approach. ACS Omega, 2021, 6, 32043-32071.	1.6	43
64	Elucidating the Glucokinase Activating Potentials of Naturally Occurring Prenylated Flavonoids: An Explicit Computational Approach. Molecules, 2021, 26, 7211.	1.7	17
65	Inhibition of TNF-Alpha Using Plant-Derived Small Molecules for Treatment of Inflammation-Mediated Diseases. Proceedings (mdpi), 2021, 83, 13.	0.2	1
66	Molecular Docking and Dynamics Studies to Explore Effective Inhibitory Peptides Against the Spike Receptor Binding Domain of SARS-CoV-2. Frontiers in Molecular Biosciences, 2021, 8, 791642.	1.6	14
67	Tobacco Smoking and Liver Cancer Risk: Potential Avenues for Carcinogenesis. Journal of Oncology, 2021, 2021, 1-11.	0.6	37
68	Phytochemical Constituents, Biological Activities, and Health-Promoting Effects of the Melissa officinalis. Oxidative Medicine and Cellular Longevity, 2021, 2021, 1-20.	1.9	39
69	LC-MS/HRMS Analysis, Anti-Cancer, Anti-Enzymatic and Anti-Oxidant Effects of Boerhavia diffusa Extracts: A Potential Raw Material for Functional Applications. Antioxidants, 2021, 10, 2003.	2.2	26
70	Plasma activated water: the next generation eco-friendly stimulant for enhancing plant seed germination, vigor and increased enzyme activity, a study on black gram (Vigna mungo L.). Plasma Chemistry and Plasma Processing, 2020, 40, 119-143.	1.1	70
71	Exploring the potent inhibitors and binding modes of phospholipase A2 through in silico investigation. Journal of Biomolecular Structure and Dynamics, 2020, 38, 4221-4231.	2.0	27
72	Proteome-wide screening for designing a multi-epitope vaccine against emerging pathogenElizabethkingia anophelisusing immunoinformatic approaches. Journal of Biomolecular Structure and Dynamics, 2020, 38, 4850-4867.	2.0	90

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73	Identification and in silico molecular modelling study of newly isolated Bacillus subtilis SI-18 strain against S9 protein of Rhizoctonia solani. Arabian Journal of Chemistry, 2020, 13, 8600-8612.	2.3	22
74	Comparative molecular investigation of the potential inhibitors against SARS-CoV-2 main protease: a molecular docking study. Journal of Biomolecular Structure and Dynamics, 2020, 39, 1-7.	2.0	26
75	Methanolic Bark Extract of Abroma augusta (L.) Induces Apoptosis in EAC Cells through Altered Expression of Apoptosis Regulatory Genes. Evidence-based Complementary and Alternative Medicine, 2020, 2020, 1-14.	0.5	7
76	Habit and habitual status with relative diversity study of avifauna of Jaipurhat district of Bangladesh. Journal of Advanced Biotechnology and Experimental Therapeutics, 2020, 3, 204.	0.4	0
77	Isolation and characterization of bacteria from two soil samples and their effect on wheat (Triticum) Tj ETQq1 1 0.784314 rgBT /Overlo 2020, 3, 254.	0.4	5
78	Assessment of structurally and functionally high-risk nsSNPs impacts on human bone morphogenetic protein receptor type IA (BMPR1A) by computational approach. Computational Biology and Chemistry, 2019, 80, 31-45.	1.1	28
79	Evaluation of antibacterial and antioxidant activity of three plant species from Morus genus. International Journal of Biosciences, 2019, 14, 183-189.	0.4	2