

Dinesh Gupta

List of Publications by Year in descending order

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Version: 2024-02-01

116
papers

3,262
citations

218677

26
h-index

175258

52
g-index

127
all docs

127
docs citations

127
times ranked

4703
citing authors

#	ARTICLE	IF	CITATIONS
1	Lead optimization, pharmacophore development and scaffold design of protein kinase CK2 inhibitors as potential COVID-19 therapeutics. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 1811-1827.	3.5	5
2	Ligand-based pharmacophore modeling of TNF- α to design novel inhibitors using virtual screening and molecular dynamics. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 1702-1718.	3.5	8
3	Insights into the structural and dynamical changes of spike glycoprotein mutations associated with SARS-CoV-2 host receptor binding. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 263-275.	3.5	29
4	Targeting SARS-CoV-2 nucleocapsid oligomerization: Insights from molecular docking and molecular dynamics simulations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 2430-2443.	3.5	29
5	Structural insights into the mechanism of human methyltransferase hPRMT4. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 10821-10834.	3.5	3
6	DriverFuse: An R package for analysis of next-generation sequencing datasets to identify cancer driver fusion genes. <i>PLoS ONE</i> , 2022, 17, e0262686.	2.5	2
7	Machine learning assisted analysis of breast cancer gene expression profiles reveals novel potential prognostic biomarkers for triple-negative breast cancer. <i>Computational and Structural Biotechnology Journal</i> , 2022, 20, 1618-1631.	4.1	17
8	Insights into the structure and dynamics of SARS-CoV-2 spike glycoprotein double mutant L452R-E484Q. <i>3 Biotech</i> , 2022, 12, 87.	2.2	5
9	BIO22-027: Exploiting Machine Learning to Unravel Prognostic Biomarkers in Lung Cancer. <i>Journal of the National Comprehensive Cancer Network: JNCCN</i> , 2022, 20, BIO22-027.	4.9	0
10	In-Silico Functional Annotation of Plasmodium falciparum Hypothetical Proteins to Identify Novel Drug Targets. <i>Frontiers in Genetics</i> , 2022, 13, 821516.	2.3	3
11	Latent Tuberculosis Infection Diagnosis among Household Contacts in a High Tuberculosis-Burden Area: a Comparison between Transcript Signature and Interferon Gamma Release Assay. <i>Microbiology Spectrum</i> , 2022, 10, e0244521.	3.0	4
12	Anti-Fungal Drug Anidulafungin Inhibits SARS-CoV-2 Spike-Induced Syncytia Formation by Targeting ACE2-Spike Protein Interaction. <i>Frontiers in Genetics</i> , 2022, 13, 866474.	2.3	13
13	ProtPathDB: A Web-based Resource of Parasite Proteases. <i>Current Bioinformatics</i> , 2022, 17, 710-722.	1.5	0
14	Bazedoxifene, a Postmenopausal Drug, Acts as an Antimalarial and Inhibits Hemozoin Formation. <i>Microbiology Spectrum</i> , 2022, 10, .	3.0	4
15	Heme Detoxification Protein (<i>Pf</i> HDP) is essential for the hemoglobin uptake and metabolism in <i>Plasmodium falciparum</i> . <i>FASEB BioAdvances</i> , 2022, 4, 662-674.	2.4	5
16	Screening Malaria-box compounds to identify potential inhibitors against SARS-CoV-2 Mpro, using molecular docking and dynamics simulation studies. <i>European Journal of Pharmacology</i> , 2021, 890, 173664.	3.5	25
17	<i>In-silico</i> profiling and structural insights into the impact of nSNPs in the <i>P. falciparum</i> acetyl-CoA transporter gene to understand the mechanism of drug resistance in malaria. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 558-569.	3.5	2
18	Unsupervised subtyping and methylation landscape of pancreatic ductal adenocarcinoma. <i>Heliyon</i> , 2021, 7, e06000.	3.2	11

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19	Virus-Free Improved Food in the Era of Bacterial Immunity. Concepts and Strategies in Plant Sciences, 2021, , 63-96.	0.5	0
20	Simultaneous Inhibition of SARS-CoV-2 Entry Pathways by Cyclosporine. ACS Chemical Neuroscience, 2021, 12, 930-944.	3.5	20
21	Structural stability predictions and molecular dynamics simulations of RBD and HR1 mutations associated with SARS-CoV-2 spike glycoprotein. Journal of Biomolecular Structure and Dynamics, 2021, , 1-13.	3.5	11
22	Machine Learning Assisted Prediction of Prognostic Biomarkers Associated With COVID-19, Using Clinical and Proteomics Data. Frontiers in Genetics, 2021, 12, 636441.	2.3	17
23	Computational Design of Novel Allosteric Inhibitors for Plasmodium falciparum DegP. Molecules, 2021, 26, 2742.	3.8	5
24	A Plasmodium falciparum protein tyrosine phosphatase inhibitor identified from the ChEMBL database blocks parasite growth. FEBS Open Bio, 2021, 11, 1921-1929.	2.3	1
25	Detection of truncated isoforms of human neuroserpin lacking the reactive center loop: Implications in noninhibitory role. IUBMB Life, 2021, 73, 941-952.	3.4	1
26	The landscape of microRNAs in plant viral infections. Plant Gene, 2021, 26, 100293.	2.3	2
27	Atomic Resolution Homology Models and Molecular Dynamics Simulations of Plasmodium falciparum Tubulins. ACS Omega, 2021, 6, 17510-17522.	3.5	9
28	Plasmodium falciparum DDX17 is an RNA helicase crucial for parasite development. Biochemistry and Biophysics Reports, 2021, 26, 101000.	1.3	2
29	The structural, functional, and dynamic effect of Tau tubulin kinase1 upon a mutation: A neurodegenerative hotspot. Journal of Cellular Biochemistry, 2021, 122, 1653-1664.	2.6	11
30	Identification of COVID-19 prognostic markers and therapeutic targets through meta-analysis and validation of Omics data from nasopharyngeal samples. EBioMedicine, 2021, 70, 103525.	6.1	27
31	Plasmodium falciparum metacaspase-2 capture its natural substrate in a non-canonical way. Journal of Biochemistry, 2021, 170, 639-653.	1.7	2
32	Targeting cathepsins: A potential link between COVID-19 and associated neurological manifestations. Heliyon, 2021, 7, e08089.	3.2	11
33	A molecular journey to check the conformational dynamics of tau tubulin kinase 2 mutations associated with Alzheimer's disease. RSC Advances, 2021, 11, 1320-1331.	3.6	12
34	Artemisinin Binds and Inhibits the Activity of Plasmodium falciparum Ddi1, a Retroviral Aspartyl Protease. Pathogens, 2021, 10, 1465.	2.8	5
35	Classifying juvenile onset primary open angle glaucoma using cluster analysis. British Journal of Ophthalmology, 2020, 104, 827-835.	3.9	10
36	Computational prediction and experimental validation of the activator function of C2- ¹² -D-glucopyranosyl-1,3,6,7-tetrahydroxyxanthone on pancreatic and hepatic hexokinase. Journal of Biomolecular Structure and Dynamics, 2020, 38, 2976-2987.	3.5	3

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37	Artificial Intelligence-Based Classification of Chest X-Ray Images into COVID-19 and Other Infectious Diseases. <i>International Journal of Biomedical Imaging</i> , 2020, 2020, 1-10.	3.9	87
38	Metagenomic analysis of the fecal microbiome of an adult elephant reveals the diversity of CAZymes related to lignocellulosic biomass degradation. <i>Symbiosis</i> , 2020, 81, 209-222.	2.3	11
39	Indian major basmati paddy seed varieties images dataset. <i>Data in Brief</i> , 2020, 33, 106460.	1.0	3
40	Dataset of mutational analysis, miRNAs targeting SARS-CoV-2 genes and host gene expression in SARS-CoV and SARS-CoV-2 infections. <i>Data in Brief</i> , 2020, 32, 106207.	1.0	5
41	Identification of Novel SARS-CoV-2 Drug Targets by Host MicroRNAs and Transcription Factors Co-regulatory Interaction Network Analysis. <i>Frontiers in Genetics</i> , 2020, 11, 571274.	2.3	52
42	Identification and characterization of a novel isoform of heparin cofactor <scp>II</scp> in human liver. <i>IUBMB Life</i> , 2020, 72, 2180-2193.	3.4	4
43	Integrative analyses of SARS-CoV-2 genomes from different geographical locations reveal unique features potentially consequential to host-virus interaction, pathogenesis and clues for novel therapies. <i>Heliyon</i> , 2020, 6, e04658.	3.2	104
44	Classification models for Invasive Ductal Carcinoma Progression, based on gene expression data-trained supervised machine learning. <i>Scientific Reports</i> , 2020, 10, 4113.	3.3	23
45	Plasmodium Condensin Core Subunits SMC2/SMC4 Mediate Atypical Mitosis and Are Essential for Parasite Proliferation and Transmission. <i>Cell Reports</i> , 2020, 30, 1883-1897.e6.	6.4	22
46	Changes in strand 6B and helix B during neuroserpin inhibition: Implication in severity of clinical phenotype. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2020, 1868, 140363.	2.3	4
47	<i>Plasmodium</i> DEH is ER-localized and crucial for oocyst mitotic division during malaria transmission. <i>Life Science Alliance</i> , 2020, 3, e202000879.	2.8	6
48	Whole-Genome Sequence of Drug-Resistant Mycobacterium tuberculosis Strain S7, Isolated from a Patient with Pulmonary Tuberculosis. <i>Microbiology Resource Announcements</i> , 2020, 9, .	0.6	1
49	S.Typhi derived OmpC peptide conjugated with Vi-polysaccharide evokes better immune response than free Vi-polysaccharide in mice. <i>Biologicals</i> , 2019, 62, 50-56.	1.4	4
50	ApicoTFdb: the comprehensive web repository of apicomplexan transcription factors and transcription-associated co-factors. <i>Database: the Journal of Biological Databases and Curation</i> , 2019, .	3.0	2
51	A genome-wide analysis of coatomer protein (COP) subunits of apicomplexan parasites and their evolutionary relationships. <i>BMC Genomics</i> , 2019, 20, 98.	2.8	5
52	PAmiRDB: A web resource for plant miRNAs targeting viruses. <i>Scientific Reports</i> , 2019, 9, 4627.	3.3	10
53	A novel identification approach for discovery of 5-HydroxyTryptamine 2A antagonists: combination of 2D/3D similarity screening, molecular docking and molecular dynamics. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 931-943.	3.5	15
54	iRSVPred: A Web Server for Artificial Intelligence Based Prediction of Major Basmati Paddy Seed Varieties. <i>Frontiers in Plant Science</i> , 2019, 10, 1791.	3.6	7

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55	A consensus-guided approach yields a heat-stable alkane-producing enzyme and identifies residues promoting thermostability. <i>Journal of Biological Chemistry</i> , 2018, 293, 9148-9161.	3.4	20
56	Investigation of Multiple Resistance Mechanisms in Voriconazole-Resistant <i>Aspergillus flavus</i> Clinical Isolates from a Chest Hospital Surveillance in Delhi, India. <i>Antimicrobial Agents and Chemotherapy</i> , 2018, 62, .	3.2	39
57	Role of CYP1B1, p.E229K and p.R368H mutations among 120 families with sporadic juvenile onset open-angle glaucoma. <i>Graefe's Archive for Clinical and Experimental Ophthalmology</i> , 2018, 256, 355-362.	1.9	13
58	High throughput <i>in silico</i> identification and characterization of <i>Plasmodium falciparum</i> PRL phosphatase inhibitors. <i>Journal of Biomolecular Structure and Dynamics</i> , 2018, 36, 3531-3540.	3.5	9
59	Host Lipid Rafts Play a Major Role in Binding and Endocytosis of Influenza A Virus. <i>Viruses</i> , 2018, 10, 650.	3.3	47
60	Biochemical characterization of <i>Plasmodium</i> complement factors binding protein for its role in immune modulation. <i>Biochemical Journal</i> , 2018, 475, 2877-2891.	3.7	3
61	Altered Pathway Analyzer: A gene expression dataset analysis tool for identification and prioritization of differentially regulated and network rewired pathways. <i>Scientific Reports</i> , 2017, 7, 40450.	3.3	12
62	A hydrophobic patch surrounding Trp154 in human neuroserpin controls the helix F dynamics with implications in inhibition and aggregation. <i>Scientific Reports</i> , 2017, 7, 42987.	3.3	8
63	RNAi Suppressors: Biology and Mechanisms. <i>RNA Technologies</i> , 2017, , 199-230.	0.3	11
64	Proteomic Identification and Analysis of Arginine-Methylated Proteins of <i>Plasmodium falciparum</i> at Asexual Blood Stages. <i>Journal of Proteome Research</i> , 2017, 16, 368-383.	3.7	35
65	Exploring Heme and Hemoglobin Binding Regions of <i>Plasmodium</i> Heme Detoxification Protein for New Antimalarial Discovery. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 8298-8308.	6.4	21
66	Comparative insights into the saccharification potentials of a relatively unexplored but robust <i>Penicillium funiculosum</i> glycoside hydrolase 7 cellobiohydrolase. <i>Biotechnology for Biofuels</i> , 2017, 10, 71.	6.2	30
67	PRmePRed: A protein arginine methylation prediction tool. <i>PLoS ONE</i> , 2017, 12, e0183318.	2.5	28
68	KiPho: malaria parasite kinome and phosphatome portal. <i>Database: the Journal of Biological Databases and Curation</i> , 2017, 2017, .	3.0	1
69	An RNAi-based high-throughput screening assay to identify small molecule inhibitors of hepatitis B virus replication. <i>Journal of Biological Chemistry</i> , 2017, 292, 12577-12588.	3.4	14
70	Evaluation of efficacy of the fixed vs unfixed combination of latanoprost and timolol in patients of open-angle glaucoma and ocular hypertension insufficiently controlled on timolol and latanoprost monotherapy. <i>National Journal of Physiology, Pharmacy and Pharmacology</i> , 2017, , 1.	0.1	0
71	Identification of CYP1B1-specific candidate inhibitors using combination of <i>in silico</i> screening, integrated knowledge-based filtering, and molecular dynamics simulations. <i>Chemical Biology and Drug Design</i> , 2016, 88, 730-739.	3.2	4
72	Widespread occurrence of lysine methylation in <i>Plasmodium falciparum</i> proteins at asexual blood stages. <i>Scientific Reports</i> , 2016, 6, 35432.	3.3	18

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73	Gene Network Rewiring to Study Melanoma Stage Progression and Elements Essential for Driving Melanoma. PLoS ONE, 2015, 10, e0142443.	2.5	9
74	Comparative insight into nucleotide excision repair components of Plasmodium falciparum. DNA Repair, 2015, 28, 60-72.	2.8	10
75	3â€² and 5â€² microRNA-end post-biogenesis modifications in plant transcriptomes: Evidences from small RNA next generation sequencing data analysis. Biochemical and Biophysical Research Communications, 2015, 467, 892-899.	2.1	5
76	Machine learning for biomarker identification in cancer research â€“ developments toward its clinical application. Personalized Medicine, 2015, 12, 371-387.	1.5	40
77	miRMOD: a tool for identification and analysis of 5â€² and 3â€² miRNA modifications in Next Generation Sequencing small RNA data. PeerJ, 2015, 3, e1332.	2.0	21
78	Supervised Learning Classification Models for Prediction of Plant Virus Encoded RNA Silencing Suppressors. PLoS ONE, 2014, 9, e97446.	2.5	13
79	Genome wide in silico analysis of Plasmodium falciparum phosphatome. BMC Genomics, 2014, 15, 1024.	2.8	24
80	The evolutionary dynamics of variant antigen genes in Babesia reveal a history of genomic innovation underlying host-parasite interaction. Nucleic Acids Research, 2014, 42, 7113-7131.	14.5	90
81	Classification models for clear cell renal carcinoma stage progression, based on tumor RNAseq expression trained supervised machine learning algorithms. BMC Proceedings, 2014, 8, S2.	1.6	47
82	<i>In silico</i> characterization and molecular dynamics simulation of Pfcyc-1, a cyclin homolog of <i>Plasmodium falciparum</i> . Journal of Biomolecular Structure and Dynamics, 2014, 32, 1624-1633.	3.5	0
83	GFF-Ex: a genome feature extraction package. BMC Research Notes, 2014, 7, 315.	1.4	9
84	Bacillus thuringiensis toxin, Cry1C interacts with 128HLHFHLP134 region of aminopeptidase N of agricultural pest, Spodoptera litura. Process Biochemistry, 2014, 49, 688-696.	3.7	7
85	Gene disruption reveals a dispensable role for Plasmepsin VII in the Plasmodium berghei life cycle. Molecular and Biochemical Parasitology, 2014, 195, 10-13.	1.1	17
86	Protein folding grand challenge: hydrophobic vs. hydrophilic forces. Journal of Biomolecular Structure and Dynamics, 2013, 31, 1008-1010.	3.5	0
87	Identifying Bacterial Virulent Proteins by Fusing a Set of Classifiers Based on Variants of Chou's Pseudo Amino Acid Composition and on Evolutionary Information. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2012, 9, 467-475.	3.0	156
88	Identification of mirtrons in rice using MirtronPred: A tool for predicting plant mirtrons. Genomics, 2012, 99, 370-375.	2.9	29
89	Development of target focused library against drug target of P. falciparum using SVM and Molecular docking. Journal of Cheminformatics, 2012, 4, .	6.1	0
90	Support Vector Machine Based Prediction of P. falciparum Proteasome Inhibitors and Development of Focused Library by Molecular Docking. Combinatorial Chemistry and High Throughput Screening, 2011, 14, 898-907.	1.1	7

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91	Support Vector Machine Based Classification Model for Screening Plasmodium falciparum Proliferation Inhibitors and Non-Inhibitors. Biomedical Engineering and Computational Biology, 2011, 3, BECB.S7503.	2.0	5
92	Disruption of a mitochondrial protease machinery in Plasmodium falciparum is an intrinsic signal for parasite cell death. Cell Death and Disease, 2011, 2, e231-e231.	6.3	36
93	Chaperones and foldases in endoplasmic reticulum stress signaling in plants. Plant Signaling and Behavior, 2011, 6, 232-236.	2.4	73
94	A cyanobacterial serine protease of <i>Plasmodium falciparum</i> is targeted to the apicoplast and plays an important role in its growth and development. Molecular Microbiology, 2010, 77, 873-890.	2.5	48
95	FaaPred: A SVM-Based Prediction Method for Fungal Adhesins and Adhesin-Like Proteins. PLoS ONE, 2010, 5, e9695.	2.5	37
96	Thermo and pH stable ATP-independent chaperone activity of heat-inducible Hsp70 from <i>Pennisetum glaucum</i> . Plant Signaling and Behavior, 2010, 5, 110-121.	2.4	14
97	Machine Learning Methods for Prediction of CDK-Inhibitors. PLoS ONE, 2010, 5, e13357.	2.5	9
98	ProtVirDB: a database of protozoan virulent proteins. Bioinformatics, 2009, 25, 1568-1569.	4.1	12
99	LipocalinPred: a SVM-based method for prediction of lipocalins. BMC Bioinformatics, 2009, 10, 445.	2.6	18
100	Molecular Modeling Studies of the Interaction Between Plasmodium falciparum HslU and HslV Subunits. Journal of Biomolecular Structure and Dynamics, 2009, 26, 473-479.	3.5	25
101	A systematic classification of Plasmodium falciparum P-loop NTPases: structural and functional correlation. Malaria Journal, 2009, 8, 69.	2.3	10
102	VirulentPred: a SVM based prediction method for virulent proteins in bacterial pathogens. BMC Bioinformatics, 2008, 9, 62.	2.6	250
103	CyclinPred: A SVM-Based Method for Predicting Cyclin Protein Sequences. PLoS ONE, 2008, 3, e2605.	2.5	28
104	Virtual high throughput screening (vHTS) – A perspective. Bioinformation, 2008, 3, 14-17.	0.5	53
105	Characterization and localization of Plasmodium falciparum homolog of prokaryotic ClpQ/HslV protease. Molecular and Biochemical Parasitology, 2007, 152, 139-148.	1.1	41
106	ProtRepeatsDB: a database of amino acid repeats in genomes. BMC Bioinformatics, 2006, 7, 336.	2.6	33
107	A database for Plasmodium falciparum protein models. Bioinformation, 2005, 1, 50-51.	0.5	1
108	Distribution of proline-rich (PxxP) motifs in distinct proteomes: functional and therapeutic implications for malaria and tuberculosis. Protein Engineering, Design and Selection, 2004, 17, 175-182.	2.1	50

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109	PlasmoDB: the Plasmodium genome resource. A database integrating experimental and computational data. <i>Nucleic Acids Research</i> , 2003, 31, 212-215.	14.5	329
110	PlasmoDB: the Plasmodium genome resource. An integrated database providing tools for accessing, analyzing and mapping expression and sequence data (both finished and unfinished). <i>Nucleic Acids Research</i> , 2002, 30, 87-90.	14.5	110
111	The Plasmodium genome database. <i>Nature</i> , 2002, 419, 490-492.	27.8	156
112	The 3' End of Hepatitis E Virus (HEV) Genome Binds Specifically to the Viral RNA-Dependent RNA Polymerase (RdRp). <i>Virology</i> , 2001, 282, 87-101.	2.4	135
113	The ORF3 Protein of Hepatitis E Virus Binds to Src Homology 3 Domains and Activates MAPK. <i>Journal of Biological Chemistry</i> , 2001, 276, 42389-42400.	3.4	132
114	Cloning, sequencing, and expression of the hepatitis E virus (HEV) nonstructural open reading frame 1 (ORF1). <i>Journal of Medical Virology</i> , 2000, 60, 275-283.	5.0	102
115	Cloning, sequencing, and expression of the hepatitis E virus (HEV) nonstructural open reading frame 1 (ORF1). , 2000, 60, 275.		1
116	Natural selection plays a significant role in governing the codon usage bias in the novel SARS-CoV-2 variants of concern (VOC). <i>PeerJ</i> , 0, 10, e13562.	2.0	4