Punit Kaur

List of Publications by Year in descending order

84 papers	1,389 citations	394286 19 h-index	395590 33 g-index
89 all docs	89 docs citations	89 times ranked	2193 citing authors

#	Article	IF	Citations
1	N-acetylglucosamine-phosphatidylinositol de-N-acetylase as a novel target for probing potential inhibitor against Leishmania donovani. Journal of Biomolecular Structure and Dynamics, 2023, 41, 1904-1918.	2.0	4
2	Comprehensive omics studies of p53 mutants in human cancer. Briefings in Functional Genomics, 2023, 22, 97-108.	1.3	6
3	Structure prediction and discovery of inhibitors against phosphopantothenoyl cysteine synthetase of Acinetobacter baumannii. Journal of Biomolecular Structure and Dynamics, 2022, 40, 11405-11417.	2.0	4
4	Identification and structural studies of natural inhibitors against SARS-CoV-2 viral RNA methyltransferase (NSP16). Journal of Biomolecular Structure and Dynamics, 2022, 40, 13965-13975.	2.0	14
5	Identification of novel natural MurD ligase inhibitors as potential antimicrobial agents targeting Acinetobacter baumannii: In silico screening and biological evaluation. Journal of Biomolecular Structure and Dynamics, 2022, 40, 14051-14066.	2.0	3
6	Identification of polypharmacological anticancerous molecules against Aurora kinase family of proteins. Journal of Cellular Biochemistry, 2022, 123, 719-735.	1.2	8
7	Deciphering the mechanism of p73 recognition of p53 response elements using the crystal structure of p73-DNA complexes and computational studies. International Journal of Biological Macromolecules, 2022, 206, 40-50.	3.6	2
8	Genome-wide identification of carbapenem-resistant Gram-negative bacterial (CR-GNB) isolates retrieved from hospitalized patients in Bihar, India. Scientific Reports, 2022, 12, 8477.	1.6	8
9	Structural analysis of LpqY, a substrate-binding protein from the SugABC transporter of Mycobacterium tuberculosis, provides insights into its trehalose specificity. Acta Crystallographica Section D: Structural Biology, 2022, 78, 835-845.	1.1	3
10	Identification of bioactive molecule from Withania somnifera (Ashwagandha) as SARS-CoV-2 main protease inhibitor. Journal of Biomolecular Structure and Dynamics, 2021, 39, 5668-5681.	2.0	105
11	Identification of potential drug candidates to combat COVID-19: a structural study using the main protease (mpro) of SARS-CoV-2. Journal of Biomolecular Structure and Dynamics, 2021, 39, 6649-6659.	2.0	25
12	Identification of promising drug candidates against NSP16 of SARS-CoV-2 through computational drug repurposing study. Journal of Biomolecular Structure and Dynamics, 2021, 39, 6713-6727.	2.0	20
13	Mutation Spectrum of Tuberous Sclerosis Complex Patients in Indian Population. Journal of Pediatric Genetics, 2021, 10, 274-283.	0.3	1
14	Corrigendum to â€œSpectrum of amyloglucosidase mutations in Asian Indian patients with Glycogen storage disease type <scp>III</scp>. Am J Med Genet Part A. 2020;<scp>182A</scp>:1190â€“1,200â€• American Journal of Medical Genetics, Part A, 2021, 185, 1008-1010.	0.7	0
15	Potassium-induced partial inhibition of lactoperoxidase: structure of the complex of lactoperoxidase with potassium ion at 2.20ÂÃ... resolution. Journal of Biological Inorganic Chemistry, 2021, 26, 149-159.	1.1	4
16	AMR-Diag: Neural network based genotype-to-phenotype prediction of resistance towards Î²-lactams in Escherichia coli and Klebsiella pneumoniae. Computational and Structural Biotechnology Journal, 2021, 19, 1896-1906.	1.9	38
17	Structure of Yak Lactoperoxidase at 1.55ÂÃ... Resolution. Protein Journal, 2021, 40, 8-18.	0.7	5
18	Curcumin rescue p53Y220C in BxPC-3 pancreatic adenocarcinomas cell line: Evidence-based on computational, biophysical, and in vivo studies. Biochimica Et Biophysica Acta - General Subjects, 2021, 1865, 129807.	1.1	7

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19	Structural analysis of COVID-19 spike protein in recognizing the ACE2 receptor of different mammalian species and its susceptibility to viral infection. 3 Biotech, 2021, 11, 109.	1.1	18
20	Heteroarene-fused anthraquinone derivatives as potential modulators for human aurora kinase B. Biochimie, 2021, 182, 152-165.	1.3	9
21	Structural insights into the transient closed conformation and pH dependent ATPase activity of S.Typhi GyraseB N- terminal domain. Archives of Biochemistry and Biophysics, 2021, 701, 108786.	1.4	3
22	Cardioprotective effects of azilsartan compared with that of telmisartan on an in vivo model of myocardial ischemiaâ€reperfusion injury. Journal of Biochemical and Molecular Toxicology, 2021, 35, e22785.	1.4	6
23	Genome-wide identification of potential biomarkers in multiple myeloma using meta-analysis of mRNA and miRNA expression data. Scientific Reports, 2021, 11, 10957.	1.6	13
24	Evolving scenario of big data and Artificial Intelligence (AI) in drug discovery. Molecular Diversity, 2021, 25, 1439-1460.	2.1	38
25	Structure of a ternary complex of lactoperoxidase with iodide and hydrogen peroxide at 1.77ÂÃ... resolution. Journal of Inorganic Biochemistry, 2021, 220, 111461.	1.5	9
26	Computational Intelligence in Drug Repurposing for COVID-19. Studies in Computational Intelligence, 2021, , 273-294.	0.7	6
27	Exome sequencing identifies procollagen-lysine 2-oxoglutarate 5-dioxygenase 2 mutations in primary congenital and juvenile glaucoma. Indian Journal of Ophthalmology, 2021, 69, 2710.	0.5	4
28	Structural and functional insights into the spike protein mutations of emerging SARS-CoV-2 variants. Cellular and Molecular Life Sciences, 2021, 78, 7967-7989.	2.4	40
29	Efficacy of Quercetin as a potent sensitizer of Î²2-AR in combating the impairment of fluid clearance in lungs of rats under hypoxia. Respiratory Physiology and Neurobiology, 2020, 273, 103334.	0.7	6
30	Pathogenic/likely pathogenic variants in the SHOX, GHR and IGFALS genes among Indian children with idiopathic short stature. Journal of Pediatric Endocrinology and Metabolism, 2020, 33, 79-88.	0.4	15
31	Allosteric inhibition and kinetic characterization of Klebsiella pneumoniae CysE: An emerging drug target. International Journal of Biological Macromolecules, 2020, 151, 1240-1249.	3.6	7
32	The molecular mechanism involved in cardioprotection by the dietary flavonoid fisetin as an agonist of PPAR-Î³ in a murine model of myocardial infarction. Archives of Biochemistry and Biophysics, 2020, 694, 108572.	1.4	21
33	Structure based drug discovery and in vitro activity testing for DNA gyrase inhibitors of Salmonella enterica serovar Typhi. Bioorganic Chemistry, 2020, 104, 104244.	2.0	6
34	Structure-Based Virtual Screening and Biochemical Validation to Discover a Potential Inhibitor of the SARS-CoV-2 Main Protease. ACS Omega, 2020, 5, 33151-33161.	1.6	27
35	Genomic profiling of antimicrobial resistance genes in clinical isolates of Salmonella Typhi from patients infected with Typhoid fever in India. Scientific Reports, 2020, 10, 8299.	1.6	41
36	Drug repurposing approach to target FtsZ cell division protein from Salmonella Typhi. International Journal of Biological Macromolecules, 2020, 159, 1073-1083.	3.6	10

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37	Spectrum of amyloglucosidase mutations in Asian Indian patients with Glycogen storage disease type III. American Journal of Medical Genetics, Part A, 2020, 182, 1190-1200.	0.7	6
38	The pivot point arginines identified in the Î²-pinwheel structure of C-terminal domain from Salmonella Typhi DNA Gyrase A subunit. Scientific Reports, 2020, 10, 7817.	1.6	2
39	Discovery of Novel DNA Gyrase Inhibitors Against Salmonella Typhi using Structure Based Drug Delivery Approach. Biophysical Journal, 2020, 118, 72a-73a.	0.2	1
40	Structural and conformational behavior of MurE ligase from Salmonella enterica serovar Typhi at different temperature and pH conditions. International Journal of Biological Macromolecules, 2020, 150, 389-399.	3.6	8
41	Binding and structural studies of the complexes of type 1 ribosome inactivating protein from <scp>Momordica balsamina</scp> with uracil and uridine. Proteins: Structure, Function and Bioinformatics, 2019, 87, 99-109.	1.5	1
42	Decoding of novel missense TSC2 gene variants using in-silico methods. BMC Medical Genetics, 2019, 20, 164.	2.1	4
43	Structure model of ferrochelatase from Salmonella Typhi elucidating metalation mechanism. International Journal of Biological Macromolecules, 2019, 127, 585-593.	3.6	6
44	Azithromycin resistance mechanisms in typhoidal salmonellae in India: A 25 years analysis. Indian Journal of Medical Research, 2019, 149, 404.	0.4	16
45	New antitumor anthra[2,3-b]furan-3-carboxamides: Synthesis and structure-activity relationship. European Journal of Medicinal Chemistry, 2018, 148, 128-139.	2.6	26
46	Estimation of structure and stability of MurE ligase from Salmonella enterica serovar Typhi. International Journal of Biological Macromolecules, 2018, 109, 375-382.	3.6	5
47	Search of multiple hot spots on the surface of peptidyl-tRNA hydrolase: structural, binding and antibacterial studies. Biochemical Journal, 2018, 475, 547-560.	1.7	5
48	A glycoprotein from mammary gland secreted during involution promotes apoptosis: Structural and biological studies. Archives of Biochemistry and Biophysics, 2018, 644, 72-80.	1.4	0
49	Structural basis of activation of mammalian heme peroxidases. Progress in Biophysics and Molecular Biology, 2018, 133, 49-55.	1.4	16
50	NGSPanPipe: A Pipeline for Pan-genome Identification in Microbial Strains from Experimental Reads. Advances in Experimental Medicine and Biology, 2018, 1052, 39-49.	0.8	4
51	Identification of Shared Molecular Signatures Indicate the Susceptibility of Endometriosis to Multiple Sclerosis. Frontiers in Genetics, 2018, 9, 42.	1.1	16
52	Effect of chemical denaturants on the conformational stability of GyrB subunit of DNA gyrase from Salmonella enterica serovar Typhi. International Journal of Biological Macromolecules, 2017, 103, 165-174.	3.6	2
53	Application of whole exome sequencing in elucidating the phenotype and genotype spectrum of junctional epidermolysis bullosa: A preliminary experience of a tertiary care centre in India. Journal of Dermatological Science, 2017, 86, 30-36.	1.0	16
54	Structure of bovine lactoperoxidase with a partially linked heme moiety at 1.98Ã... resolution. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2017, 1865, 329-335.	1.1	14

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55	Design of anti-thyroid drugs: Binding studies and structure determination of the complex of lactoperoxidase with 2-mercaptoimidazole at 2.30 Ã... resolution. Proteins: Structure, Function and Bioinformatics, 2017, 85, 1882-1890.	1.5	3
56	Asparagine Synthetase deficiency-report of a novel mutation and review of literature. Metabolic Brain Disease, 2017, 32, 1889-1900.	1.4	24
57	Binding studies and structure determination of the recombinantly produced type-II 3-dehydroquinate dehydratase from Acinetobacter baumannii. International Journal of Biological Macromolecules, 2017, 94, 459-465.	3.6	4
58	Structure and binding studies of proliferating cell nuclear antigen from Leishmania donovani. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2017, 1865, 1395-1405.	1.1	3
59	Structure of iron saturated <scp>C</scp>â€lobe of bovine lactoferrin at p<scp>H</scp> 6.8 indicates a weakening of iron coordination. Proteins: Structure, Function and Bioinformatics, 2016, 84, 591-599.	1.5	23
60	Serum 5-LOX: a progressive protein marker for breast cancer and new approach for therapeutic target. Carcinogenesis, 2016, 37, 912-917.	1.3	30
61	Binding and structural studies of the complexes of type 1 ribosome inactivating protein from Momordica balsamina with cytosine, cytidine, and cytidine diphosphate. Biochemistry and Biophysics Reports, 2015, 4, 134-140.	0.7	3
62	Structure Based In Silico Analysis of Quinolone Resistance in Clinical Isolates of Salmonella Typhi from India. PLoS ONE, 2015, 10, e0126560.	1.1	26
63	Structures and binding studies of the complexes of phospholipase A2 with five inhibitors. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2015, 1854, 269-277.	1.1	24
64	Current Overview of Allergens of Plant Pathogenesis Related Protein Families. Scientific World Journal, The, 2014, 2014, 1-19.	0.8	170
65	Crystal structure of peptidylâ€tRNA hydrolase from a Gramâ€positive bacterium, Streptococcus pyogenes at 2.19 Ã... resolution shows the closed structure of the substrateâ€binding cleft. FEBS Open Bio, 2014, 4, 915-922.	1.0	12
66	Structure of the ironâ€free true Câ€terminal half of bovine lactoferrin produced by tryptic digestion and its functional significance in the gut. FEBS Journal, 2014, 281, 2871-2882.	2.2	11
67	Structural and binding studies of peptidyl-tRNA hydrolase from Pseudomonas aeruginosa provide a platform for the structure-based inhibitor design against peptidyl-tRNA hydrolase. Biochemical Journal, 2014, 463, 329-337.	1.7	17
68	Identification of a high affinity selective inhibitor of Polo-like kinase 1 for cancer chemotherapy by computational approach. Journal of Molecular Graphics and Modelling, 2014, 51, 104-112.	1.3	4
69	Pharmacophore Mapping, In Silico Screening and Molecular Docking to Identify Selective Trypanosoma brucei Pteridine Reductase Inhibitors. Molecular Informatics, 2014, 33, 124-134.	1.4	4
70	Structural and functional insights into peptidyl-tRNA hydrolase. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2014, 1844, 1279-1288.	1.1	29
71	Preparation and Antimicrobial Action of Three Tryptic Digested Functional Molecules of Bovine Lactoferrin. PLoS ONE, 2014, 9, e90011.	1.1	26
72	Antimicrobial Lactoferrin Peptides: The Hidden Players in the Protective Function of a Multifunctional Protein. International Journal of Peptides, 2013, 2013, 1-12.	0.7	98

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73	Cloning, Expression, and Purification of Nucleoside Diphosphate Kinase fromAcinetobacter baumannii. Enzyme Research, 2013, 2013, 1-4.	1.8	5
74	3D-QSAR based pharmacophore modeling and virtual screening for identification of novel pteridine reductase inhibitors. Journal of Molecular Modeling, 2012, 18, 1701-1711.	0.8	26
75	Structural analysis of a secretory phospholipase A2 from Clonorchis sinensis: therapeutic implications for hepatic fibrosis. FASEB Journal, 2012, 26, 964.1.	0.2	1
76	Structure-based in-silico rational design of a selective peptide inhibitor for thymidine monophosphate kinase of mycobacterium tuberculosis. Journal of Molecular Modeling, 2011, 17, 1173-1182.	0.8	14
77	Structureâ€Based In silico Design of aHighâ€Affinity Dipeptide Inhibitor for Novel Protein Drug Target Shikimate Kinase of Mycobacterium tuberculosis. Chemical Biology and Drug Design, 2010, 76, 277-284.	1.5	14
78	Human group III phospholipase A2 as a drug target: structural analysis and ligand binding studies. FASEB Journal, 2010, 24, 681.7.	0.2	0
79	Backbone-side-chain interactions in serine Synthesis, crystal structure and solution conformation of a linear model peptide N-Boc-l-Ser-l-Phe-OCH3. International Journal of Peptide and Protein Research, 2009, 48, 299-303.	0.1	2
80	Crystal structures of complexes of phospholipase A 2 with natural and synthetic inhibitors. FASEB Journal, 2007, 21, A638.	0.2	0
81	Indian Scorpion PLA ₂ : A functional convergence. FASEB Journal, 2006, 20, A474.	0.2	0
82	Structure of a Serine Protease Proteinase K from Tritirachium album limber at 0.98 Ã... Resolution. Biochemistry, 2001, 40, 3080-3088.	1.2	128
83	Contributory presentations/posters. Journal of Biosciences, 1999, 24, 33-198.	0.5	0
84	Design of Peptides Using Î±,Î²-Dehydro-residues: Synthesis, Crystal Structure and Molecular Conformation ofN-Boc-L-Val-Î”Pheâ€“Î”Phe-L-Ala-OCH3. Journal of Peptide Science, 1996, 2, 357-363.	0.8	3