

Shankar Prasad Kanaujia

List of Publications by Year in descending order

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41
papers

303
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1040056

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360
citing authors

#	ARTICLE	IF	CITATIONS
1	Structural and functional role of invariant water molecules in matrix metalloproteinases: a data-mining approach. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022, 40, 10074-10085.	3.5	3
2	Role of an orphan substrate-binding protein MhuP in transient heme transfer in <i>Mycobacterium tuberculosis</i> . <i>International Journal of Biological Macromolecules</i> , 2022, 211, 342-356.	7.5	3
3	Exploiting the rationale behind substrate recognition by promiscuous thermophilic NDP-sugar pyrophosphorylase for expanding glycorandomization: an <i>in silico</i> study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, 39, 6099-6111.	3.5	0
4	Water-mediated structural rearrangement establishes active conformation of caspases for apoptosis and inflammation. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021, , 1-14.	3.5	0
5	Structural and thermodynamic insights into the novel dinucleotide-binding protein of ABC transporter unveils its moonlighting function. <i>FEBS Journal</i> , 2021, 288, 4614-4636.	4.7	3
6	Acyldepsipeptide activated ClpP1P2 macromolecule of <i>Leptospira</i> , an ideal Achilles heel to hamper the cell survival and deregulate ClpP proteolytic activity. <i>Research in Microbiology</i> , 2021, 172, 103797.	2.1	4
7	Conserved features of the <i>scp</i> MlaD domain aid the trafficking of hydrophobic molecules. <i>Proteins: Structure, Function and Bioinformatics</i> , 2021, 89, 1473-1488.	2.6	1
8	Identification and characterization of metal uptake ABC transporters in <i>Mycobacterium tuberculosis</i> unveil their ligand specificity. <i>International Journal of Biological Macromolecules</i> , 2021, 185, 324-337.	7.5	4
9	An updated classification and mechanistic insights into ligand binding of the substrate-binding proteins. <i>FEBS Letters</i> , 2021, 595, 2395-2409.	2.8	15
10	Structural and thermodynamic insights into a novel Mg ²⁺ citrate-binding protein from the ABC transporter superfamily. <i>Acta Crystallographica Section D: Structural Biology</i> , 2021, 77, 1516-1534.	2.3	1
11	Structural and thermodynamic correlation illuminates the selective transport mechanism of disaccharide β -glucosides through ABC transporter. <i>FEBS Journal</i> , 2020, 287, 1576-1597.	4.7	12
12	Conformational Trapping of a β -Glucosides-Binding Protein Unveils the Selective Two-Step Ligand-Binding Mechanism of ABC Importers. <i>Journal of Molecular Biology</i> , 2020, 432, 5711-5734.	4.2	8
13	An insight into bacterial phospholipase C classification and their translocation through Tat and Sec pathways: A data mining study. <i>Meta Gene</i> , 2019, 20, 100547.	0.6	4
14	Designating ligand specificities to metal uptake ABC transporters in <i>Thermus thermophilus</i> HB8. <i>Metallomics</i> , 2019, 11, 597-612.	2.4	15
15	Design of novel PhMTNA inhibitors, targeting neurological disorder through homology modeling, molecular docking, and dynamics approaches. <i>Journal of Receptor and Signal Transduction Research</i> , 2019, 39, 28-38.	2.5	7
16	Role of Structural Features in Oligomerization, Active-Site Integrity and Ligand Binding of Ribose-1,5-Bisphosphate Isomerase. <i>Computational and Structural Biotechnology Journal</i> , 2019, 17, 333-344.	4.1	5
17	Identification and characterization of ABC transporters for carbohydrate uptake in <i>Thermus thermophilus</i> HB8. <i>Gene</i> , 2019, 696, 135-148.	2.2	15
18	Structural insights into the catalytic mechanism of 5-methylthioribose 1-phosphate isomerase. <i>Journal of Structural Biology</i> , 2019, 205, 67-77.	2.8	3

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19	Archaeal and eukaryal translation initiation factor 1 differ in their RNA interacting loops. <i>FEBS Letters</i> , 2018, 592, 1602-1610.	2.8	2
20	A presumed homologue of the regulatory subunits of eIF2B functions as ribose-1,5-bisphosphate isomerase in <i>Pyrococcus horikoshii</i> OT3. <i>Scientific Reports</i> , 2018, 8, 1891.	3.3	5
21	In silico characterization of TTHA0596: A potential Zn ²⁺ binding protein of ATP-binding cassette transporter. <i>Gene Reports</i> , 2017, 6, 132-141.	0.8	2
22	UgpB, a periplasmic component of the UgpABCE ATP-binding cassette transporter, predominantly follows the Sec translocation pathway. <i>Meta Gene</i> , 2017, 13, 129-139.	0.6	3
23	Computational characterization of TTHA0379: A potential glycerophosphocholine binding protein of Ugp ATP-binding cassette transporter. <i>Gene</i> , 2016, 592, 260-268.	2.2	10
24	In silico analysis of 5' UTRs highlights the prevalence of Shine-Dalgarno and leaderless-dependent mechanisms of translation initiation in bacteria and archaea, respectively. <i>Journal of Theoretical Biology</i> , 2016, 402, 54-61.	1.7	15
25	Direct inhibition of matrix metalloproteinase-2 (MMP-2) by (âˆ”)-epigallocatechin-3-gallate: A possible role for the fibronectin type II repeats. <i>Gene</i> , 2016, 593, 126-130.	2.2	12
26	In silico analysis suggests that PH0702 and PH0208 encode for methylthioribose-1-phosphate isomerase and ribose-1,5-bisphosphate isomerase, respectively, rather than aIF2B ^{Î²} and aIF2B ^{Î³} . <i>Gene</i> , 2016, 575, 118-126.	2.2	7
27	Heterogeneous behavior of metalloproteins toward metal ion binding and selectivity: insights from molecular dynamics studies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2016, 34, 1470-1485.	3.5	7
28	Role of invariant water molecules and water-mediated ionic interactions in D-xylose isomerase from <i>Streptomyces rubiginosus</i> . <i>Journal of Biomolecular Structure and Dynamics</i> , 2013, 31, 376-384.	3.5	2
29	Crystal structures and binding studies of atovaquone and its derivatives with cytochrome bc1: a molecular basis for drug design. <i>CrystEngComm</i> , 2013, 15, 4871.	2.6	10
30	Structure of SAICAR synthetase from <i>Pyrococcus horikoshii</i> OT3: Insights into thermal stability. <i>International Journal of Biological Macromolecules</i> , 2013, 53, 7-19.	7.5	6
31	Crystal structures, dynamics and functional implications of molybdenum-cofactor biosynthesis protein MogA from two thermophilic organisms. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2011, 67, 2-16.	0.7	4
32	Free and ATP-bound structures of Ap ₄ A hydrolase from <i>Aquifex aeolicus</i> V5. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010, 66, 116-124.	2.5	7
33	Structures of apo and GTP-bound molybdenum cofactor biosynthesis protein MoaC from <i>Thermus thermophilus</i> HB8. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2010, 66, 821-833.	2.5	22
34	Structural and functional role of water molecules in bovine pancreatic phospholipase A ₂ : a data-mining approach. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2009, 65, 74-84.	2.5	21
35	Structures and molecular-dynamics studies of three active-site mutants of bovine pancreatic phospholipase A ₂ . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2008, 64, 1003-1011.	2.5	3
36	Observation of a calcium-binding site in the Î³-class carbonic anhydrase from <i>Pyrococcus horikoshii</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2008, 64, 1012-1019.	2.5	48

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37	Crystallization and preliminary crystallographic analysis of molybdenum-cofactor biosynthesis protein C from <i>Thermus thermophilus</i> . <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2007, 63, 27-29.	0.7	4
38	Cloning, expression, purification, crystallization and preliminary X-ray crystallographic study of DHNA synthetase from <i>Geobacillus kaustophilus</i> . <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2007, 63, 103-105.	0.7	4
39	Cloning, expression, purification, crystallization and preliminary X-ray crystallographic study of molybdopterin synthase from <i>Thermus thermophilus</i> HB8. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2007, 63, 324-326.	0.7	2
40	Preliminary X-ray crystallographic study of glucose dehydrogenase from <i>Thermus thermophilus</i> HB8. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2007, 63, 446-448.	0.7	1
41	Suggestive evidence for the involvement of the second calcium and surface loop in interfacial binding: monoclinic and trigonal crystal structures of a quadruple mutant of phospholipase A2. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2006, 62, 717-724.	2.5	3