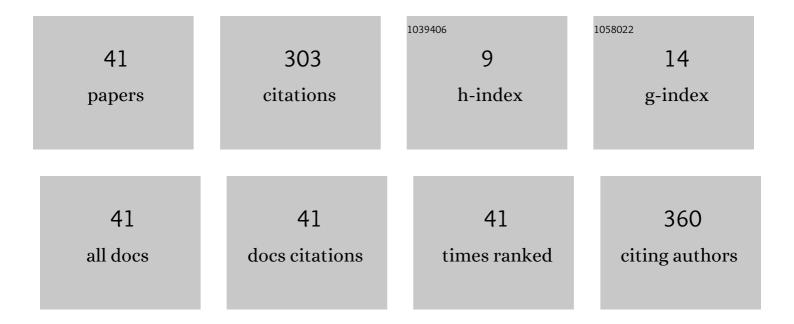
## Shankar Prasad Kanaujia

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Structural and functional role of invariant water molecules in matrix metalloproteinases: a data-mining approach. Journal of Biomolecular Structure and Dynamics, 2022, 40, 10074-10085.	2.0	3
2	Role of an orphan substrate-binding protein MhuP in transient heme transfer in Mycobacterium tuberculosis. International Journal of Biological Macromolecules, 2022, 211, 342-356.	3.6	3
3	Exploiting the rationale behind substrate recognition by promiscuous thermophilic NDP-sugar pyrophosphorylase for expanding glycorandomization: an <i>in silico</i> study. Journal of Biomolecular Structure and Dynamics, 2021, 39, 6099-6111.	2.0	0
4	Water-mediated structural rearrangement establishes active conformation of caspases for apoptosis and inflammation. Journal of Biomolecular Structure and Dynamics, 2021, , 1-14.	2.0	0
5	Structural and thermodynamic insights into the novel dinucleotideâ€binding protein of ABC transporter unveils its moonlighting function. FEBS Journal, 2021, 288, 4614-4636.	2.2	3
6	Acyldepsipeptide activated ClpP1P2 macromolecule of Leptospira, an ideal Achilles' heel to hamper the cell survival and deregulate ClpP proteolytic activity. Research in Microbiology, 2021, 172, 103797.	1.0	4
7	Conserved features of the <scp>MlaD</scp> domain aid the trafficking of hydrophobic molecules. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1473-1488.	1.5	1
8	Identification and characterization of metal uptake ABC transporters in Mycobacterium tuberculosis unveil their ligand specificity. International Journal of Biological Macromolecules, 2021, 185, 324-337.	3.6	4
9	An updated classification and mechanistic insights into ligand binding of the substrateâ€binding proteins. FEBS Letters, 2021, 595, 2395-2409.	1.3	15
10	Structural and thermodynamic insights into a novel Mg <sup>2+</sup> –citrate-binding protein from the ABC transporter superfamily. Acta Crystallographica Section D: Structural Biology, 2021, 77, 1516-1534.	1.1	1
11	Structural and thermodynamic correlation illuminates the selective transport mechanism of disaccharide αâ€glycosides through ABC transporter. FEBS Journal, 2020, 287, 1576-1597.	2.2	12
12	Conformational Trapping of a β-Glucosides-Binding Protein Unveils the Selective Two-Step Ligand-Binding Mechanism of ABC Importers. Journal of Molecular Biology, 2020, 432, 5711-5734.	2.0	8
13	An insight into bacterial phospholipase C classification and their translocation through Tat and Sec pathways: A data mining study. Meta Gene, 2019, 20, 100547.	0.3	4
14	Designating ligand specificities to metal uptake ABC transporters in <i>Thermus thermophilus</i> HB8. Metallomics, 2019, 11, 597-612.	1.0	15
15	Design of novel <i>Ph</i> MTNA inhibitors, targeting neurological disorder through homology modeling, molecular docking, and dynamics approaches. Journal of Receptor and Signal Transduction Research, 2019, 39, 28-38.	1.3	7
16	Role of Structural Features in Oligomerization, Active-Site Integrity and Ligand Binding of Ribose-1,5-Bisphosphate Isomerase. Computational and Structural Biotechnology Journal, 2019, 17, 333-344.	1.9	5
17	Identification and characterization of ABC transporters for carbohydrate uptake in Thermus thermophilus HB8. Gene, 2019, 696, 135-148.	1.0	15
18	Structural insights into the catalytic mechanism of 5-methylthioribose 1-phosphate isomerase. Journal of Structural Biology, 2019, 205, 67-77.	1.3	3

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19	Archaeal and eukaryal translation initiation factor 1 differ in their RNA interacting loops. FEBS Letters, 2018, 592, 1602-1610.	1.3	2
20	A presumed homologue of the regulatory subunits of eIF2B functions as ribose-1,5-bisphosphate isomerase in Pyrococcus horikoshii OT3. Scientific Reports, 2018, 8, 1891.	1.6	5
21	In silico characterization of TTHA0596: A potential Zn 2+ binding protein of ATP-binding cassette transporter. Gene Reports, 2017, 6, 132-141.	0.4	2
22	UgpB, a periplasmic component of the UgpABCE ATP-binding cassette transporter, predominantly follows the Sec translocation pathway. Meta Gene, 2017, 13, 129-139.	0.3	3
23	Computational characterization of TTHA0379: A potential glycerophosphocholine binding protein of Ugp ATP-binding cassette transporter. Gene, 2016, 592, 260-268.	1.0	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. Journal of Theoretical Biology, 2016, 402, 54-61.	0.8	15
25	Direct inhibition of matrix metalloproteinase-2 (MMP-2) by (â^')-epigallocatechin-3-gallate: A possible role for the fibronectin type II repeats. Gene, 2016, 593, 126-130.	1.0	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 alF2Bβ and alF2Bδ. Gene, 2016, 575, 118-126.	1.0	7
27	Heterogeneous behavior of metalloproteins toward metal ion binding and selectivity: insights from molecular dynamics studies. Journal of Biomolecular Structure and Dynamics, 2016, 34, 1470-1485.	2.0	7
28	Role of invariant water molecules and water-mediated ionic interactions in D-xylose isomerase fromStreptomyces rubiginosus. Journal of Biomolecular Structure and Dynamics, 2013, 31, 376-384.	2.0	2
29	Crystal structures and binding studies of atovaquone and its derivatives with cytochrome bc1: a molecular basis for drug design. CrystEngComm, 2013, 15, 4871.	1.3	10
30	Structure of SAICAR synthetase from Pyrococcus horikoshii OT3: Insights into thermal stability. International Journal of Biological Macromolecules, 2013, 53, 7-19.	3.6	6
31	Crystal structures, dynamics and functional implications of molybdenum-cofactor biosynthesis protein MogA from two thermophilic organisms. Acta Crystallographica Section F: Structural Biology Communications, 2011, 67, 2-16.	0.7	4
32	Free and ATP-bound structures of Ap <sub>4</sub> A hydrolase from <i>Aquifex aeolicus</i> V5. Acta Crystallographica Section D: Biological Crystallography, 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. Acta Crystallographica Section D: Biological Crystallography, 2010, 66, 821-833.	2.5	22
34	Structural and functional role of water molecules in bovine pancreatic phospholipase A <sub>2</sub> : a data-mining approach. Acta Crystallographica Section D: Biological Crystallography, 2009, 65, 74-84.	2.5	21
35	Structures and molecular-dynamics studies of three active-site mutants of bovine pancreatic phospholipase A <sub>2</sub> . Acta Crystallographica Section D: Biological Crystallography, 2008, 64, 1003-1011.	2.5	3
36	Observation of a calcium-binding site in the γ-class carbonic anhydrase from <i>Pyrococcus horikoshii</i> . Acta Crystallographica Section D: Biological Crystallography, 2008, 64, 1012-1019.	2.5	48

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37	Crystallization and preliminary crystallographic analysis of molybdenum-cofactor biosynthesis protein C fromThermus thermophilus. Acta Crystallographica Section F: Structural Biology Communications, 2007, 63, 27-29.	0.7	4
38	Cloning, expression, purification, crystallization and preliminary X-ray crystallographic study of DHNA synthetase fromGeobacillus kaustophilus. Acta Crystallographica Section F: Structural Biology Communications, 2007, 63, 103-105.	0.7	4
39	Cloning, expression, purification, crystallization and preliminary X-ray crystallographic study of molybdopterin synthase fromThermus thermophilusHB8. Acta Crystallographica Section F: Structural Biology Communications, 2007, 63, 324-326.	0.7	2
40	Preliminary X-ray crystallographic study of glucose dehydrogenase fromThermus thermophilusHB8. Acta Crystallographica Section F: Structural Biology Communications, 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. Acta Crystallographica Section D: Biological Crystallography, 2006, 62, 717-724.	2.5	3