Nagendra Singh

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Crystal Structure of Lactoperoxidase at 2.4ÂÃ Resolution. Journal of Molecular Biology, 2008, 376, 1060-1075.	2.0	102
2	A physiological connection between tmRNA and peptidyl-tRNA hydrolase functions in Escherichia coli. Nucleic Acids Research, 2004, 32, 6028-6037.	6.5	68
3	Structural Plasticity and Enzyme Action: Crystal Structures of Mycobacterium tuberculosis Peptidyl-tRNA Hydrolase. Journal of Molecular Biology, 2007, 372, 186-193.	2.0	58
4	Inhibition of Lactoperoxidase by Its Own Catalytic Product: Crystal Structure of the Hypothiocyanate-Inhibited Bovine Lactoperoxidase at 2.3-Ã Resolution. Biophysical Journal, 2009, 96, 646-654.	0.2	54
5	Molecular basis for nonspecificity of nonsteroidal anti-inflammatory drugs (NSAIDs). Drug Discovery Today, 2015, 20, 863-873.	3.2	53
6	Identification of potential inhibitors of SARS-COV-2 endoribonuclease (EndoU) from FDA approved drugs: a drug repurposing approach to find therapeutics for COVID-19. Journal of Biomolecular Structure and Dynamics, 2021, 39, 4201-4211.	2.0	52
7	Aptamer-Based TB Antigen Tests for the Rapid Diagnosis of Pulmonary Tuberculosis: Potential Utility in Screening for Tuberculosis. ACS Infectious Diseases, 2018, 4, 1718-1726.	1.8	51
8	Structural Evidence of Substrate Specificity in Mammalian Peroxidases. Journal of Biological Chemistry, 2009, 284, 14849-14856.	1.6	50
9	Mode of Binding of the Tuberculosis Prodrug Isoniazid to Heme Peroxidases. Journal of Biological Chemistry, 2010, 285, 1569-1576.	1.6	45
10	Binding Modes of Aromatic Ligands to Mammalian Heme Peroxidases with Associated Functional Implications. Journal of Biological Chemistry, 2009, 284, 20311-20318.	1.6	39
11	Identification of a novel and potent inhibitor of phospholipase A2 in a medicinal plant: Crystal structure at 1.93Ã and Surface Plasmon Resonance analysis of phospholipase A2 complexed with berberine. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2011, 1814, 657-663.	1.1	39
12	Structural Basis of Recognition of Pathogen-associated Molecular Patterns and Inhibition of Proinflammatory Cytokines by Camel Peptidoglycan Recognition Protein. Journal of Biological Chemistry, 2011, 286, 16208-16217.	1.6	36
13	Specific binding of non-steroidal anti-inflammatory drugs (NSAIDs) to phospholipase A2: structure of the complex formed between phospholipase A2and diclofenac at 2.7â€Â resolution. Acta Crystallographica Section D: Biological Crystallography, 2006, 62, 410-416.	2.5	32
14	The Structural Basis for the Prevention of Nonsteroidal Antiinflammatory Drug-Induced Gastrointestinal Tract Damage by the C-Lobe of Bovine Colostrum Lactoferrin. Biophysical Journal, 2009, 97, 3178-3186.	0.2	32
15	Biochemical studies and crystal structure determination of dihydrodipicolinate synthase from Pseudomonas aeruginosa. International Journal of Biological Macromolecules, 2011, 48, 779-787.	3.6	29
16	Evidence for a role of initiation factor 3 in recycling of ribosomal complexes stalled on mRNAs in Escherichia coli. Nucleic Acids Research, 2005, 33, 5591-5601.	6.5	27
17	Simultaneous inhibition of antiâ€coagulation and inflammation: crystal structure of phospholipase A ₂ complexed with indomethacin at 1.4 à resolution reveals the presence of the new common ligandâ€binding site. Journal of Molecular Recognition, 2009, 22, 437-445.	1.1	27
18	Polysaccharide binding sites in hyaluronate lyase – crystal structures of native phage–encoded hyaluronate lyase and its complexes with ascorbic acid and lactose. FEBS Journal, 2009, 276, 3392-3402.	2.2	27

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19	Phospholipase A2 as a Target Protein for Nonsteroidal Anti-Inflammatory Drugs (NSAIDs): Crystal Structure of the Complex Formed between Phospholipase A2 and Oxyphenbutazone at 1.6 A Resolution. Biochemistry, 2004, 43, 14577-14583.	1.2	26
20	Crystal structures of the complexes of a group IIA phospholipase A 2 with two natural antiâ€inflammatory agents, anisic acid, and atropine reveal a similar mode of binding. Proteins: Structure, Function and Bioinformatics, 2006, 64, 89-100.	1.5	25
21	First structural evidence for the mode of diffusion of aromatic ligands and ligand-induced closure of the hydrophobic channel in heme peroxidases. Journal of Biological Inorganic Chemistry, 2010, 15, 1099-1107.	1.1	24
22	Detection of native peptides as potent inhibitors of enzymes. FEBS Journal, 2005, 272, 562-572.	2.2	23
23	Crystal structure of a secretory signalling glycoprotein from sheep at 2.0Ã resolution. Journal of Structural Biology, 2006, 156, 505-516.	1.3	22
24	The Mode of Inhibitor Binding to Peptidyl-tRNA Hydrolase: Binding Studies and Structure Determination of Unbound and Bound Peptidyl-tRNA Hydrolase from Acinetobacter baumannii. PLoS ONE, 2013, 8, e67547.	1.1	21
25	<i>In silico</i> identification and validation of natural antiviral compounds as potential inhibitors of SARS-CoV-2 methyltransferase. Journal of Biomolecular Structure and Dynamics, 2022, 40, 6534-6544.	2.0	21
26	Crystal structure of a novel phospholipase A2 from Naja naja sagittifera with a strong anticoagulant activity. Toxicon, 2005, 46, 865-875.	0.8	20
27	Structural Elements of Ligand Recognition Site in Secretory Phospholipase A2 and Structure-Based Design of Specific Inhibitors. Current Topics in Medicinal Chemistry, 2007, 7, 757-764.	1.0	20
28	Structure of the zinc-saturated C-terminal lobe of bovine lactoferrin at 2.0â€Ã resolution. Acta Crystallographica Section D: Biological Crystallography, 2005, 61, 1107-1115.	2.5	19
29	Non-steroidal anti-inflammatory drugs as potent inhibitors of phospholipase A2: structure of the complex of phospholipase A2with niflumic acid at 2.5â€Ã resolution. Acta Crystallographica Section D: Biological Crystallography, 2005, 61, 1579-1586.	2.5	19
30	Substituted hydrazinecarbothioamide as potent antitubercular agents: Synthesis and quantitative structure–activity relationship (QSAR). Bioorganic and Medicinal Chemistry Letters, 2010, 20, 2597-2600.	1.0	18
31	Synthesis, Structure–Activity Relationship and Docking Studies of Substituted Aryl Thiazolyl Phenylsulfonamides as Potential Protein Tyrosine Phosphataseâ€1B Inhibitors. ChemMedChem, 2012, 7, 1185-1190.	1.6	16
32	Exploring potential inhibitor of SARS-CoV2 replicase from FDA approved drugs using insilico drug discovery methods. Journal of Biomolecular Structure and Dynamics, 2022, 40, 5507-5514.	2.0	16
33	Crystal Structure of the Peptidoglycan Recognition Protein at 1.8ÂÃ Resolution Reveals Dual Strategy to Combat Infection Through Two Independent Functional Homodimers. Journal of Molecular Biology, 2008, 378, 923-932.	2.0	14
34	Crystal structure of a heterodimer of phospholipase A2 from Naja naja sagittifera at 2.3 Ã resolution reveals the presence of a new PLA2-like protein with a novel cys 32-Cys 49 disulphide bridge with a bound sugar at the substrate-binding site. Proteins: Structure, Function and Bioinformatics, 2005, 62, 329-337.	1.5	13
35	Crystal structure determination and inhibition studies of a novel xylanase and α â€amylase inhibitor protein (XAIP) from <i>Scadoxus multiflorus</i> . FEBS Journal, 2010, 277, 2868-2882.	2.2	12
36	Identification of a novel and potent small molecule inhibitor of SRPK1: mechanism of dual inhibition of SRPK1 for the inhibition of cancer progression. Aging, 2021, 13, 163-180.	1.4	12

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37	Carbohydrate-binding properties of goat secretory glycoprotein (SPC-40) and its functional implications: structures of the native glycoprotein and its four complexes with chitin-like oligosaccharides. Acta Crystallographica Section D: Biological Crystallography, 2007, 63, 437-446.	2.5	11
38	Specific interactions of C-terminal half (C-lobe) of lactoferrin protein with edible sugars: Binding and structural studies with implications on diabetes. International Journal of Biological Macromolecules, 2010, 47, 50-59.	3.6	11
39	Crystal structure of the complex of group I PLA2 with a group II-specific peptide Leu-Ala-Ile-Tyr-Ser (LAIYS) at 2.6 Ã resolution. Journal of Drug Targeting, 2005, 13, 367-374.	2.1	9
40	Crystal structure of a highly acidic neurotoxin from scorpion Buthus tamulus at $2.2\zeta^{2}$ resolution reveals novel structural features. Journal of Structural Biology, 2006, 155, 52-62.	1.3	9
41	Traditional Nutritional and Health Practices Targeting Lifestyle Behavioral Changes in Humans. Journal of Lifestyle Medicine, 2020, 10, 67-73.	0.3	9
42	Crystal structure of peptidyl-tRNA hydrolase from mycobacterium smegmatis reveals novel features related to enzyme dynamics. International Journal of Biochemistry and Molecular Biology, 2012, 3, 58-69.	0.1	9
43	Lactoferrin-melanin interaction and its possible implications in melanin polymerization: Crystal structure of the complex formed between mare lactoferrin and melanin monomers at 2.7-A resolution. Proteins: Structure, Function and Bioinformatics, 2001, 45, 229-236.	1.5	7
44	Crystal structure of a calcium-induced dimer of two isoforms of cobra phospholipase A2 at 1.6 Ã resolution. Proteins: Structure, Function and Bioinformatics, 2005, 59, 856-863.	1.5	7
45	Cloning, expression, purification, crystallization and preliminary X-ray analysis of peptidyl-tRNA hydrolase fromMycobacterium tuberculosis. Acta Crystallographica Section F: Structural Biology Communications, 2006, 62, 913-915.	0.7	7
46	Isolation, purification, crystallization and preliminary crystallographic studies of amaryllin, a plant pathogenesis-related protein from <i>Amaryllis belladonna</i> . Acta Crystallographica Section F: Structural Biology Communications, 2009, 65, 635-637.	0.7	6
47	Structure of the zinc-induced heterodimer of two calcium-free isoforms of phospholipase A2fromNaja naja sagittiferaat 2.7â€Â resolution. Acta Crystallographica Section D: Biological Crystallography, 2005, 61, 302-308.	2.5	5
48	Structural and binding studies of C-terminal half (C-lobe) of lactoferrin protein with COX-2-specific non-steroidal anti-inflammatory drugs (NSAIDs). Archives of Biochemistry and Biophysics, 2010, 500, 196-202.	1.4	5
49	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
50	Bioengineering of crop plants for improved tetrahydrofolate production. Bioengineered, 2018, 9, 152-158.	1.4	5
51	Identification and evaluation of quercetin as a potential inhibitor of naphthoate synthase fromEnterococcus faecalis. Journal of Molecular Recognition, 2019, 32, e2802.	1.1	5
52	Expression of Regucalcin, a calcium-binding protein is regulated by hypoxia-inducible factor-1α. Life Sciences, 2022, 292, 120278.	2.0	5
53	Modulation of inhibitory activity of xylanase - α-amylase inhibitor protein (XAIP): binding studies and crystal structure determination of XAIP- II from Scadoxus multiflorus at 1.2 Ã resolution. BMC Structural Biology, 2010, 10, 41.	2.3	4
54	Identification of hot spot residues on serine-arginine protein kinase-1 by molecular dynamics simulation studies. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1579-1587.	2.0	4

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55	Purification and preliminary X-ray crystallographic studies of β-microseminoprotein from human seminal plasma. Acta Crystallographica Section F: Structural Biology Communications, 2009, 65, 518-521.	0.7	3
56	Recombinant overexpression of dihydroneopterin aldolase catalyst potentially regulates folateâ€biofortification. Journal of Basic Microbiology, 2017, 57, 517-524.	1.8	3
57	Direct detection of Mycobacterium tuberculosis rifampin resistance in bio-safe stained sputum smears. PLoS ONE, 2017, 12, e0189149.	1.1	3
58	Structural studies on dihydrouridine synthase A (DusA) from Pseudomonas aeruginosa. International Journal of Biological Macromolecules, 2019, 132, 254-264.	3.6	3
59	Isolation, purification, crystallization and preliminary crystallographic studies of sagitoxin, an oligomeric cardiotoxin from the venom ofNaja naja saggitifera. Acta Crystallographica Section F: Structural Biology Communications, 2008, 64, 545-547.	0.7	1
60	Tryptophan as a three-way switch in regulating the function of the secretory signalling glycoprotein (SPS-40) from mammary glands: structure of SPS-40 complexed with 2-methylpentane-2,4-diol at 1.6â€Ã resolution. Acta Crystallographica Section D: Biological Crystallography, 2009, 65, 375-378.	2.5	1
61	Crystal structures of complexes of phospholipase A 2 with natural and synthetic inhibitors. FASEB Journal, 2007, 21, A638.	0.2	0