K Sekar

List of Publications by Year
in descending order

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83	2,153	236612	243296
papers	citations	25 h-index	44 g-index

83	83	83	2272
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	A novel mode of carbohydrate recognition in jacalin, a Moraceae plant lectin with a Î²-prism fold. Nature Structural Biology, 1996, 3, 596-603.	9.7	224
2	Ramachandran Plot on The Web (2.0). Protein and Peptide Letters, 2007, 14, 669-671.	0.4	124
3	3dSS: 3D structural superposition. Nucleic Acids Research, 2006, 34, W128-W132.	6.5	104
4	Crystal structures of artocarpin, a Moraceae lectin with mannose specificity, and its complex with methyl-Î±-d-mannose: implications to the generation of carbohydrate specificity. Journal of Molecular Biology, 2002, 317, 237-247.	2.0	97
5	Câ€“halogenâ€¦Ï€ interactions in proteins: a database study. Crystal Engineering, 2003, 6, 69-77.	0.7	86
6	Online_DPI: a web server to calculate the diffraction precision index for a protein structure. Journal of Applied Crystallography, 2015, 48, 939-942.	1.9	79
7	Crystal Structure of the Jacalinâ€“T-antigen Complex and a Comparative Study of Lectinâ€“T-antigen Complexes. Journal of Molecular Biology, 2002, 321, 637-645.	2.0	77
8	Ramachandran plot on the web. Bioinformatics, 2002, 18, 1548-1549.	1.8	69
9	X-ray Analysis of Mycobacterium smegmatis Dps and a Comparative Study Involving Other Dps and Dps-like Molecules. Journal of Molecular Biology, 2004, 339, 1103-1113.	2.0	67
10	Evolution, Homology Conservation, and Identification of Unique Sequence Signatures in GH19 Family Chitinases. Journal of Molecular Evolution, 2010, 70, 466-478.	0.8	66
11	Structure of Mycobacterium tuberculosis Single-stranded DNA-binding Protein. Variability in Quaternary Structure and Its Implications. Journal of Molecular Biology, 2003, 331, 385-393.	2.0	62
12	Unusual sugar specificity of banana lectin from Musa paradisiaca and its probable evolutionary origin. Crystallographic and modelling studies. Glycobiology, 2005, 15, 1025-1032.	1.3	61
13	Structural Basis for the Energetics of Jacalinâ€“Sugar Interactions: Promiscuity Versus Specificity. Journal of Molecular Biology, 2005, 347, 181-188.	2.0	60
14	An Insight to the Dynamics of Conserved Water Molecular Triad in IMPDH II (Human): Recognition of Cofactor and Substrate to Catalytic Arg 322. Journal of Biomolecular Structure and Dynamics, 2009, 27, 149-158.	2.0	60
15	Structural Basis of the Carbohydrate Specificities of Jacalin: An X-ray and Modeling Study. Journal of Molecular Biology, 2003, 332, 217-228.	2.0	58
16	Phospholipase A2Engineering. Structural and Functional Roles of the Highly Conserved Active Site Residue Aspartate-99â€. Biochemistry, 1997, 36, 3104-3114.	1.2	53
17	Structural Basis of the Anionic Interface Preference and Activation of Pancreatic Phospholipase A2. Biochemistry, 2000, 39, 12312-12323.	1.2	52
18	Crystal Structure of the Complex of Bovine Pancreatic Phospholipase A2with the Inhibitor 1-Hexadecyl-3-(trifluoroethyl)-sn-glycero-2-phosphomethanolâ€,â€¡. Biochemistry, 1997, 36, 14186-14191.	1.2	49

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19	Role of N and C-terminal Tails in DNA Binding and Assembly in Dps: Structural Studies of Mycobacterium smegmatis Dps Deletion Mutants. Journal of Molecular Biology, 2007, 370, 752-767.	2.0	49
20	PSAP: protein structure analysis package. Journal of Applied Crystallography, 2007, 40, 773-777.	1.9	41
21	Phospholipase A2Engineering. Deletion of the C-Terminus Segment Changes Substrate Specificity and Uncouples Calcium and Substrate Binding at the Zwitterionic Interfaceâ€‚â‡. Biochemistry, 1996, 35, 12164-12174.	1.2	37
22	A FAST Pattern Matching Algorithm. Journal of Chemical Information and Computer Sciences, 2004, 44, 1251-1256.	2.8	33
23	Structure ofMycobacterium smegmatissingle-stranded DNA-binding protein and a comparative study involving homologus SSBs: biological implications of structural plasticity and variability in quaternary association. Acta Crystallographica Section D: Biological Crystallography, 2005, 61, 1140-1148.	2.5	29
24	Crystal Structures of the Free and Anisic Acid Bound Triple Mutant of Phospholipase A2. Journal of Molecular Biology, 2003, 333, 367-376.	2.0	28
25	Conserved Water Mediated H-bonding Dynamics of Inhibitor, Cofactor, Asp 364 and Asn 303 in Human IMPDH II. Journal of Biomolecular Structure and Dynamics, 2009, 26, 497-507.	2.0	28
26	ProSTRIP: A method to find similar structural repeats in three-dimensional protein structures. Computational Biology and Chemistry, 2010, 34, 126-130.	1.1	25
27	RepEx: Repeat extractor for biological sequences. Genomics, 2013, 102, 403-408.	1.3	25
28	PDB Goodies â€“ a web-based GUI to manipulate the Protein Data Bank file. Acta Crystallographica Section D: Biological Crystallography, 2002, 58, 1385-1386.	2.5	24
29	Structural biology of Mycobacterium tuberculosis proteins: The Indian efforts. Tuberculosis, 2011, 91, 456-468.	0.8	22
30	Water-mediated ionic interactions in protein structures. Journal of Biosciences, 2011, 36, 253-263.	0.5	22
31	Structure, dynamics, and interactions of jacalin. Insights from molecular dynamics simulations examined in conjunction with results of Xâ€ray studies. Proteins: Structure, Function and Bioinformatics, 2009, 77, 760-777.	1.5	21
32	Observation of Additional Calcium Ion in the Crystal Structure of the Triple Mutant K56,120,121M of Bovine Pancreatic Phospholipase A2. Journal of Molecular Biology, 2002, 324, 755-762.	2.0	19
33	Purification, crystallization and preliminary X-ray structure analysis of the banana lectin fromMusa paradisiaca. Acta Crystallographica Section D: Biological Crystallography, 2004, 60, 2104-2106.	2.5	18
34	Structure of the Complex of Bovine Pancreatic Phospholipase A2 with a Transition-State Analogue. Acta Crystallographica Section D: Biological Crystallography, 1998, 54, 334-341.	2.5	16
35	Ion pairs in non-redundant protein structures. Journal of Biosciences, 2007, 32, 693-704.	0.5	16
36	C-halogenâ€¦pi interactions in nucleic acids: a database study. Journal of Chemical Sciences, 2020, 132, 1.	0.7	15

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37	High-resolution refinement of orthorhombic bovine pancreatic phospholipase A2. Acta Crystallographica Section D: Biological Crystallography, 1999, 55, 46-50.	2.5	14
38	Fragment Finder: a web-based software to identify similar three-dimensional structural motif. Nucleic Acids Research, 2005, 33, W85-W88.	6.5	14
39	CADB: Conformation Angles DataBase of proteins. Nucleic Acids Research, 2003, 31, 448-451.	6.5	12
40	Structures of the catalytic site mutants D99A and H48Q and the calcium-loop mutant D49E of phospholipase A2. Acta Crystallographica Section D: Biological Crystallography, 1999, 55, 443-447.	2.5	11
41	THGS: a web-based database of Transmembrane Helices in Genome Sequences. Nucleic Acids Research, 2004, 32, 125D-128.	6.5	10
42	Conserved water-mediated recognition and dynamics of NAD+(carboxamide group) to hIMPDH enzyme: water mimic approach toward the design of isoform-selective inhibitor. Journal of Biomolecular Structure and Dynamics, 2014, 32, 1248-1262.	2.0	10
43	WAP: water analysis package â€“ a Web-based package to calculate geometrical parameters between water oxygen and protein atoms. Journal of Applied Crystallography, 2003, 36, 167-168.	1.9	8
44	Crystallization and preliminary X-ray diffraction analysis ofMycobacterium smegmatisDps. Acta Crystallographica Section D: Biological Crystallography, 2003, 59, 2254-2256.	2.5	8
45	A redetermination of the structure of the triple mutantâ€…(K53,56,120M)â€…ofâ€…phospholipase A2at 1.6â€…Ã… resolution using sulfur-SAS at 1.54â€…Ã… wavelength. Acta Crystallographica Section D: Biological Crystallography, 2004, 60, 1586-1590.	2.5	8
46	Hydrogen Bonds Computing Server (HBCS): an online web server to compute hydrogen-bond interactions and their precision. Journal of Applied Crystallography, 2016, 49, 642-645.	1.9	8
47	Side-chain conformation angles of amino acids: effect of temperature factor cut-off. Journal of Structural Biology, 2003, 143, 181-184.	1.3	7
48	RPMS: Ramachandran plot for multiple structures. Journal of Applied Crystallography, 2008, 41, 219-221.	1.9	7
49	Recognition of active and inactive catalytic triads: A template based approach. International Journal of Biological Macromolecules, 2010, 46, 317-323.	3.6	7
50	New biochemical insight of conserved water molecules at catalytic and structural Zn2+ ions in human matrix metalloproteinase-I: a study by MD-simulation. Journal of Molecular Modeling, 2017, 23, 57.	0.8	7
51	RepEx: A web server to extract sequence repeats from protein and DNA sequences. Computational Biology and Chemistry, 2019, 78, 424-430.	1.1	7
52	Crystal and Molecular Structure of an Acridinedione. Crystal Research and Technology, 2002, 37, 1029-1037.	0.6	6
53	SSEP: secondary structural elements of proteins. Nucleic Acids Research, 2003, 31, 3404-3405.	6.5	6
54	SSEP-2.0: Secondary Structural Elements of Proteins. Acta Crystallographica Section D: Biological Crystallography, 2005, 61, 634-636.	2.5	6

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55	Structural Biology of Recombinant Bovine Pancreatic Phospholipase A2 and its Inhibitor Complexes. Current Topics in Medicinal Chemistry, 2007, 7, 779-785.	1.0	6
56	1.72 Ã... Resolution Refinement of the Trigonal Form of Bovine Pancreatic Phospholipase A2. Acta Crystallographica Section D: Biological Crystallography, 1998, 54, 342-346.	2.5	5
57	WAP(version 2.0): an updated computing and visualization server for water molecules. Journal of Applied Crystallography, 2008, 41, 952-954.	1.9	5
58	Role of water molecules and ion pairs in Dps and related ferritin-like structures. International Journal of Biological Macromolecules, 2008, 43, 333-338.	3.6	5
59	Fragment Finder 2.0: a computing server to identify structurally similar fragments. Journal of Applied Crystallography, 2012, 45, 332-334.	1.9	5
60	Crystal and molecular structure of 1-methyl-3-ethyl-2,6-diphenyl-4-piperidone and a study of the geometry of the 4-piperidone ring. Journal of Crystallographic and Spectroscopic Research, 1993, 23, 101-105.	0.3	4
61	Crystal and molecular structure of 2,6-bis(4-fluorobenzylidene)cyclohexanone. Crystal Research and Technology, 2003, 38, 822-828.	0.6	4
62	Crystal and molecular structure of 2,6-bis(4-chlorophenyl)-3-phenylpiperidin-4-one. Crystal Research and Technology, 2003, 38, 918-921.	0.6	4
63	CAP: conformation angles package--displaying the conformation angles of side chains in proteins. Bioinformatics, 2003, 19, 1043-1044.	1.8	4
64	SEM (Symmetry Equivalent Molecules): a web-based GUI to generate and visualize the macromolecules. Nucleic Acids Research, 2003, 31, 3356-3358.	6.5	4
65	Atomic resolution (0.97â€...Ã...) structure of the triple mutant (K53,56,121M) of bovine pancreatic phospholipase A2. Acta Crystallographica Section F: Structural Biology Communications, 2005, 61, 3-7.	0.7	4
66	Conformational Angles Database (CADB-3.0). Protein and Peptide Letters, 2007, 14, 665-668.	0.4	4
67	Structure of 4-piperidone derivatives. I. 3-Methyl-2,6-diphenyl-4-piperidone. Acta Crystallographica Section C: Crystal Structure Communications, 1990, 46, 1153-1155.	0.4	3
68	Structure of 4-piperidone derivatives. II. 2,6-Bis(p-methoxyphenyl)-3,5-dimethyl-4-piperidone. Acta Crystallographica Section C: Crystal Structure Communications, 1990, 46, 1338-1340.	0.4	3
69	BSDD: Biomolecules Segment Display Device--a web-based interactive display tool. Nucleic Acids Research, 2004, 32, W645-W648.	6.5	3
70	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
71	Large cryptic internal sequence repeats in protein structures from Homo sapiens. Journal of Biosciences, 2009, 34, 103-112.	0.5	3
72	ACMS: a database of alternate conformations found in the atoms of main and side chains of protein structures. Journal of Applied Crystallography, 2019, 52, 910-913.	1.9	3

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73	Atomic resolution structure of the double mutant (K53,56M) of bovine pancreatic phospholipase A2. Acta Crystallographica Section F: Structural Biology Communications, 2006, 62, 1-5.	0.7	2
74	MLDB: macromolecule ligand database. Journal of Applied Crystallography, 2010, 43, 200-202.	1.9	2
75	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
76	An algorithm to find distant repeats in a pair of protein sequences. Pattern Recognition Letters, 2010, 31, 2161-2169.	2.6	1
77	SSMBS: a web server to locate sequentially separated motifs in biological sequences. Journal of Applied Crystallography, 2010, 43, 203-205.	1.9	1
78	IMRPS: Inserted and Modified Residues in Protein Structures. A database. Journal of Applied Crystallography, 2020, 53, 569-573.	1.9	1
79	X-ray Analysis of Mycobacterium smegmatis Dps and a Comparative Study Involving Other Dps and Dps-like Molecules. Journal of Molecular Biology, 2004, 339, 1103-1103.	2.0	0
80	Third calcium ion found in an inhibitor-bound phospholipase A2. Acta Crystallographica Section D: Biological Crystallography, 2006, 62, 392-397.	2.5	0
81	NIMS: a database on nucleobase compounds and their interactions in macromolecular structures. Journal of Applied Crystallography, 2016, 49, 1093-1098.	1.9	0
82	PlaneFinder: a methodology to find the best plane for a set of atoms involved in the metal coordination in protein structures. Journal of Applied Crystallography, 2018, 51, 1251-1256.	1.9	0
83	An Algorithm to Find All Identical Motifs in Multiple Biological Sequences. Lecture Notes in Computer Science, 2010, , 137-148.	1.0	0