

K Sekar

List of Publications by Year in descending order

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Version: 2024-02-01

83
papers

2,153
citations

236612

25
h-index

243296

44
g-index

83
all docs

83
docs citations

83
times ranked

2272
citing authors

| # | ARTICLE | IF | CITATIONS |
|----|--|-----|-----------|
| 1 | C-halogenâ€¦pi interactions in nucleic acids: a database study. <i>Journal of Chemical Sciences</i> , 2020, 132, 1. | 0.7 | 15 |
| 2 | IMRPS: Inserted and Modified Residues in Protein Structures. A database. <i>Journal of Applied Crystallography</i> , 2020, 53, 569-573. | 1.9 | 1 |
| 3 | RepEx: A web server to extract sequence repeats from protein and DNA sequences. <i>Computational Biology and Chemistry</i> , 2019, 78, 424-430. | 1.1 | 7 |
| 4 | ACMS: a database of alternate conformations found in the atoms of main and side chains of protein structures. <i>Journal of Applied Crystallography</i> , 2019, 52, 910-913. | 1.9 | 3 |
| 5 | PlaneFinder: a methodology to find the best plane for a set of atoms involved in the metal coordination in protein structures. <i>Journal of Applied Crystallography</i> , 2018, 51, 1251-1256. | 1.9 | 0 |
| 6 | New biochemical insight of conserved water molecules at catalytic and structural Zn ²⁺ ions in human matrix metalloproteinase-I: a study by MD-simulation. <i>Journal of Molecular Modeling</i> , 2017, 23, 57. | 0.8 | 7 |
| 7 | NIMS: a database on nucleobase compounds and their interactions in macromolecular structures. <i>Journal of Applied Crystallography</i> , 2016, 49, 1093-1098. | 1.9 | 0 |
| 8 | <i>Hydrogen Bonds Computing Server</i> (<i>HBCS</i>): an online web server to compute hydrogen-bond interactions and their precision. <i>Journal of Applied Crystallography</i> , 2016, 49, 642-645. | 1.9 | 8 |
| 9 | <i>Online_DPI</i>: a web server to calculate the diffraction precision index for a protein structure. <i>Journal of Applied Crystallography</i> , 2015, 48, 939-942. | 1.9 | 79 |
| 10 | Conserved water-mediated recognition and dynamics of NAD ⁺ (carboxamide group) to hIMPDPH enzyme: water mimic approach toward the design of isoform-selective inhibitor. <i>Journal of Biomolecular Structure and Dynamics</i> , 2014, 32, 1248-1262. | 2.0 | 10 |
| 11 | 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. | 2.0 | 2 |
| 12 | RepEx: Repeat extractor for biological sequences. <i>Genomics</i> , 2013, 102, 403-408. | 1.3 | 25 |
| 13 | Fragment Finder 2.0: a computing server to identify structurally similar fragments. <i>Journal of Applied Crystallography</i> , 2012, 45, 332-334. | 1.9 | 5 |
| 14 | Structural biology of <i>Mycobacterium tuberculosis</i> proteins: The Indian efforts. <i>Tuberculosis</i> , 2011, 91, 456-468. | 0.8 | 22 |
| 15 | Water-mediated ionic interactions in protein structures. <i>Journal of Biosciences</i> , 2011, 36, 253-263. | 0.5 | 22 |
| 16 | Evolution, Homology Conservation, and Identification of Unique Sequence Signatures in GH19 Family Chitinases. <i>Journal of Molecular Evolution</i> , 2010, 70, 466-478. | 0.8 | 66 |
| 17 | An algorithm to find distant repeats in a pair of protein sequences. <i>Pattern Recognition Letters</i> , 2010, 31, 2161-2169. | 2.6 | 1 |
| 18 | ProSTRIP: A method to find similar structural repeats in three-dimensional protein structures. <i>Computational Biology and Chemistry</i> , 2010, 34, 126-130. | 1.1 | 25 |

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|----|--|-----|-----------|
| 19 | SSMBS: a web server to locate sequentially separated motifs in biological sequences. Journal of Applied Crystallography, 2010, 43, 203-205. | 1.9 | 1 |
| 20 | MLDB: macromolecule ligand database. Journal of Applied Crystallography, 2010, 43, 200-202. | 1.9 | 2 |
| 21 | Recognition of active and inactive catalytic triads: A template based approach. International Journal of Biological Macromolecules, 2010, 46, 317-323. | 3.6 | 7 |
| 22 | An Algorithm to Find All Identical Motifs in Multiple Biological Sequences. Lecture Notes in Computer Science, 2010, , 137-148. | 1.0 | 0 |
| 23 | Large cryptic internal sequence repeats in protein structures from Homo sapiens. Journal of Biosciences, 2009, 34, 103-112. | 0.5 | 3 |
| 24 | Structure, dynamics, and interactions of jacalin. Insights from molecular dynamics simulations examined in conjunction with results of X-ray studies. Proteins: Structure, Function and Bioinformatics, 2009, 77, 760-777. | 1.5 | 21 |
| 25 | 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 |
| 26 | 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 |
| 27 | <i>RPMS</i>: Ramachandran plot for multiple structures. Journal of Applied Crystallography, 2008, 41, 219-221. | 1.9 | 7 |
| 28 | <i>WAP</i> (version 2.0): an updated computing and visualization server for water molecules. Journal of Applied Crystallography, 2008, 41, 952-954. | 1.9 | 5 |
| 29 | 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 |
| 30 | Ramachandran Plot on The Web (2.0). Protein and Peptide Letters, 2007, 14, 669-671. | 0.4 | 124 |
| 31 | Conformational Angles Database (CADB-3.0). Protein and Peptide Letters, 2007, 14, 665-668. | 0.4 | 4 |
| 32 | Structural Biology of Recombinant Bovine Pancreatic Phospholipase A2 and its Inhibitor Complexes. Current Topics in Medicinal Chemistry, 2007, 7, 779-785. | 1.0 | 6 |
| 33 | 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 |
| 34 | PSAP: protein structure analysis package. Journal of Applied Crystallography, 2007, 40, 773-777. | 1.9 | 41 |
| 35 | Ion pairs in non-redundant protein structures. Journal of Biosciences, 2007, 32, 693-704. | 0.5 | 16 |
| 36 | Third calcium ion found in an inhibitor-bound phospholipase A2. Acta Crystallographica Section D: Biological Crystallography, 2006, 62, 392-397. | 2.5 | 0 |

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|----|---|-----|-----------|
| 37 | 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 |
| 38 | Atomic resolution structure of the double mutant (K53,56M) of bovine pancreatic phospholipase A2. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2006, 62, 1-5. | 0.7 | 2 |
| 39 | 3dSS: 3D structural superposition. <i>Nucleic Acids Research</i> , 2006, 34, W128-W132. | 6.5 | 104 |
| 40 | SSEP-2.0: Secondary Structural Elements of Proteins. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2005, 61, 634-636. | 2.5 | 6 |
| 41 | Structure of <i>Mycobacterium smegmatis</i> single-stranded DNA-binding protein and a comparative study involving homologous SSBs: biological implications of structural plasticity and variability in quaternary association. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2005, 61, 1140-1148. | 2.5 | 29 |
| 42 | Atomic resolution (0.97 Å) structure of the triple mutant (K53,56,121M) of bovine pancreatic phospholipase A2. <i>Acta Crystallographica Section F: Structural Biology Communications</i> , 2005, 61, 3-7. | 0.7 | 4 |
| 43 | Unusual sugar specificity of banana lectin from <i>Musa paradisiaca</i> and its probable evolutionary origin. <i>Crystallographic and modelling studies. Glycobiology</i> , 2005, 15, 1025-1032. | 1.3 | 61 |
| 44 | Fragment Finder: a web-based software to identify similar three-dimensional structural motif. <i>Nucleic Acids Research</i> , 2005, 33, W85-W88. | 6.5 | 14 |
| 45 | Structural Basis for the Energetics of Jacalin-Sugar Interactions: Promiscuity Versus Specificity. <i>Journal of Molecular Biology</i> , 2005, 347, 181-188. | 2.0 | 60 |
| 46 | BSDD: Biomolecules Segment Display Device—a web-based interactive display tool. <i>Nucleic Acids Research</i> , 2004, 32, W645-W648. | 6.5 | 3 |
| 47 | THGS: a web-based database of Transmembrane Helices in Genome Sequences. <i>Nucleic Acids Research</i> , 2004, 32, 125D-128. | 6.5 | 10 |
| 48 | A redetermination of the structure of the triple mutant (K53,56,120M) of bovine pancreatic phospholipase A2 at 1.6 Å resolution using sulfur-SAS at 1.54 Å wavelength. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2004, 60, 1586-1590. | 2.5 | 8 |
| 49 | Purification, crystallization and preliminary X-ray structure analysis of the banana lectin from <i>Musa paradisiaca</i> . <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2004, 60, 2104-2106. | 2.5 | 18 |
| 50 | A FAST Pattern Matching Algorithm. <i>Journal of Chemical Information and Computer Sciences</i> , 2004, 44, 1251-1256. | 2.8 | 33 |
| 51 | X-ray Analysis of <i>Mycobacterium smegmatis</i> Dps and a Comparative Study Involving Other Dps and Dps-like Molecules. <i>Journal of Molecular Biology</i> , 2004, 339, 1103-1103. | 2.0 | 0 |
| 52 | X-ray Analysis of <i>Mycobacterium smegmatis</i> Dps and a Comparative Study Involving Other Dps and Dps-like Molecules. <i>Journal of Molecular Biology</i> , 2004, 339, 1103-1113. | 2.0 | 67 |
| 53 | Crystal and molecular structure of 2,6-bis(4-fluorobenzylidene)cyclohexanone. <i>Crystal Research and Technology</i> , 2003, 38, 822-828. | 0.6 | 4 |
| 54 | Crystal and molecular structure of 2,6-bis(4-chlorophenyl)-3-phenylpiperidin-4-one. <i>Crystal Research and Technology</i> , 2003, 38, 918-921. | 0.6 | 4 |

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|----|--|-----|-----------|
| 55 | Câ€“halogenâ€“ interactions in proteins: a database study. <i>Crystal Engineering</i> , 2003, 6, 69-77. | 0.7 | 86 |
| 56 | WAP: water analysis package â€“ a Web-based package to calculate geometrical parameters between water oxygen and protein atoms. <i>Journal of Applied Crystallography</i> , 2003, 36, 167-168. | 1.9 | 8 |
| 57 | Crystallization and preliminary X-ray diffraction analysis of <i>Mycobacterium smegmatis</i> Dps. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2003, 59, 2254-2256. | 2.5 | 8 |
| 58 | CAP: conformation angles package--displaying the conformation angles of side chains in proteins. <i>Bioinformatics</i> , 2003, 19, 1043-1044. | 1.8 | 4 |
| 59 | Side-chain conformation angles of amino acids: effect of temperature factor cut-off. <i>Journal of Structural Biology</i> , 2003, 143, 181-184. | 1.3 | 7 |
| 60 | Crystal Structures of the Free and Anisic Acid Bound Triple Mutant of Phospholipase A2. <i>Journal of Molecular Biology</i> , 2003, 333, 367-376. | 2.0 | 28 |
| 61 | Structure of <i>Mycobacterium tuberculosis</i> Single-stranded DNA-binding Protein. Variability in Quaternary Structure and Its Implications. <i>Journal of Molecular Biology</i> , 2003, 331, 385-393. | 2.0 | 62 |
| 62 | Structural Basis of the Carbohydrate Specificities of Jacalin: An X-ray and Modeling Study. <i>Journal of Molecular Biology</i> , 2003, 332, 217-228. | 2.0 | 58 |
| 63 | CADB: Conformation Angles DataBase of proteins. <i>Nucleic Acids Research</i> , 2003, 31, 448-451. | 6.5 | 12 |
| 64 | SEM (Symmetry Equivalent Molecules): a web-based GUI to generate and visualize the macromolecules. <i>Nucleic Acids Research</i> , 2003, 31, 3356-3358. | 6.5 | 4 |
| 65 | SSEP: secondary structural elements of proteins. <i>Nucleic Acids Research</i> , 2003, 31, 3404-3405. | 6.5 | 6 |
| 66 | Ramachandran plot on the web. <i>Bioinformatics</i> , 2002, 18, 1548-1549. | 1.8 | 69 |
| 67 | Crystal structures of artocarpin, a Moraceae lectin with mannose specificity, and its complex with methyl- β -D-mannose: implications to the generation of carbohydrate specificity. <i>Journal of Molecular Biology</i> , 2002, 317, 237-247. | 2.0 | 97 |
| 68 | Crystal Structure of the Jacalinâ€“T-antigen Complex and a Comparative Study of Lectinâ€“T-antigen Complexes. <i>Journal of Molecular Biology</i> , 2002, 321, 637-645. | 2.0 | 77 |
| 69 | Observation of Additional Calcium Ion in the Crystal Structure of the Triple Mutant K56,120,121M of Bovine Pancreatic Phospholipase A2. <i>Journal of Molecular Biology</i> , 2002, 324, 755-762. | 2.0 | 19 |
| 70 | Crystal and Molecular Structure of an Acridinedione. <i>Crystal Research and Technology</i> , 2002, 37, 1029-1037. | 0.6 | 6 |
| 71 | PDB Goodies â€“ a web-based GUI to manipulate the Protein Data Bank file. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2002, 58, 1385-1386. | 2.5 | 24 |
| 72 | Structural Basis of the Anionic Interface Preference and Activation of Pancreatic Phospholipase A2. <i>Biochemistry</i> , 2000, 39, 12312-12323. | 1.2 | 52 |

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|----|--|-----|-----------|
| 73 | High-resolution refinement of orthorhombic bovine pancreatic phospholipase A2. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 1999, 55, 46-50. | 2.5 | 14 |
| 74 | Structures of the catalytic site mutants D99A and H48Q and the calcium-loop mutant D49E of phospholipase A2. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 1999, 55, 443-447. | 2.5 | 11 |
| 75 | Structure of the Complex of Bovine Pancreatic Phospholipase A2 with a Transition-State Analogue. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 1998, 54, 334-341. | 2.5 | 16 |
| 76 | 1.72 Å... Resolution Refinement of the Trigonal Form of Bovine Pancreatic Phospholipase A2. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 1998, 54, 342-346. | 2.5 | 5 |
| 77 | Phospholipase A2 Engineering. Structural and Functional Roles of the Highly Conserved Active Site Residue Aspartate-99. <i>Biochemistry</i> , 1997, 36, 3104-3114. | 1.2 | 53 |
| 78 | Crystal Structure of the Complex of Bovine Pancreatic Phospholipase A2 with the Inhibitor 1-Hexadecyl-3-(trifluoroethyl)-sn-glycero-2-phosphomethanol. <i>Biochemistry</i> , 1997, 36, 14186-14191. | 1.2 | 49 |
| 79 | Phospholipase A2 Engineering. Deletion of the C-Terminus Segment Changes Substrate Specificity and Uncouples Calcium and Substrate Binding at the Zwitterionic Interface. <i>Biochemistry</i> , 1996, 35, 12164-12174. | 1.2 | 37 |
| 80 | A novel mode of carbohydrate recognition in jacalin, a Moraceae plant lectin with a \hat{I}^2 -prism fold. <i>Nature Structural Biology</i> , 1996, 3, 596-603. | 9.7 | 224 |
| 81 | 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. <i>Journal of Crystallographic and Spectroscopic Research</i> , 1993, 23, 101-105. | 0.3 | 4 |
| 82 | Structure of 4-piperidone derivatives. I. 3-Methyl-2,6-diphenyl-4-piperidone. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 1990, 46, 1153-1155. | 0.4 | 3 |
| 83 | Structure of 4-piperidone derivatives. II. 2,6-Bis(p-methoxyphenyl)-3,5-dimethyl-4-piperidone. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 1990, 46, 1338-1340. | 0.4 | 3 |