

Debnath Pal

List of Publications by Year in descending order

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105
papers

2,705
citations

257450

24
h-index

197818

49
g-index

112
all docs

112
docs citations

112
times ranked

3570
citing authors

| # | ARTICLE | IF | CITATIONS |
|----|---|------|-----------|
| 1 | Cis peptide bonds in proteins: residues involved, their conformations, interactions and locations 1 1 Edited by J. M. Thornton. <i>Journal of Molecular Biology</i> , 1999, 294, 271-288. | 4.2 | 294 |
| 2 | More hydrogen bonds for the (structural) biologist. <i>Trends in Biochemical Sciences</i> , 2001, 26, 521-523. | 7.5 | 230 |
| 3 | The interrelationships of side-chain and main-chain conformations in proteins. <i>Progress in Biophysics and Molecular Biology</i> , 2001, 76, 1-102. | 2.9 | 189 |
| 4 | Inference of Protein Function from Protein Structure. <i>Structure</i> , 2005, 13, 121-130. | 3.3 | 175 |
| 5 | Non-hydrogen Bond Interactions Involving the Methionine Sulfur Atom. <i>Journal of Biomolecular Structure and Dynamics</i> , 2001, 19, 115-128. | 3.5 | 160 |
| 6 | Environment of tryptophan side chains in proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2000, 38, 288-300. | 2.6 | 133 |
| 7 | Disulfide bonds, their stereospecific environment and conservation in protein structures. <i>Protein Engineering, Design and Selection</i> , 2004, 17, 795-808. | 2.1 | 109 |
| 8 | Packing of aromatic rings against tryptophan residues in proteins. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 1999, 55, 1421-1427. | 2.5 | 102 |
| 9 | WebGeSTer DB—a transcription terminator database. <i>Nucleic Acids Research</i> , 2011, 39, D129-D135. | 14.5 | 100 |
| 10 | In Vivo Proton MR Spectroscopy Evaluation of Pyogenic Brain Abscesses: A Report of 194 Cases. <i>American Journal of Neuroradiology</i> , 2010, 31, 360-366. | 2.4 | 85 |
| 11 | Different Types of Interactions Involving Cysteine Sulfhydryl Group in Proteins. <i>Journal of Biomolecular Structure and Dynamics</i> , 1998, 15, 1059-1072. | 3.5 | 83 |
| 12 | On residues in the disallowed region of the Ramachandran map. <i>Biopolymers</i> , 2002, 63, 195-206. | 2.4 | 74 |
| 13 | An Enthalpy Model for Simulation of Dendritic Growth. <i>Numerical Heat Transfer, Part B: Fundamentals</i> , 2006, 50, 59-78. | 0.9 | 48 |
| 14 | An overview on 2-methyl-2,4-pentanediol in crystallization and in crystals of biological macromolecules. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2002, 58, 1722-1728. | 2.5 | 43 |
| 15 | Main-chain conformational features at different conformations of the side-chains in proteins. <i>Protein Engineering, Design and Selection</i> , 1998, 11, 631-647. | 2.1 | 38 |
| 16 | Environment of tryptophan side chains in proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2000, 38, 288-300. | 2.6 | 36 |
| 17 | New Principles of Protein Structure: Nests, Eggs—and What Next?. <i>Angewandte Chemie - International Edition</i> , 2002, 41, 4663-4665. | 13.8 | 35 |
| 18 | Serum biomarkers identification by iTRAQ and verification by MRM: S100A8/S100A9 levels predict tumor-stroma involvement and prognosis in Glioblastoma. <i>Scientific Reports</i> , 2019, 9, 2749. | 3.3 | 33 |

| # | ARTICLE | IF | CITATIONS |
|----|--|------|-----------|
| 19 | β-Sheet propensity and its correlation with parameters based on conformation. Acta Crystallographica Section D: Biological Crystallography, 2000, 56, 589-594. | 2.5 | 32 |
| 20 | Effect of Elevated CO ₂ and Temperature on Nitrogen Dynamics and Microbial Activity During Wheat (<i>Triticum aestivum</i> L.) Growth on a Subtropical Inceptisol in India. Journal of Agronomy and Crop Science, 2012, 198, 452-465. | 3.5 | 32 |
| 21 | New routes to condensed polynuclear compounds—VIII. Tetrahedron, 1973, 29, 177-184. | 1.9 | 30 |
| 22 | Nitrogen Fixation in the Phyllosphere of Tropical Plants: Occurrence of Phyllosphere Nitrogen-Fixing Micro-organisms in Eastern India and their Utility for the Growth and Nitrogen Nutrition of Host Plants. Annals of Botany, 1981, 48, 705-716. | 2.9 | 30 |
| 23 | Combining Bayes Classification and Point Group Symmetry under Boolean Framework for Enhanced Protein Quaternary Structure Inference. Structure, 2011, 19, 304-312. | 3.3 | 30 |
| 24 | A proline insertion-deletion in the spike glycoprotein fusion peptide of mouse hepatitis virus strongly alters neuropathology. Journal of Biological Chemistry, 2019, 294, 8064-8087. | 3.4 | 29 |
| 25 | New measures for estimating surface complementarity and packing at protein-protein interfaces. FEBS Letters, 2010, 584, 1163-1168. | 2.8 | 24 |
| 26 | Stereodivergent C-C Bond Formation on Arene-Chromium Template: Endo-Selective Allylation by Hosomi-Sakurai Reaction. Journal of Organic Chemistry, 1996, 61, 8362-8363. | 3.2 | 23 |
| 27 | Estimates of the loss of main-chain conformational entropy of different residues on protein folding. , 1999, 36, 332-339. | | 21 |
| 28 | On gene ontology and function annotation. Bioinformatics, 2006, 1, 97-98. | 0.5 | 21 |
| 29 | Pattern Recognition-Based Approach for Identifying Metabolites in Nuclear Magnetic Resonance-Based Metabolomics. Analytical Chemistry, 2015, 87, 7148-7155. | 6.5 | 20 |
| 30 | Bacterial siderophore mimicking iron complexes as DNA targeting antimicrobials. RSC Advances, 2016, 6, 39245-39260. | 3.6 | 19 |
| 31 | An electrophile-nucleophile interaction in metalloprotein structures. Protein Science, 1997, 6, 851-859. | 7.6 | 17 |
| 32 | Functionally important segments in proteins dissected using Gene Ontology and geometric clustering of peptide fragments. Genome Biology, 2008, 9, R52. | 9.6 | 17 |
| 33 | Development of Modular Shallow Water AUV: Issues & Trial Results. Journal of the Institution of Engineers (India): Series C, 2012, 93, 217-228. | 1.2 | 16 |
| 34 | Evaluating the predictions of the protein stability change upon single amino acid substitutions for the FXN CAG15 challenge. Human Mutation, 2019, 40, 1392-1399. | 2.5 | 16 |
| 35 | Using correlated parameters for improved ranking of protein-protein docking decoys. Journal of Computational Chemistry, 2011, 32, 787-796. | 3.3 | 15 |
| 36 | PRUNE and PROBE--two modular web services for protein-protein docking. Nucleic Acids Research, 2011, 39, W229-W234. | 14.5 | 15 |

| # | ARTICLE | IF | CITATIONS |
|----|---|-----|-----------|
| 37 | Azadirachta indica A. Juss bark extract and its Nimbin isomers restrict $\hat{\Gamma}^2$ -coronaviral infection and replication. <i>Virology</i> , 2022, 569, 13-28. | 2.4 | 15 |
| 38 | Terminal residues in protein chains: Residue preference, conformation, and interaction. <i>Biopolymers</i> , 2000, 53, 467-475. | 2.4 | 13 |
| 39 | Modeling a hybrid reactive-deliberative architecture towards realizing overall dynamic behavior of an AUV. <i>Procedia Computer Science</i> , 2010, 1, 259-268. | 2.0 | 13 |
| 40 | Push-Pull Butadienes: Evidence for a possible C?H?S hydrogen bond in 4-(methylthio)-4-nitro-1-(pyrrolidin-1-yl)buta-1,3-diene. <i>Helvetica Chimica Acta</i> , 1997, 80, 2329-2336. | 1.6 | 12 |
| 41 | The unique functional role of the C?H?S hydrogen bond in the substrate specificity and enzyme catalysis of type 1 methionine aminopeptidase. <i>Molecular BioSystems</i> , 2016, 12, 2408-2416. | 2.9 | 12 |
| 42 | Chemical Shifts to Metabolic Pathways: Identifying Metabolic Pathways Directly from a Single 2D NMR Spectrum. <i>Analytical Chemistry</i> , 2015, 87, 12197-12205. | 6.5 | 11 |
| 43 | Spike protein fusion loop controls SARS-CoV-2 fusogenicity and infectivity. <i>Journal of Structural Biology</i> , 2021, 213, 107713. | 2.8 | 11 |
| 44 | Conformational Similarity Indices Between Different Residues in Proteins and $\hat{\Gamma}^{\pm}$ -Helix Propensities. <i>Journal of Biomolecular Structure and Dynamics</i> , 2000, 18, 273-280. | 3.5 | 10 |
| 45 | Exploring the use of molecular dynamics in assessing protein variants for phenotypic alterations. <i>Human Mutation</i> , 2019, 40, 1424-1435. | 2.5 | 10 |
| 46 | Silver(i) oxide?silver halide mediated alcoholysis of O-benzoyl-myo-inositol 1,3,5-orthoformates: intramolecular assistance by the sulfonyl group. <i>Perkin Transactions II RSC</i> , 2002, , 358-365. | 1.1 | 9 |
| 47 | Production of Hydrolases by N2-fixing Microorganisms. <i>Biochemie Und Physiologie Der Pflanzen</i> , 1989, 185, 75-81. | 0.5 | 8 |
| 48 | <i>De novo</i> inference of protein function from coarse-grained dynamics. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 2443-2454. | 2.6 | 8 |
| 49 | Interaction of arsenic with gap junction protein connexin 43 alters gap junctional intercellular communication. <i>Biochimica Et Biophysica Acta - Molecular Cell Research</i> , 2018, 1865, 1423-1436. | 4.1 | 8 |
| 50 | Assessing predictions on fitness effects of missense variants in calmodulin. <i>Human Mutation</i> , 2019, 40, 1463-1473. | 2.5 | 8 |
| 51 | Assessing the performance of in silico methods for predicting the pathogenicity of variants in the gene CHEK2, among Hispanic females with breast cancer. <i>Human Mutation</i> , 2019, 40, 1612-1622. | 2.5 | 8 |
| 52 | Saccharomyces cerevisiae Hop1 Protein Zinc Finger Motif Binds to the Holliday Junction and Distorts the DNA Structure: Implications for Holliday Junction Migration. <i>Biochemistry</i> , 2007, 46, 12530-12542. | 2.5 | 7 |
| 53 | Use of Vertex Index in Structure-Activity Analysis and Design of Molecules. <i>Current Computer-Aided Drug Design</i> , 2012, 8, 128-134. | 1.2 | 7 |
| 54 | Spike Glycoprotein Is Central to Coronavirus Pathogenesis-Parallel Between m-CoV and SARS-CoV-2. <i>Annals of Neurosciences</i> , 2021, 28, 201-218. | 1.7 | 7 |

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|----|--|-----|-----------|
| 55 | Secondary structures at polypeptide-chain termini and their features. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2002, 58, 1793-1802. | 2.5 | 6 |
| 56 | Mass Spectrometry-Based Diagnosis of Hemoglobinopathies: A Potential Tool for the Screening of Genetic Disorder. <i>Biochemical Genetics</i> , 2016, 54, 816-825. | 1.7 | 6 |
| 57 | Structural analysis of glutathionyl hemoglobin using native mass spectrometry. <i>Journal of Structural Biology</i> , 2019, 208, 107386. | 2.8 | 6 |
| 58 | Inferring molecular function: contributions from functional linkages. <i>Trends in Genetics</i> , 2008, 24, 587-590. | 6.7 | 5 |
| 59 | Identifying functionally important <i>cis</i> -peptide containing segments in proteins and their utility in molecular function annotation. <i>FEBS Journal</i> , 2014, 281, 5602-5621. | 4.7 | 5 |
| 60 | Mass spectrometry based characterization of Hb Beckman variant in a falsely elevated HbA1c sample. <i>Analytical Biochemistry</i> , 2015, 489, 53-58. | 2.4 | 5 |
| 61 | Computational design of model scaffold for anion recognition based on the ϵ -NN TM motif. <i>Biopolymers</i> , 2017, 108, e22921. | 2.4 | 5 |
| 62 | Mechanisms of Arsenic-Induced Toxicity with Special Emphasis on Arsenic-Binding Proteins. , 0, , . | | 5 |
| 63 | Inferring metal binding sites in flexible regions of proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2021, 89, 1125-1133. | 2.6 | 5 |
| 64 | Molecular Dynamics of Hemoglobin Reveals Structural Alterations and Explains the Interactions Driving Sickle Cell Fibrillation. <i>Journal of Physical Chemistry B</i> , 2021, 125, 9921-9933. | 2.6 | 5 |
| 65 | Estimates of the loss of main-chain conformational entropy of different residues on protein folding. <i>Proteins: Structure, Function and Bioinformatics</i> , 1999, 36, 332-9. | 2.6 | 5 |
| 66 | Information content of molecular graph and prediction of gas phase thermal entropy of organic compounds. <i>Journal of Mathematical Chemistry</i> , 2013, 51, 2718-2730. | 1.5 | 4 |
| 67 | Two new atom centered fragment descriptors and scoring function enhance classification of antibacterial activity. <i>Journal of Molecular Modeling</i> , 2014, 20, 2164. | 1.8 | 4 |
| 68 | Molecular Dynamics Information Improves <i>cis</i> -Peptide-Based Function Annotation of Proteins. <i>Journal of Proteome Research</i> , 2017, 16, 2936-2946. | 3.7 | 4 |
| 69 | Ebolavirus interferon antagonists' protein interaction perspectives to combat pathogenesis. <i>Briefings in Functional Genomics</i> , 2018, 17, 392-401. | 2.7 | 4 |
| 70 | ReneGENE-DP: Accelerated Parallel Dynamic Programming for Genome Informatics. , 2018, , . | | 4 |
| 71 | Aggregation of M3 (E376D) variant of alpha1- antitrypsin. <i>Scientific Reports</i> , 2020, 10, 8290. | 3.3 | 4 |
| 72 | Clusters of hairpins induce intrinsic transcription termination in bacteria. <i>Scientific Reports</i> , 2021, 11, 16194. | 3.3 | 4 |

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|----|---|-----|-----------|
| 73 | Assessment of Adaptive Breast Cancer Screening Policies for Improved Mortality Reduction in Low to Middle Income Countries. <i>Asian Pacific Journal of Cancer Prevention</i> , 2017, 18, 2375-2380. | 1.2 | 4 |
| 74 | Network-based identification of miRNAs and transcription factors and in silico drug screening targeting Î-secretase involved in Alzheimer's disease. <i>Heliyon</i> , 2021, 7, e08502. | 3.2 | 4 |
| 75 | MD DaVis: interactive data visualization of protein molecular dynamics. <i>Bioinformatics</i> , 2022, 38, 3299-3301. | 4.1 | 4 |
| 76 | Graphical representation of the salient conformational features of protein residues. <i>Protein Engineering, Design and Selection</i> , 1999, 12, 523-526. | 2.1 | 3 |
| 77 | Avoiding acidic region streaking in two-dimensional gel electrophoresis: Case study with two bacterial whole cell protein extracts. <i>Journal of Biosciences</i> , 2014, 39, 631-642. | 1.1 | 3 |
| 78 | Pipeline for inferring protein function from dynamics using coarse-grained molecular mechanics forcefield. <i>Computers in Biology and Medicine</i> , 2017, 83, 134-142. | 7.0 | 3 |
| 79 | Molecular insights of inhibition in sickle hemoglobin polymerization upon glutathionylation: hydrogen/deuterium exchange mass spectrometry and molecular dynamics simulation-based approach. <i>Biochemical Journal</i> , 2018, 475, 2153-2166. | 3.7 | 3 |
| 80 | Predicting gas phase entropy of select hydrocarbon classes through specific information-theoretical molecular descriptors. <i>SAR and QSAR in Environmental Research</i> , 2019, 30, 491-505. | 2.2 | 3 |
| 81 | Exo-selective intermolecular Diels-Ålder reaction by PyrI4 and AbnU on non-natural substrates. <i>Communications Chemistry</i> , 2021, 4, . | 4.5 | 3 |
| 82 | Global Asymptotic Stability of a Non-linear Population Model of Diabetes Mellitus. <i>Springer Proceedings in Mathematics and Statistics</i> , 2018, , 351-357. | 0.2 | 3 |
| 83 | Combinatorial Design of Molecule using Activity-Linked Substructural Topological Information as Applied to Antitubercular Compounds. <i>Current Computer-Aided Drug Design</i> , 2018, 15, 67-81. | 1.2 | 3 |
| 84 | Functional Linkages Can Reveal Protein Complexes for Structure Determination. <i>Structure</i> , 2007, 15, 1079-1089. | 3.3 | 2 |
| 85 | dockYard- a repository to assist modeling of protein-protein docking. <i>Journal of Molecular Modeling</i> , 2011, 17, 599-606. | 1.8 | 2 |
| 86 | Role of Vertex Index in Substructure Identification and Activity Prediction: A Study on Antitubercular Activity of a Series of Acid Alkyl Ester Derivatives. <i>Croatica Chemica Acta</i> , 2014, 87, 39-47. | 0.4 | 2 |
| 87 | AccuRA: Accurate alignment of short reads on scalable reconfigurable accelerators. , 2016, , . | | 2 |
| 88 | New facets of larger Nest motifs in proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2020, 88, 1413-1422. | 2.6 | 2 |
| 89 | A computational framework for modeling functional protein-protein interactions. <i>Proteins: Structure, Function and Bioinformatics</i> , 2021, 89, 1353-1364. | 2.6 | 2 |
| 90 | DJ-1-Nrf2 axis is activated upon murine Î2-coronavirus infection in the CNS. <i>Brain Disorders</i> , 2021, 4, 100021. | 1.7 | 2 |

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|-----|--|-----|-----------|
| 91 | Sustained AMPK Activation and Proline Metabolism Play Critical Roles in the Survival of Matrix-Deprived Transformed Cells. <i>Frontiers in Cell and Developmental Biology</i> , 2021, 9, 771366. | 3.7 | 2 |
| 92 | Combinatorial Drug Discovery from Activity-Related Substructure Identification. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2019, , 71-108. | 0.6 | 1 |
| 93 | Usefulness of graph vertex complexity and class partial information content in explaining gas phase thermal entropy of chemical compounds. <i>Journal of Mathematical Chemistry</i> , 2020, 58, 887-892. | 1.5 | 1 |
| 94 | Environment of tryptophan side chains in proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2000, 38, 288-300. | 2.6 | 1 |
| 95 | ReneGENE-GI: Empowering Precision Genomics with FPGAs on HPCs. <i>Lecture Notes in Computer Science</i> , 2018, , 178-191. | 1.3 | 1 |
| 96 | ReneGENE-Novo: Co-designed Algorithm-Architecture for Accelerated Preprocessing and Assembly of Genomic Short Reads. <i>Lecture Notes in Computer Science</i> , 2018, , 564-577. | 1.3 | 1 |
| 97 | Effect of land use on soil carbon fractions. <i>Journal of the Indian Society of Soil Science</i> , 2020, 68, 392-399. | 0.2 | 1 |
| 98 | A Graph-Based Framework for Multiscale Modeling of Physiological Transport. <i>Frontiers in Network Physiology</i> , 2022, 1, . | 1.8 | 1 |
| 99 | Somatic mutation analyses of stem-like cells in gingivobuccal oral squamous cell carcinoma reveals DNA damage response genes. <i>Genomics</i> , 2022, 114, 110308. | 2.9 | 1 |
| 100 | Two Consecutive Prolines in the Fusion Peptide of Murine β -Coronavirus Spike Protein Predominantly Determine Fusogenicity and May Be Essential but Not Sufficient to Cause Demyelination. <i>Viruses</i> , 2022, 14, 834. | 3.3 | 1 |
| 101 | Effects of dynamic impacts on human bones. <i>Journal of Biosciences</i> , 1980, 2, 139-144. | 1.1 | 0 |
| 102 | Interface of Apoptotic Protein Complexes Has Distinct Properties. <i>In Silico Biology</i> , 2009, 9, 365-378. | 0.9 | 0 |
| 103 | Numerical simulation of a glucose sensitive composite membrane closed-loop insulin delivery system. <i>Bioprocess and Biosystems Engineering</i> , 2017, 40, 1453-1462. | 3.4 | 0 |
| 104 | Towards Accelerated Genome Informatics on Parallel HPC Platforms: The ReneGENE-GI Perspective. <i>Journal of Signal Processing Systems</i> , 2020, 92, 1197-1213. | 2.1 | 0 |
| 105 | Differential Regulation of DJ α 1 in Glial Cells upon MHV α 59 α -Induced Oxidative Stress. <i>FASEB Journal</i> , 2020, 34, 1-1. | 0.5 | 0 |