Debnath Pal

List of Publications by Year
in descending order

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105 papers	2,705 citations	257101 24 h-index	197535 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 1Edited by J. M. Thornton. Journal of Molecular Biology, 1999, 294, 271-288.	2.0	294
2	More hydrogen bonds for the (structural) biologist. Trends in Biochemical Sciences, 2001, 26, 521-523.	3.7	230
3	The interrelationships of side-chain and main-chain conformations in proteins. Progress in Biophysics and Molecular Biology, 2001, 76, 1-102.	1.4	189
4	Inference of Protein Function from Protein Structure. Structure, 2005, 13, 121-130.	1.6	175
5	Non-hydrogen Bond Interactions Involving the Methionine Sulfur Atom. Journal of Biomolecular Structure and Dynamics, 2001, 19, 115-128.	2.0	160
6	Environment of tryptophan side chains in proteins. Proteins: Structure, Function and Bioinformatics, 2000, 38, 288-300.	1.5	133
7	Disulfide bonds, their stereospecific environment and conservation in protein structures. Protein Engineering, Design and Selection, 2004, 17, 795-808.	1.0	109
8	Packing of aromatic rings against tryptophan residues in proteins. Acta Crystallographica Section D: Biological Crystallography, 1999, 55, 1421-1427.	2.5	102
9	WebGeSTer DBâ€”a transcription terminator database. Nucleic Acids Research, 2011, 39, D129-D135.	6.5	100
10	In Vivo Proton MR Spectroscopy Evaluation of Pyogenic Brain Abscesses: A Report of 194 Cases. American Journal of Neuroradiology, 2010, 31, 360-366.	1.2	85
11	Different Types of Interactions Involving Cysteine Sulfhydryl Group in Proteins. Journal of Biomolecular Structure and Dynamics, 1998, 15, 1059-1072.	2.0	83
12	On residues in the disallowed region of the Ramachandran map. Biopolymers, 2002, 63, 195-206.	1.2	74
13	An Enthalpy Model for Simulation of Dendritic Growth. Numerical Heat Transfer, Part B: Fundamentals, 2006, 50, 59-78.	0.6	48
14	An overview on 2-methyl-2,4-pentanediol in crystallization and in crystals of biological macromolecules. Acta Crystallographica Section D: Biological Crystallography, 2002, 58, 1722-1728.	2.5	43
15	Main-chain conformational features at different conformations of the side-chains in proteins. Protein Engineering, Design and Selection, 1998, 11, 631-647.	1.0	38
16	Environment of tryptophan side chains in proteins. Proteins: Structure, Function and Bioinformatics, 2000, 38, 288-300.	1.5	36
17	New Principles of Protein Structure: Nests, Eggsâ€”and What Next?. Angewandte Chemie - International Edition, 2002, 41, 4663-4665.	7.2	35
18	Serum biomarkers identification by iTRAQ and verification by MRM: S100A8/S100A9 levels predict tumor-stroma involvement and prognosis in Glioblastoma. Scientific Reports, 2019, 9, 2749.	1.6	33

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19	Î²-Sheet propensity and its correlation withparameters based on conformation. Acta Crystallographica Section D: Biological Crystallography, 2000, 56, 589-594.	2.5	32
20	Effect of Elevated CO₂ and Temperature on Nitrogen Dynamics and Microbial Activity During Wheat (Triticum aestivum L.) Growth on a Subtropical Inceptisol in India. Journal of Agronomy and Crop Science, 2012, 198, 452-465.	1.7	32
21	New routes to condensed polynuclear compoundsâ€"VIII. Tetrahedron, 1973, 29, 177-184.	1.0	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.	1.4	30
23	Combining Bayes Classification and Point Group Symmetry under Boolean Framework for Enhanced Protein Quaternary Structure Inference. Structure, 2011, 19, 304-312.	1.6	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.	1.6	29
25	New measures for estimating surface complementarity and packing at proteinâ€"protein interfaces. FEBS Letters, 2010, 584, 1163-1168.	1.3	24
26	Stereodivergent Câ^'C Bond Formation on Areneâ^'Chromium Template:ÂEndo-Selective Allylation by Hosomiâ^'Sakurai Reactionâ€. Journal of Organic Chemistry, 1996, 61, 8362-8363.	1.7	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. Bioinformation, 2006, 1, 97-98.	0.2	21
29	Pattern Recognition-Based Approach for Identifying Metabolites in Nuclear Magnetic Resonance-Based Metabolomics. Analytical Chemistry, 2015, 87, 7148-7155.	3.2	20
30	Bacterial siderophore mimicking iron complexes as DNA targeting antimicrobials. RSC Advances, 2016, 6, 39245-39260.	1.7	19
31	An electrophileâ€nucleophile interaction in metalloprotein structures. Protein Science, 1997, 6, 851-859.	3.1	17
32	Functionally important segments in proteins dissected using Gene Ontology and geometric clustering of peptide fragments. Genome Biology, 2008, 9, R52.	13.9	17
33	Development of Modular Shallow Water AUV: Issues & Trial Results. Journal of the Institution of Engineers (India): Series C, 2012, 93, 217-228.	0.7	16
34	Evaluating the predictions of the protein stability change upon single amino acid substitutions for the FXN CAGI5 challenge. Human Mutation, 2019, 40, 1392-1399.	1.1	16
35	Using correlated parameters for improved ranking of proteinâ€"protein docking decoys. Journal of Computational Chemistry, 2011, 32, 787-796.	1.5	15
36	PRUNE and PROBE--two modular web services for protein-protein docking. Nucleic Acids Research, 2011, 39, W229-W234.	6.5	15

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37	Azadirachta indica A. Juss bark extract and its Nimbin isomers restrict Î²-coronaviral infection and replication. Virology, 2022, 569, 13-28.	1.1	15
38	Terminal residues in protein chains: Residue preference, conformation, and interaction. Biopolymers, 2000, 53, 467-475.	1.2	13
39	Modeling a hybrid reactive-deliberative architecture towards realizing overall dynamic behavior of an AUV. Procedia Computer Science, 2010, 1, 259-268.	1.2	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. Helvetica Chimica Acta, 1997, 80, 2329-2336.	1.0	12
41	The unique functional role of the Câ€“Hâ‹¯S hydrogen bond in the substrate specificity and enzyme catalysis of type 1 methionine aminopeptidase. Molecular BioSystems, 2016, 12, 2408-2416.	2.9	12
42	Chemical Shifts to Metabolic Pathways: Identifying Metabolic Pathways Directly from a Single 2D NMR Spectrum. Analytical Chemistry, 2015, 87, 12197-12205.	3.2	11
43	Spike protein fusion loop controls SARS-CoV-2 fusogenicity and infectivity. Journal of Structural Biology, 2021, 213, 107713.	1.3	11
44	Conformational Similarity Indices Between Different Residues in Proteins and Î±-Helix Propensities. Journal of Biomolecular Structure and Dynamics, 2000, 18, 273-280.	2.0	10
45	Exploring the use of molecular dynamics in assessing protein variants for phenotypic alterations. Human Mutation, 2019, 40, 1424-1435.	1.1	10
46	Silver(i) oxideâ€“silver halide mediated alcoholysis of O-benzoyl-myo-inositol 1,3,5-orthoformates: intramolecular assistance by the sulfonyl group. Perkin Transactions II RSC, 2002, , 358-365.	1.1	9
47	Production of Hydrolases by N2-fixing Microorganisms. Biochemie Und Physiologie Der Pflanzen, 1989, 185, 75-81.	0.5	8
48	De novoinference of protein function from coarse-grained dynamics. Proteins: Structure, Function and Bioinformatics, 2014, 82, 2443-2454.	1.5	8
49	Interaction of arsenic with gap junction protein connexin 43 alters gap junctional intercellular communication. Biochimica Et Biophysica Acta - Molecular Cell Research, 2018, 1865, 1423-1436.	1.9	8
50	Assessing predictions on fitness effects of missense variants in calmodulin. Human Mutation, 2019, 40, 1463-1473.	1.1	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. Human Mutation, 2019, 40, 1612-1622.	1.1	8
52	Saccharomyces cerevisiae Hop1 Protein Zinc Finger Motif Binds to the Holliday Junction and Distorts the DNA Structure:â€‰ Implications for Holliday Junction Migration. Biochemistry, 2007, 46, 12530-12542.	1.2	7
53	Use of Vertex Index in Structure-Activity Analysis and Design of Molecules. Current Computer-Aided Drug Design, 2012, 8, 128-134.	0.8	7
54	Spike Glycoprotein Is Central to Coronavirus Pathogenesis-Parallel Between m-CoV and SARS-CoV-2. Annals of Neurosciences, 2021, 28, 201-218.	0.9	7

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55	Secondary structures at polypeptide-chain termini and their features. Acta Crystallographica Section D: Biological Crystallography, 2002, 58, 1793-1802.	2.5	6
56	Mass Spectrometry-Based Diagnosis of Hemoglobinopathies: A Potential Tool for the Screening of Genetic Disorder. Biochemical Genetics, 2016, 54, 816-825.	0.8	6
57	Structural analysis of glutathionyl hemoglobin using native mass spectrometry. Journal of Structural Biology, 2019, 208, 107386.	1.3	6
58	Inferring molecular function: contributions from functional linkages. Trends in Genetics, 2008, 24, 587-590.	2.9	5
59	Identifying functionally important cisâ€peptide containing segments in proteins and their utility in molecular function annotation. FEBS Journal, 2014, 281, 5602-5621.	2.2	5
60	Mass spectrometry based characterization of Hb Beckman variant in a falsely elevated HbA1c sample. Analytical Biochemistry, 2015, 489, 53-58.	1.1	5
61	Computational design of model scaffold for anion recognition based on the â€˜C^{Î±}NNâ€™ motif. Biopolymers, 2017, 108, e22921.	1.2	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. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1125-1133.	1.5	5
64	Molecular Dynamics of Hemoglobin Reveals Structural Alterations and Explains the Interactions Driving Sickle Cell Fibrillation. Journal of Physical Chemistry B, 2021, 125, 9921-9933.	1.2	5
65	Estimates of the loss of main-chain conformational entropy of different residues on protein folding. Proteins: Structure, Function and Bioinformatics, 1999, 36, 332-9.	1.5	5
66	Information content of molecular graph and prediction of gas phase thermal entropy of organic compounds. Journal of Mathematical Chemistry, 2013, 51, 2718-2730.	0.7	4
67	Two new atom centered fragment descriptors and scoring function enhance classification of antibacterial activity. Journal of Molecular Modeling, 2014, 20, 2164.	0.8	4
68	Molecular Dynamics Information Improves cis-Peptide-Based Function Annotation of Proteins. Journal of Proteome Research, 2017, 16, 2936-2946.	1.8	4
69	Ebolavirus interferon antagonistsâ€”protein interaction perspectives to combat pathogenesis. Briefings in Functional Genomics, 2018, 17, 392-401.	1.3	4
70	ReneGENE-DP: Accelerated Parallel Dynamic Programming for Genome Informatics. , 2018, , .		4
71	Aggregation of M3 (E376D) variant of alpha1- antitrypsin. Scientific Reports, 2020, 10, 8290.	1.6	4
72	Clusters of hairpins induce intrinsic transcription termination in bacteria. Scientific Reports, 2021, 11, 16194.	1.6	4

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73	Assessment of Adaptive Breast Cancer Screening Policies for Improved Mortality Reduction in Low to Middle Income Countries. Asian Pacific Journal of Cancer Prevention, 2017, 18, 2375-2380.	0.5	4
74	Network-based identification of miRNAs and transcription factors and in silico drug screening targeting Î´-secretase involved in Alzheimer's disease. Heliyon, 2021, 7, e08502.	1.4	4
75	MD DaVis: interactive data visualization of protein molecular dynamics. Bioinformatics, 2022, 38, 3299-3301.	1.8	4
76	Graphical representation of the salient conformational features of protein residues. Protein Engineering, Design and Selection, 1999, 12, 523-526.	1.0	3
77	Avoiding acidic region streaking in two-dimensional gel electrophoresis: Case study with two bacterial whole cell protein extracts. Journal of Biosciences, 2014, 39, 631-642.	0.5	3
78	Pipeline for inferring protein function from dynamics using coarse-grained molecular mechanics forcefield. Computers in Biology and Medicine, 2017, 83, 134-142.	3.9	3
79	Molecular insights of inhibition in sickle hemoglobin polymerization upon glutathionylation: hydrogen/deuterium exchange mass spectrometry and molecular dynamics simulation-based approach. Biochemical Journal, 2018, 475, 2153-2166.	1.7	3
80	Predicting gas phase entropy of select hydrocarbon classes through specific information-theoretical molecular descriptors. SAR and QSAR in Environmental Research, 2019, 30, 491-505.	1.0	3
81	Exo-selective intermolecular Dielsâ€“Alder reaction by Pyrl4 and AbnU on non-natural substrates. Communications Chemistry, 2021, 4, .	2.0	3
82	Global Asymptotic Stability of a Non-linear Population Model of Diabetes Mellitus. Springer Proceedings in Mathematics and Statistics, 2018, , 351-357.	0.1	3
83	Combinatorial Design of Molecule using Activity-Linked Substructural Topological Information as Applied to Antitubercular Compounds. Current Computer-Aided Drug Design, 2018, 15, 67-81.	0.8	3
84	Functional Linkages Can Reveal Protein Complexes for Structure Determination. Structure, 2007, 15, 1079-1089.	1.6	2
85	dockYardâ€“a repository to assist modeling of protein-protein docking. Journal of Molecular Modeling, 2011, 17, 599-606.	0.8	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. Croatica Chemica Acta, 2014, 87, 39-47.	0.1	2
87	AccuRA: Accurate alignment of short reads on scalable reconfigurable accelerators. , 2016, , .		2
88	New facets of larger Nest motifs in proteins. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1413-1422.	1.5	2
89	A computational framework for modeling functional proteinâ€protein interactions. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1353-1364.	1.5	2
90	DJ-1-Nrf2 axis is activated upon murine Î²-coronavirus infection in the CNS. Brain Disorders, 2021, 4, 100021.	1.1	2

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91	Sustained AMPK Activation and Proline Metabolism Play Critical Roles in the Survival of Matrix-Deprived Transformed Cells. Frontiers in Cell and Developmental Biology, 2021, 9, 771366.	1.8	2
92	Combinatorial Drug Discovery from Activity-Related Substructure Identification. Challenges and Advances in Computational Chemistry and Physics, 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. Journal of Mathematical Chemistry, 2020, 58, 887-892.	0.7	1
94	Environment of tryptophan side chains in proteins. , 2000, 38, 288.		1
95	ReneGENE-GI: Empowering Precision Genomics with FPGAs on HPCs. Lecture Notes in Computer Science, 2018, , 178-191.	1.0	1
96	ReneGENE-Novo: Co-designed Algorithm-Architecture for Accelerated Preprocessing and Assembly of Genomic Short Reads. Lecture Notes in Computer Science, 2018, , 564-577.	1.0	1
97	Effect of land use on soil carbon fractions. Journal of the Indian Society of Soil Science, 2020, 68, 392-399.	0.1	1
98	A Graph-Based Framework for Multiscale Modeling of Physiological Transport. Frontiers in Network Physiology, 2022, 1, .	0.8	1
99	Somatic mutation analyses of stem-like cells in gingivobuccal oral squamous cell carcinoma reveals DNA damage response genes. Genomics, 2022, 114, 110308.	1.3	1
100	Two Consecutive Prolines in the Fusion Peptide of Murine Î²-Coronavirus Spike Protein Predominantly Determine Fusogenicity and May Be Essential but Not Sufficient to Cause Demyelination. Viruses, 2022, 14, 834.	1.5	1
101	Effects of dynamic impacts on human bones. Journal of Biosciences, 1980, 2, 139-144.	0.5	0
102	Interface of Apoptotic Protein Complexes Has Distinct Properties. In Silico Biology, 2009, 9, 365-378.	0.4	0
103	Numerical simulation of a glucose sensitive composite membrane closed-loop insulin delivery system. Bioprocess and Biosystems Engineering, 2017, 40, 1453-1462.	1.7	0
104	Towards Accelerated Genome Informatics on Parallel HPC Platforms: The ReneGENE-GI Perspective. Journal of Signal Processing Systems, 2020, 92, 1197-1213.	1.4	0
105	Differential Regulation of DJâ€1 in Glial Cells upon MHVâ€A59 â€Induced Oxidative Stress. FASEB Journal, 2020, 34, 1-1.	0.2	0