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	A Graph-Based Framework for Multiscale Modeling of Physiological Transport. Frontiers in Network Physiology, 2022, 1, .	1.8	1
2	Somatic mutation analyses of stem-like cells in gingivobuccal oral squamous cell carcinoma reveals DNA damage response genes. Genomics, 2022, 114, 110308.	2.9	1
3	Azadirachta indica A. Juss bark extract and its Nimbin isomers restrict Î²-coronaviral infection and replication. Virology, 2022, 569, 13-28.	2.4	15
4	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.	3.3	1
5	MD DaVis: interactive data visualization of protein molecular dynamics. Bioinformatics, 2022, 38, 3299-3301.	4.1	4
6	Inferring metal binding sites in flexible regions of proteins. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1125-1133.	2.6	5
7	Spike protein fusion loop controls SARS-CoV-2 fusogenicity and infectivity. Journal of Structural Biology, 2021, 213, 107713.	2.8	11
8	A computational framework for modeling functional proteinâ€protein interactions. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1353-1364.	2.6	2
9	Molecular Dynamics of Hemoglobin Reveals Structural Alterations and Explains the Interactions Driving Sickle Cell Fibrillation. Journal of Physical Chemistry B, 2021, 125, 9921-9933.	2.6	5
10	Exo-selective intermolecular Dielsâ€“Alder reaction by PyrI4 and AbnU on non-natural substrates. Communications Chemistry, 2021, 4, .	4.5	3
11	Clusters of hairpins induce intrinsic transcription termination in bacteria. Scientific Reports, 2021, 11, 16194.	3.3	4
12	DJ-1-Nrf2 axis is activated upon murine Î²-coronavirus infection in the CNS. Brain Disorders, 2021, 4, 100021.	1.7	2
13	Spike Glycoprotein Is Central to Coronavirus Pathogenesis-Parallel Between m-CoV and SARS-CoV-2. Annals of Neurosciences, 2021, 28, 201-218.	1.7	7
14	Network-based identification of miRNAs and transcription factors and in silico drug screening targeting Î³-secretase involved in Alzheimer's disease. Heliyon, 2021, 7, e08502.	3.2	4
15	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.	3.7	2
16	Towards Accelerated Genome Informatics on Parallel HPC Platforms: The ReneGENE-GI Perspective. Journal of Signal Processing Systems, 2020, 92, 1197-1213.	2.1	0
17	Aggregation of M3 (E376D) variant of alpha1- antitrypsin. Scientific Reports, 2020, 10, 8290.	3.3	4
18	New facets of larger Nest motifs in proteins. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1413-1422.	2.6	2

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19	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.	1.5	1
20	Effect of land use on soil carbon fractions. Journal of the Indian Society of Soil Science, 2020, 68, 392-399.	0.2	1
21	Differential Regulation of DJâ€1 in Glial Cells upon MHVâ€A59 â€Induced Oxidative Stress. FASEB Journal, 2020, 34, 1-1.	0.5	0
22	Assessing predictions on fitness effects of missense variants in calmodulin. Human Mutation, 2019, 40, 1463-1473.	2.5	8
23	Structural analysis of glutathionyl hemoglobin using native mass spectrometry. Journal of Structural Biology, 2019, 208, 107386.	2.8	6
24	Evaluating the predictions of the protein stability change upon single amino acid substitutions for the FXN CAGI5 challenge. Human Mutation, 2019, 40, 1392-1399.	2.5	16
25	Predicting gas phase entropy of select hydrocarbon classes through specific information-theoretical molecular descriptors. SAR and QSAR in Environmental Research, 2019, 30, 491-505.	2.2	3
26	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.	2.5	8
27	Exploring the use of molecular dynamics in assessing protein variants for phenotypic alterations. Human Mutation, 2019, 40, 1424-1435.	2.5	10
28	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
29	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.	3.3	33
30	Combinatorial Drug Discovery from Activity-Related Substructure Identification. Challenges and Advances in Computational Chemistry and Physics, 2019, , 71-108.	0.6	1
31	Ebolavirus interferon antagonistsâ€"protein interaction perspectives to combat pathogenesis. Briefings in Functional Genomics, 2018, 17, 392-401.	2.7	4
32	ReneGENE-DP: Accelerated Parallel Dynamic Programming for Genome Informatics. , 2018, , .		4
33	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.	4.1	8
34	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.	3.7	3
35	Global Asymptotic Stability of a Non-linear Population Model of Diabetes Mellitus. Springer Proceedings in Mathematics and Statistics, 2018, , 351-357.	0.2	3
36	ReneGENE-GI: Empowering Precision Genomics with FPGAs on HPCs. Lecture Notes in Computer Science, 2018, , 178-191.	1.3	1

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37	ReneGENE-Novo: Co-designed Algorithm-Architecture for Accelerated Preprocessing and Assembly of Genomic Short Reads. Lecture Notes in Computer Science, 2018, , 564-577.	1.3	1
38	Combinatorial Design of Molecule using Activity-Linked Substructural Topological Information as Applied to Antitubercular Compounds. Current Computer-Aided Drug Design, 2018, 15, 67-81.	1.2	3
39	Pipeline for inferring protein function from dynamics using coarse-grained molecular mechanics forcefield. Computers in Biology and Medicine, 2017, 83, 134-142.	7.0	3
40	Molecular Dynamics Information Improves cis-Peptide-Based Function Annotation of Proteins. Journal of Proteome Research, 2017, 16, 2936-2946.	3.7	4
41	Numerical simulation of a glucose sensitive composite membrane closed-loop insulin delivery system. Bioprocess and Biosystems Engineering, 2017, 40, 1453-1462.	3.4	0
42	Computational design of model scaffold for anion recognition based on the â€˜C^{Î±}NNâ€™ motif. Biopolymers, 2017, 108, e22921.	2.4	5
43	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.	1.2	4
44	Mass Spectrometry-Based Diagnosis of Hemoglobinopathies: A Potential Tool for the Screening of Genetic Disorder. Biochemical Genetics, 2016, 54, 816-825.	1.7	6
45	AccuRA: Accurate alignment of short reads on scalable reconfigurable accelerators. , 2016, , .		2
46	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
47	Bacterial siderophore mimicking iron complexes as DNA targeting antimicrobials. RSC Advances, 2016, 6, 39245-39260.	3.6	19
48	Chemical Shifts to Metabolic Pathways: Identifying Metabolic Pathways Directly from a Single 2D NMR Spectrum. Analytical Chemistry, 2015, 87, 12197-12205.	6.5	11
49	Pattern Recognition-Based Approach for Identifying Metabolites in Nuclear Magnetic Resonance-Based Metabolomics. Analytical Chemistry, 2015, 87, 7148-7155.	6.5	20
50	Mass spectrometry based characterization of Hb Beckman variant in a falsely elevated HbA1c sample. Analytical Biochemistry, 2015, 489, 53-58.	2.4	5
51	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.	0.4	2
52	Identifying functionally important cisâ€peptide containing segments in proteins and their utility in molecular function annotation. FEBS Journal, 2014, 281, 5602-5621.	4.7	5
53	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.	1.1	3
54	Two new atom centered fragment descriptors and scoring function enhance classification of antibacterial activity. Journal of Molecular Modeling, 2014, 20, 2164.	1.8	4

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55	De novoinference of protein function from coarse-grained dynamics. Proteins: Structure, Function and Bioinformatics, 2014, 82, 2443-2454.	2.6	8
56	Information content of molecular graph and prediction of gas phase thermal entropy of organic compounds. Journal of Mathematical Chemistry, 2013, 51, 2718-2730.	1.5	4
57	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
58	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.	3.5	32
59	Use of Vertex Index in Structure-Activity Analysis and Design of Molecules. Current Computer-Aided Drug Design, 2012, 8, 128-134.	1.2	7
60	Combining Bayes Classification and Point Group Symmetry under Boolean Framework for Enhanced Protein Quaternary Structure Inference. Structure, 2011, 19, 304-312.	3.3	30
61	dockYardâ€“a repository to assist modeling of protein-protein docking. Journal of Molecular Modeling, 2011, 17, 599-606.	1.8	2
62	Using correlated parameters for improved ranking of proteinâ€“protein docking decoys. Journal of Computational Chemistry, 2011, 32, 787-796.	3.3	15
63	PRUNE and PROBE--two modular web services for protein-protein docking. Nucleic Acids Research, 2011, 39, W229-W234.	14.5	15
64	WebGeSTer DBâ€”a transcription terminator database. Nucleic Acids Research, 2011, 39, D129-D135.	14.5	100
65	New measures for estimating surface complementarity and packing at proteinâ€“protein interfaces. FEBS Letters, 2010, 584, 1163-1168.	2.8	24
66	Modeling a hybrid reactive-deliberative architecture towards realizing overall dynamic behavior of an AUV. Procedia Computer Science, 2010, 1, 259-268.	2.0	13
67	In Vivo Proton MR Spectroscopy Evaluation of Pyogenic Brain Abscesses: A Report of 194 Cases. American Journal of Neuroradiology, 2010, 31, 360-366.	2.4	85
68	Interface of Apoptotic Protein Complexes Has Distinct Properties. In Silico Biology, 2009, 9, 365-378.	0.9	0
69	Inferring molecular function: contributions from functional linkages. Trends in Genetics, 2008, 24, 587-590.	6.7	5
70	Functionally important segments in proteins dissected using Gene Ontology and geometric clustering of peptide fragments. Genome Biology, 2008, 9, R52.	9.6	17
71	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.	2.5	7
72	Functional Linkages Can Reveal Protein Complexes for Structure Determination. Structure, 2007, 15, 1079-1089.	3.3	2

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73	An Enthalpy Model for Simulation of Dendritic Growth. Numerical Heat Transfer, Part B: Fundamentals, 2006, 50, 59-78.	0.9	48
74	On gene ontology and function annotation. Bioinformation, 2006, 1, 97-98.	0.5	21
75	Inference of Protein Function from Protein Structure. Structure, 2005, 13, 121-130.	3.3	175
76	Disulfide bonds, their stereospecific environment and conservation in protein structures. Protein Engineering, Design and Selection, 2004, 17, 795-808.	2.1	109
77	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
78	New Principles of Protein Structure: Nests, Eggsâ€”and What Next?. Angewandte Chemie - International Edition, 2002, 41, 4663-4665.	13.8	35
79	On residues in the disallowed region of the Ramachandran map. Biopolymers, 2002, 63, 195-206.	2.4	74
80	Secondary structures at polypeptide-chain termini and their features. Acta Crystallographica Section D: Biological Crystallography, 2002, 58, 1793-1802.	2.5	6
81	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
82	Non-hydrogen Bond Interactions Involving the Methionine Sulfur Atom. Journal of Biomolecular Structure and Dynamics, 2001, 19, 115-128.	3.5	160
83	The interrelationships of side-chain and main-chain conformations in proteins. Progress in Biophysics and Molecular Biology, 2001, 76, 1-102.	2.9	189
84	More hydrogen bonds for the (structural) biologist. Trends in Biochemical Sciences, 2001, 26, 521-523.	7.5	230
85	Terminal residues in protein chains: Residue preference, conformation, and interaction. Biopolymers, 2000, 53, 467-475.	2.4	13
86	Environment of tryptophan side chains in proteins. Proteins: Structure, Function and Bioinformatics, 2000, 38, 288-300.	2.6	133
87	Î²-Sheet propensity and its correlation withparameters based on conformation. Acta Crystallographica Section D: Biological Crystallography, 2000, 56, 589-594.	2.5	32
88	Conformational Similarity Indices Between Different Residues in Proteins and Î±-Helix Propensities. Journal of Biomolecular Structure and Dynamics, 2000, 18, 273-280.	3.5	10
89	Environment of tryptophan side chains in proteins. Proteins: Structure, Function and Bioinformatics, 2000, 38, 288-300.	2.6	1
90	Environment of tryptophan side chains in proteins. Proteins: Structure, Function and Bioinformatics, 2000, 38, 288-300.	2.6	36

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91	Graphical representation of the salient conformational features of protein residues. Protein Engineering, Design and Selection, 1999, 12, 523-526.	2.1	3
92	Packing of aromatic rings against tryptophan residues in proteins. Acta Crystallographica Section D: Biological Crystallography, 1999, 55, 1421-1427.	2.5	102
93	Estimates of the loss of main-chain conformational entropy of different residues on protein folding. , 1999, 36, 332-339.		21
94	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.	4.2	294
95	Estimates of the loss of main-chain conformational entropy of different residues on protein folding. Proteins: Structure, Function and Bioinformatics, 1999, 36, 332-9.	2.6	5
96	Different Types of Interactions Involving Cysteine Sulfhydryl Group in Proteins. Journal of Biomolecular Structure and Dynamics, 1998, 15, 1059-1072.	3.5	83
97	Main-chain conformational features at different conformations of the side-chains in proteins. Protein Engineering, Design and Selection, 1998, 11, 631-647.	2.1	38
98	An electrophileâ€nucleophile interaction in metalloprotein structures. Protein Science, 1997, 6, 851-859.	7.6	17
99	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.	1.6	12
100	Stereodivergent Câ^'C Bond Formation on Areneâ^'Chromium Template:ÂEndo-Selective Allylation by Hosomiâ^'Sakurai Reactionâ€. Journal of Organic Chemistry, 1996, 61, 8362-8363.	3.2	23
101	Production of Hydrolases by N2-fixing Microorganisms. Biochemie Und Physiologie Der Pflanzen, 1989, 185, 75-81.	0.5	8
102	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
103	Effects of dynamic impacts on human bones. Journal of Biosciences, 1980, 2, 139-144.	1.1	0
104	New routes to condensed polynuclear compoundsâ€"VIII. Tetrahedron, 1973, 29, 177-184.	1.9	30
105	Mechanisms of Arsenic-Induced Toxicity with Special Emphasis on Arsenic-Binding Proteins. , 0, , .		5