Debasisa Mohanty

List of Publications by Year
in descending order

72 papers	3,396 citations	172457 29 h-index	144013 57 g-index
75 all docs	75 docs citations	75 times ranked	4015 citing authors

#	Article	IF	Citations
1	Kupyaphores are zinc homeostatic metallophores required for colonization of Mycobacterium tuberculosis. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	19
2	Allosteric regulation of the inactive to active state conformational transition in CDPK1 protein of Plasmodium falciparum. International Journal of Biological Macromolecules, 2022, 215, 489-500.	7.5	1
3	Pf-Phospho: a machine learning-based phosphorylation sites prediction tool for Plasmodium proteins. Briefings in Bioinformatics, 2022, 23, .	6.5	2
4	A machine learning-based method for prediction of macrocyclization patterns of polyketides and non-ribosomal peptides. Bioinformatics, 2021, 37, 603-611.	4.1	10
5	SMMPPI: a machine learning-based approach for prediction of modulators of proteinâ€“protein interactions and its application for identification of novel inhibitors for RBD:hACE2 interactions in SARS-CoV-2. Briefings in Bioinformatics, 2021, 22, .	6.5	22
6	RiPPMiner-Genome: A Web Resource for Automated Prediction of Crosslinked Chemical Structures of RiPPs by Genome Mining. Journal of Molecular Biology, 2021, 433, 166887.	4.2	19
7	LipidII interaction with specific residues of Mycobacterium tuberculosis PknB extracytoplasmic domain governs its optimal activation. Nature Communications, 2019, 10, 1231.	12.8	42
8	Sequence- and structure-based analysis of proteins involved in miRNA biogenesis. Journal of Biomolecular Structure and Dynamics, 2018, 36, 139-151.	3.5	5
9	Deciphering evolution of immune recognition in antibodies. BMC Structural Biology, 2018, 18, 19.	2.3	4
10	Molecular Dynamics Simulations for Deciphering the Structural Basis of Recognition of Pre-let-7 miRNAs by LIN28. Biochemistry, 2017, 56, 723-735.	2.5	5
11	SBSPKSv2: structure-based sequence analysis of polyketide synthases and non-ribosomal peptide synthetases. Nucleic Acids Research, 2017, 45, W72-W79.	14.5	47
12	RiPPMiner: a bioinformatics resource for deciphering chemical structures of RiPPs based on prediction of cleavage and cross-links. Nucleic Acids Research, 2017, 45, W80-W88.	14.5	100
13	In silico methods for linking genes and secondary metabolites: The way forward. Synthetic and Systems Biotechnology, 2016, 1, 80-88.	3.7	35
14	Understanding the molecular basis of substrate binding specificity of PTB domains. Scientific Reports, 2016, 6, 31418.	3.3	7
15	modPDZpep: a web resource for structure based analysis of human PDZ-mediated interaction networks. Biology Direct, 2016, 11, 48.	4.6	2
16	novPTMenzy: a database for enzymes involved in novel post-translational modifications. Database: the Journal of Biological Databases and Curation, 2015, 2015, bav039.	3.0	3
17	Deciphering the Molecular Basis of Functional Divergence in AMPylating Enzymes by Molecular Dynamics Simulations and Structure Guided Phylogeny. Biochemistry, 2015, 54, 5209-5224.	2.5	8
18	In silico identification of AMPylating enzymes and study of their divergent evolution. Scientific Reports, 2015, 5, 10804.	3.3	32

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19	Deciphering kinaseâ€“substrate relationships by analysis of domain-specific phosphorylation network. Bioinformatics, 2014, 30, 1730-1738.	4.1	17
20	Genome-Wide Search for Eliminylating Domains Reveals Novel Function for BLES03-Like Proteins. Genome Biology and Evolution, 2014, 6, 2017-2033.	2.5	2
21	Structure-Based Multiscale Approach for Identification of Interaction Partners of PDZ Domains. Journal of Chemical Information and Modeling, 2014, 54, 1143-1156.	5.4	8
22	Mechanism of Autophosphorylation of Mycobacterial PknB Explored by Molecular Dynamics Simulations. Biochemistry, 2014, 53, 4715-4726.	2.5	10
23	Prediction of inter domain interactions in modular polyketide synthases by docking and correlated mutation analysis. Journal of Biomolecular Structure and Dynamics, 2013, 31, 17-29.	3.5	3
24	STRUCTURAL BIOINFORMATICS APPROACHES FOR DECIPHERING BIOSYNTHETIC CODE OF SECONDARY METABOLITES. , 2013, , 428-442.		0
25	An In Silico Analysis of the Binding Modes and Binding Affinities of Small Molecule Modulators of PDZ-Peptide Interactions. PLoS ONE, 2013, 8, e71340.	2.5	18
26	Modeling holo-ACP:DH and holo-ACP:KR complexes of modular polyketide synthases: a docking and molecular dynamics study. BMC Structural Biology, 2012, 12, 10.	2.3	18
27	Novel insights into the regulation of malarial calciumâ€dependent protein kinase 1. FASEB Journal, 2012, 26, 3212-3221.	0.5	26
28	Retrobiosynthetic Approach Delineates the Biosynthetic Pathway and the Structure of the Acyl Chain of Mycobacterial Glycopeptidolipids*. Journal of Biological Chemistry, 2012, 287, 30677-30687.	3.4	17
29	Molecular Dynamics Simulations onPars Intercerebralis MajorPeptide-C (PMP-C) Reveal the Role of Glycosylation and Disulfide Bonds in its Enhanced Structural Stability and Function. Journal of Biomolecular Structure and Dynamics, 2012, 29, 905-920.	3.5	8
30	Inter-domain movements in polyketide synthases: a molecular dynamics study. Molecular BioSystems, 2012, 8, 1157.	2.9	8
31	RECQL4 is essential for the transport of p53 to mitochondria in normal human cells in the absence of exogenous stress. Journal of Cell Science, 2012, 125, 2509-22.	2.0	88
32	Fatty acyl-AMP ligases and polyketide synthases are unique enzymes of lipid biosynthetic machinery in Mycobacterium tuberculosis. Tuberculosis, 2011, 91, 448-455.	1.9	18
33	Role of glycosylation in structure and stability of Erythrina corallodendron lectin (EcorL): A molecular dynamics study. Protein Science, 2011, 20, 465-481.	7.6	22
34	Two Functionally Distinctive Phosphopantetheinyl Transferases from Amoeba Dictyostelium discoideum. PLoS ONE, 2011, 6, e24262.	2.5	5
35	Computational Methods for Identification of Novel Secondary Metabolite Biosynthetic Pathways by Genome Analysis. , 2011, , 380-405.		4
36	Genome scale prediction of substrate specificity for acyl adenylate superfamily of enzymes based on active site residue profiles. BMC Bioinformatics, 2010, 11, 57.	2.6	33

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37	SBSPKS: structure based sequence analysis of polyketide synthases. Nucleic Acids Research, 2010, 38, W487-W496.	14.5	162
38	Identification of substrates for Ser/Thr kinases using residue-based statistical pair potentials. Bioinformatics, 2010, 26, 189-197.	4.1	11
39	Chk1-Dependent Constitutive Phosphorylation of BLM Helicase at Serine 646 Decreases after DNA Damage. Molecular Cancer Research, 2010, 8, 1234-1247.	3.4	22
40	Structure-based identification of MHC binding peptides: Benchmarking of prediction accuracy. Molecular BioSystems, 2010, 6, 2508.	2.9	12
41	Towards Prediction of Metabolic Products of Polyketide Synthases: An In Silico Analysis. PLoS Computational Biology, 2009, 5, e1000351.	3.2	73
42	RegAnalyst: a web interface for the analysis of regulatory motifs, networks and pathways. Nucleic Acids Research, 2009, 37, W193-W201.	14.5	16
43	Mechanistic and functional insights into fatty acid activation in Mycobacterium tuberculosis. Nature Chemical Biology, 2009, 5, 166-173.	8.0	119
44	The Role of Metal Ions in Substrate Recognition and Stability of Concanavalin A: A Molecular Dynamics Study. Biophysical Journal, 2009, 96, 21-34.	0.5	42
45	In silico analysis of methyltransferase domains involved in biosynthesis of secondary metabolites. BMC Bioinformatics, 2008, 9, 454.	2.6	73
46	Dissecting the Functional Role of Polyketide Synthases in Dictyostelium discoideum. Journal of Biological Chemistry, 2008, 283, 11348-11354.	3.4	35
47	Novel Intermolecular Iterative Mechanism for Biosynthesis of Mycoketide Catalyzed by a Bimodular Polyketide Synthase. PLoS Biology, 2008, 6, e163.	5.6	30
48	MODPROPEP: a program for knowledge-based modeling of protein-peptide complexes. Nucleic Acids Research, 2007, 35, W549-W555.	14.5	36
49	PAR-3D: a server to predict protein active site residues. Nucleic Acids Research, 2007, 35, W503-W505.	14.5	34
50	Versatile polyketide enzymatic machinery for the biosynthesis of complex mycobacterial lipids. Natural Product Reports, 2007, 24, 267.	10.3	101
51	Versatility of polyketide synthases in generating metabolic diversity. Current Opinion in Structural Biology, 2007, 17, 736-743.	5.7	68
52	A genetic locus required for iron acquisition inMycobacterium tuberculosis. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 2069-2074.	7.1	113
53	SEARCHGTr: a program for analysis of glycosyltransferases involved in glycosylation of secondary metabolites. Nucleic Acids Research, 2005, 33, W220-W225.	14.5	38
54	Promiscuous Fatty Acyl CoA Ligases Produce Acyl-CoA and Acyl-SNAC Precursors for Polyketide Biosynthesis. Journal of the American Chemical Society, 2005, 127, 9388-9389.	13.7	40

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55	Dissecting the Mechanism and Assembly of a Complex Virulence Mycobacterial Lipid. Molecular Cell, 2005, 17, 631-643.	9.7	143
56	NRPS-PKS: a knowledge-based resource for analysis of NRPS/PKS megasynthases. Nucleic Acids Research, 2004, 32, W405-W413.	14.5	262
57	Enzymic activation and transfer of fatty acids as acyl-adenylates in mycobacteria. Nature, 2004, 428, 441-445.	27.8	264
58	Computational Approach for Prediction of Domain Organization and Substrate Specificity of Modular Polyketide Synthases. Journal of Molecular Biology, 2003, 328, 335-363.	4.2	202
59	A New Family of Type III Polyketide Synthases in Mycobacterium tuberculosis. Journal of Biological Chemistry, 2003, 278, 44780-44790.	3.4	101
60	SEARCHPKS: a program for detection and analysis of polyketide synthase domains. Nucleic Acids Research, 2003, 31, 3654-3658.	14.5	103
61	De novo predictions of the quaternary structure of leucine zippers and other coiled coils. International Journal of Quantum Chemistry, 1999, 75, 165-176.	2.0	5
62	Correlation between knowledge-based and detailed atomic potentials: Application to the unfolding of the GCN4 leucine zipper. Proteins: Structure, Function and Bioinformatics, 1999, 35, 447-452.	2.6	30
63	De Novo Simulations of the Folding Thermodynamics of the GCN4 Leucine Zipper. Biophysical Journal, 1999, 77, 54-69.	0.5	31
64	Dynamics of peptide folding. , 1998, , .		0
65	Kinetics of peptide folding: computer simulations of SYPFDV and peptide variants in water 1 1Edited by G. von Heijne. Journal of Molecular Biology, 1997, 272, 423-442.	4.2	69
66	Chain folding and A:T pairing in human telomeric DNA: a model-building and molecular dynamics study. Biophysical Journal, 1995, 69, 1046-1067.	0.5	21
67	Conformational polymorphism in telomeric structures: Loop orientation and interloop pairing in d(G4TnG4). Biopolymers, 1994, 34, 1187-1211.	2.4	23
68	Conformational polymorphism in G-tetraplex structures: strand reversal by base flipover or sugar flipover. Nucleic Acids Research, 1993, 21, 1767-1774.	14.5	35
69	Hairpin and parallel quartet structures for telomeric sequences. Nucleic Acids Research, 1992, 20, 4061-4067.	14.5	396
70	DNA Polymorphism and Local Variation in Base-Pair Orientation: A Theoretical Rationale. Journal of Biomolecular Structure and Dynamics, 1991, 9, 127-142.	3.5	12
71	Biosynthesis of Mycobacterial Lipids by Multifunctional Polyketide Synthases. , 0, , 235-248.		2
72	Computational Methods for Identification of Novel Secondary Metabolite Biosynthetic Pathways by Genome Analysis. , 0, , 1642-1666.		0