Debasisa Mohanty

List of Publications by Year
in descending order

72 papers	3,396 citations	172207 29 h-index	143772 57 g-index
75 all docs	75 docs citations	75 times ranked	4015 citing authors

#	Article	IF	Citations
1	Hairpin and parallel quartet structures for telomeric sequences. Nucleic Acids Research, 1992, 20, 4061-4067.	6.5	396
2	Enzymic activation and transfer of fatty acids as acyl-adenylates in mycobacteria. Nature, 2004, 428, 441-445.	13.7	264
3	NRPS-PKS: a knowledge-based resource for analysis of NRPS/PKS megasynthases. Nucleic Acids Research, 2004, 32, W405-W413.	6.5	262
4	Computational Approach for Prediction of Domain Organization and Substrate Specificity of Modular Polyketide Synthases. Journal of Molecular Biology, 2003, 328, 335-363.	2.0	202
5	SBSPKS: structure based sequence analysis of polyketide synthases. Nucleic Acids Research, 2010, 38, W487-W496.	6.5	162
6	Dissecting the Mechanism and Assembly of a Complex Virulence Mycobacterial Lipid. Molecular Cell, 2005, 17, 631-643.	4.5	143
7	Mechanistic and functional insights into fatty acid activation in Mycobacterium tuberculosis. Nature Chemical Biology, 2009, 5, 166-173.	3.9	119
8	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.	3.3	113
9	SEARCHPKS: a program for detection and analysis of polyketide synthase domains. Nucleic Acids Research, 2003, 31, 3654-3658.	6.5	103
10	A New Family of Type III Polyketide Synthases in Mycobacterium tuberculosis. Journal of Biological Chemistry, 2003, 278, 44780-44790.	1.6	101
11	Versatile polyketide enzymatic machinery for the biosynthesis of complex mycobacterial lipids. Natural Product Reports, 2007, 24, 267.	5.2	101
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.	6.5	100
13	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.	1.2	88
14	In silico analysis of methyltransferase domains involved in biosynthesis of secondary metabolites. BMC Bioinformatics, 2008, 9, 454.	1.2	73
15	Towards Prediction of Metabolic Products of Polyketide Synthases: An In Silico Analysis. PLoS Computational Biology, 2009, 5, e1000351.	1.5	73
16	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.	2.0	69
17	Versatility of polyketide synthases in generating metabolic diversity. Current Opinion in Structural Biology, 2007, 17, 736-743.	2.6	68
18	SBSPKSv2: structure-based sequence analysis of polyketide synthases and non-ribosomal peptide synthetases. Nucleic Acids Research, 2017, 45, W72-W79.	6.5	47

#	Article	IF	Citations
19	The Role of Metal Ions in Substrate Recognition and Stability of Concanavalin A: A Molecular Dynamics Study. Biophysical Journal, 2009, 96, 21-34.	0.2	42
20	LipidII interaction with specific residues of Mycobacterium tuberculosis PknB extracytoplasmic domain governs its optimal activation. Nature Communications, 2019, 10, 1231.	5.8	42
21	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.	6.6	40
22	SEARCHGTr: a program for analysis of glycosyltransferases involved in glycosylation of secondary metabolites. Nucleic Acids Research, 2005, 33, W220-W225.	6.5	38
23	MODPROPEP: a program for knowledge-based modeling of protein-peptide complexes. Nucleic Acids Research, 2007, 35, W549-W555.	6.5	36
24	Conformational polymorphism in G-tetraplex structures: strand reversal by base flipover or sugar flipover. Nucleic Acids Research, 1993, 21, 1767-1774.	6.5	35
25	Dissecting the Functional Role of Polyketide Synthases in Dictyostelium discoideum. Journal of Biological Chemistry, 2008, 283, 11348-11354.	1.6	35
26	In silico methods for linking genes and secondary metabolites: The way forward. Synthetic and Systems Biotechnology, 2016, 1, 80-88.	1.8	35
27	PAR-3D: a server to predict protein active site residues. Nucleic Acids Research, 2007, 35, W503-W505.	6.5	34
28	Genome scale prediction of substrate specificity for acyl adenylate superfamily of enzymes based on active site residue profiles. BMC Bioinformatics, 2010, 11, 57.	1.2	33
29	In silico identification of AMPylating enzymes and study of their divergent evolution. Scientific Reports, 2015, 5, 10804.	1.6	32
30	De Novo Simulations of the Folding Thermodynamics of the GCN4 Leucine Zipper. Biophysical Journal, 1999, 77, 54-69.	0.2	31
31	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.	1.5	30
32	Novel Intermolecular Iterative Mechanism for Biosynthesis of Mycoketide Catalyzed by a Bimodular Polyketide Synthase. PLoS Biology, 2008, 6, e163.	2.6	30
33	Novel insights into the regulation of malarial calciumâ€dependent protein kinase 1. FASEB Journal, 2012, 26, 3212-3221.	0.2	26
34	Conformational polymorphism in telomeric structures: Loop orientation and interloop pairing in d(G4TnG4). Biopolymers, 1994, 34, 1187-1211.	1.2	23
35	Chk1-Dependent Constitutive Phosphorylation of BLM Helicase at Serine 646 Decreases after DNA Damage. Molecular Cancer Research, 2010, 8, 1234-1247.	1.5	22
36	Role of glycosylation in structure and stability of Erythrina corallodendron lectin (EcorL): A molecular dynamics study. Protein Science, 2011, 20, 465-481.	3.1	22

#	Article	IF	Citations
37	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, .	3.2	22
38	Chain folding and A:T pairing in human telomeric DNA: a model-building and molecular dynamics study. Biophysical Journal, 1995, 69, 1046-1067.	0.2	21
39	RiPPMiner-Genome: A Web Resource for Automated Prediction of Crosslinked Chemical Structures of RiPPs by Genome Mining. Journal of Molecular Biology, 2021, 433, 166887.	2.0	19
40	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, .	3.3	19
41	Fatty acyl-AMP ligases and polyketide synthases are unique enzymes of lipid biosynthetic machinery in Mycobacterium tuberculosis. Tuberculosis, 2011, 91, 448-455.	0.8	18
42	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
43	An In Silico Analysis of the Binding Modes and Binding Affinities of Small Molecule Modulators of PDZ-Peptide Interactions. PLoS ONE, 2013, 8, e71340.	1.1	18
44	Retrobiosynthetic Approach Delineates the Biosynthetic Pathway and the Structure of the Acyl Chain of Mycobacterial Glycopeptidolipids*. Journal of Biological Chemistry, 2012, 287, 30677-30687.	1.6	17
45	Deciphering kinaseâ€“substrate relationships by analysis of domain-specific phosphorylation network. Bioinformatics, 2014, 30, 1730-1738.	1.8	17
46	RegAnalyst: a web interface for the analysis of regulatory motifs, networks and pathways. Nucleic Acids Research, 2009, 37, W193-W201.	6.5	16
47	DNA Polymorphism and Local Variation in Base-Pair Orientation: A Theoretical Rationale. Journal of Biomolecular Structure and Dynamics, 1991, 9, 127-142.	2.0	12
48	Structure-based identification of MHC binding peptides: Benchmarking of prediction accuracy. Molecular BioSystems, 2010, 6, 2508.	2.9	12
49	Identification of substrates for Ser/Thr kinases using residue-based statistical pair potentials. Bioinformatics, 2010, 26, 189-197.	1.8	11
50	Mechanism of Autophosphorylation of Mycobacterial PknB Explored by Molecular Dynamics Simulations. Biochemistry, 2014, 53, 4715-4726.	1.2	10
51	A machine learning-based method for prediction of macrocyclization patterns of polyketides and non-ribosomal peptides. Bioinformatics, 2021, 37, 603-611.	1.8	10
52	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.	2.0	8
53	Inter-domain movements in polyketide synthases: a molecular dynamics study. Molecular BioSystems, 2012, 8, 1157.	2.9	8
54	Structure-Based Multiscale Approach for Identification of Interaction Partners of PDZ Domains. Journal of Chemical Information and Modeling, 2014, 54, 1143-1156.	2.5	8

#	Article	IF	Citations
55	Deciphering the Molecular Basis of Functional Divergence in AMPylating Enzymes by Molecular Dynamics Simulations and Structure Guided Phylogeny. Biochemistry, 2015, 54, 5209-5224.	1.2	8
56	Understanding the molecular basis of substrate binding specificity of PTB domains. Scientific Reports, 2016, 6, 31418.	1.6	7
57	De novo predictions of the quaternary structure of leucine zippers and other coiled coils. International Journal of Quantum Chemistry, 1999, 75, 165-176.	1.0	5
58	Molecular Dynamics Simulations for Deciphering the Structural Basis of Recognition of Pre-let-7 miRNAs by LIN28. Biochemistry, 2017, 56, 723-735.	1.2	5
59	Sequence- and structure-based analysis of proteins involved in miRNA biogenesis. Journal of Biomolecular Structure and Dynamics, 2018, 36, 139-151.	2.0	5
60	Two Functionally Distinctive Phosphopantetheinyl Transferases from Amoeba Dictyostelium discoideum. PLoS ONE, 2011, 6, e24262.	1.1	5
61	Deciphering evolution of immune recognition in antibodies. BMC Structural Biology, 2018, 18, 19.	2.3	4
62	Computational Methods for Identification of Novel Secondary Metabolite Biosynthetic Pathways by Genome Analysis. , 2011, , 380-405.		4
63	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.	2.0	3
64	novPTMenzy: a database for enzymes involved in novel post-translational modifications. Database: the Journal of Biological Databases and Curation, 2015, 2015, bav039.	1.4	3
65	Genome-Wide Search for Eliminylating Domains Reveals Novel Function for BLES03-Like Proteins. Genome Biology and Evolution, 2014, 6, 2017-2033.	1.1	2
66	modPDZpep: a web resource for structure based analysis of human PDZ-mediated interaction networks. Biology Direct, 2016, 11, 48.	1.9	2
67	Biosynthesis of Mycobacterial Lipids by Multifunctional Polyketide Synthases. , 0, , 235-248.		2
68	Pf-Phospho: a machine learning-based phosphorylation sites prediction tool for Plasmodium proteins. Briefings in Bioinformatics, 2022, 23, .	3.2	2
69	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.	3.6	1
70	Dynamics of peptide folding. , 1998, , .		0
71	STRUCTURAL BIOINFORMATICS APPROACHES FOR DECIPHERING BIOSYNTHETIC CODE OF SECONDARY METABOLITES. , 2013, , 428-442.		0
72	Computational Methods for Identification of Novel Secondary Metabolite Biosynthetic Pathways by Genome Analysis. , 0, , 1642-1666.		0