

# Debasisa Mohanty

## List of Publications by Year in descending order

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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	Kupyaphores are zinc homeostatic metallophores required for colonization of <i>Mycobacterium tuberculosis</i> . Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	3.3	19
2	Allosteric regulation of the inactive to active state conformational transition in CDPK1 protein of <i>Plasmodium falciparum</i> . International Journal of Biological Macromolecules, 2022, 215, 489-500.	3.6	1
3	Pf-Phospho: a machine learning-based phosphorylation sites prediction tool for <i>Plasmodium</i> proteins. Briefings in Bioinformatics, 2022, 23, .	3.2	2
4	A machine learning-based method for prediction of macrocyclization patterns of polyketides and non-ribosomal peptides. Bioinformatics, 2021, 37, 603-611.	1.8	10
5	SMMPPi: a machine learning-based approach for prediction of modulators of protein-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
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.	2.0	19
7	LipidII interaction with specific residues of <i>Mycobacterium tuberculosis</i> PknB extracytoplasmic domain governs its optimal activation. Nature Communications, 2019, 10, 1231.	5.8	42
8	Sequence- and structure-based analysis of proteins involved in miRNA biogenesis. Journal of Biomolecular Structure and Dynamics, 2018, 36, 139-151.	2.0	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.	1.2	5
11	SBSPKSv2: structure-based sequence analysis of polyketide synthases and non-ribosomal peptide synthetases. Nucleic Acids Research, 2017, 45, W72-W79.	6.5	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.	6.5	100
13	In silico methods for linking genes and secondary metabolites: The way forward. Synthetic and Systems Biotechnology, 2016, 1, 80-88.	1.8	35
14	Understanding the molecular basis of substrate binding specificity of PTB domains. Scientific Reports, 2016, 6, 31418.	1.6	7
15	modPDZpep: a web resource for structure based analysis of human PDZ-mediated interaction networks. Biology Direct, 2016, 11, 48.	1.9	2
16	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
17	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
18	In silico identification of AMPylating enzymes and study of their divergent evolution. Scientific Reports, 2015, 5, 10804.	1.6	32

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19	Deciphering kinase-substrate relationships by analysis of domain-specific phosphorylation network. <i>Bioinformatics</i> , 2014, 30, 1730-1738.	1.8	17
20	Genome-Wide Search for Eliminating Domains Reveals Novel Function for BLES03-Like Proteins. <i>Genome Biology and Evolution</i> , 2014, 6, 2017-2033.	1.1	2
21	Structure-Based Multiscale Approach for Identification of Interaction Partners of PDZ Domains. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 1143-1156.	2.5	8
22	Mechanism of Autophosphorylation of Mycobacterial PknB Explored by Molecular Dynamics Simulations. <i>Biochemistry</i> , 2014, 53, 4715-4726.	1.2	10
23	Prediction of inter domain interactions in modular polyketide synthases by docking and correlated mutation analysis. <i>Journal of Biomolecular Structure and Dynamics</i> , 2013, 31, 17-29.	2.0	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. <i>PLoS ONE</i> , 2013, 8, e71340.	1.1	18
26	Modeling holo-ACP:DH and holo-ACP:KR complexes of modular polyketide synthases: a docking and molecular dynamics study. <i>BMC Structural Biology</i> , 2012, 12, 10.	2.3	18
27	Novel insights into the regulation of malarial calcium-dependent protein kinase 1. <i>FASEB Journal</i> , 2012, 26, 3212-3221.	0.2	26
28	Retrobiosynthetic Approach Delineates the Biosynthetic Pathway and the Structure of the Acyl Chain of Mycobacterial Glycopeptidolipids*. <i>Journal of Biological Chemistry</i> , 2012, 287, 30677-30687.	1.6	17
29	Molecular Dynamics Simulations on Pars Intercerebralis Major Peptide-C (PMP-C) Reveal the Role of Glycosylation and Disulfide Bonds in its Enhanced Structural Stability and Function. <i>Journal of Biomolecular Structure and Dynamics</i> , 2012, 29, 905-920.	2.0	8
30	Inter-domain movements in polyketide synthases: a molecular dynamics study. <i>Molecular BioSystems</i> , 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. <i>Journal of Cell Science</i> , 2012, 125, 2509-22.	1.2	88
32	Fatty acyl-AMP ligases and polyketide synthases are unique enzymes of lipid biosynthetic machinery in <i>Mycobacterium tuberculosis</i> . <i>Tuberculosis</i> , 2011, 91, 448-455.	0.8	18
33	Role of glycosylation in structure and stability of <i>Erythrina corallodendron</i> lectin (EcorL): A molecular dynamics study. <i>Protein Science</i> , 2011, 20, 465-481.	3.1	22
34	Two Functionally Distinctive Phosphopantetheinyl Transferases from <i>Amoeba Dictyostelium discoideum</i> . <i>PLoS ONE</i> , 2011, 6, e24262.	1.1	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. <i>BMC Bioinformatics</i> , 2010, 11, 57.	1.2	33

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37	SBSPKS: structure based sequence analysis of polyketide synthases. <i>Nucleic Acids Research</i> , 2010, 38, W487-W496.	6.5	162
38	Identification of substrates for Ser/Thr kinases using residue-based statistical pair potentials. <i>Bioinformatics</i> , 2010, 26, 189-197.	1.8	11
39	Chk1-Dependent Constitutive Phosphorylation of BLM Helicase at Serine 646 Decreases after DNA Damage. <i>Molecular Cancer Research</i> , 2010, 8, 1234-1247.	1.5	22
40	Structure-based identification of MHC binding peptides: Benchmarking of prediction accuracy. <i>Molecular BioSystems</i> , 2010, 6, 2508.	2.9	12
41	Towards Prediction of Metabolic Products of Polyketide Synthases: An In Silico Analysis. <i>PLoS Computational Biology</i> , 2009, 5, e1000351.	1.5	73
42	RegAnalyst: a web interface for the analysis of regulatory motifs, networks and pathways. <i>Nucleic Acids Research</i> , 2009, 37, W193-W201.	6.5	16
43	Mechanistic and functional insights into fatty acid activation in <i>Mycobacterium tuberculosis</i> . <i>Nature Chemical Biology</i> , 2009, 5, 166-173.	3.9	119
44	The Role of Metal Ions in Substrate Recognition and Stability of Concanavalin A: A Molecular Dynamics Study. <i>Biophysical Journal</i> , 2009, 96, 21-34.	0.2	42
45	In silico analysis of methyltransferase domains involved in biosynthesis of secondary metabolites. <i>BMC Bioinformatics</i> , 2008, 9, 454.	1.2	73
46	Dissecting the Functional Role of Polyketide Synthases in <i>Dictyostelium discoideum</i> . <i>Journal of Biological Chemistry</i> , 2008, 283, 11348-11354.	1.6	35
47	Novel Intermolecular Iterative Mechanism for Biosynthesis of Mycoketide Catalyzed by a Bimodular Polyketide Synthase. <i>PLoS Biology</i> , 2008, 6, e163.	2.6	30
48	MODPROPEP: a program for knowledge-based modeling of protein-peptide complexes. <i>Nucleic Acids Research</i> , 2007, 35, W549-W555.	6.5	36
49	PAR-3D: a server to predict protein active site residues. <i>Nucleic Acids Research</i> , 2007, 35, W503-W505.	6.5	34
50	Versatile polyketide enzymatic machinery for the biosynthesis of complex mycobacterial lipids. <i>Natural Product Reports</i> , 2007, 24, 267.	5.2	101
51	Versatility of polyketide synthases in generating metabolic diversity. <i>Current Opinion in Structural Biology</i> , 2007, 17, 736-743.	2.6	68
52	A genetic locus required for iron acquisition in <i>Mycobacterium tuberculosis</i> . <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 2069-2074.	3.3	113
53	SEARCHGTr: a program for analysis of glycosyltransferases involved in glycosylation of secondary metabolites. <i>Nucleic Acids Research</i> , 2005, 33, W220-W225.	6.5	38
54	Promiscuous Fatty Acyl CoA Ligases Produce Acyl-CoA and Acyl-SNAC Precursors for Polyketide Biosynthesis. <i>Journal of the American Chemical Society</i> , 2005, 127, 9388-9389.	6.6	40

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55	Dissecting the Mechanism and Assembly of a Complex Virulence Mycobacterial Lipid. <i>Molecular Cell</i> , 2005, 17, 631-643.	4.5	143
56	NRPS-PKS: a knowledge-based resource for analysis of NRPS/PKS megasynthases. <i>Nucleic Acids Research</i> , 2004, 32, W405-W413.	6.5	262
57	Enzymic activation and transfer of fatty acids as acyl-adenylates in mycobacteria. <i>Nature</i> , 2004, 428, 441-445.	13.7	264
58	Computational Approach for Prediction of Domain Organization and Substrate Specificity of Modular Polyketide Synthases. <i>Journal of Molecular Biology</i> , 2003, 328, 335-363.	2.0	202
59	A New Family of Type III Polyketide Synthases in <i>Mycobacterium tuberculosis</i> . <i>Journal of Biological Chemistry</i> , 2003, 278, 44780-44790.	1.6	101
60	SEARCHPKS: a program for detection and analysis of polyketide synthase domains. <i>Nucleic Acids Research</i> , 2003, 31, 3654-3658.	6.5	103
61	De novo predictions of the quaternary structure of leucine zippers and other coiled coils. <i>International Journal of Quantum Chemistry</i> , 1999, 75, 165-176.	1.0	5
62	Correlation between knowledge-based and detailed atomic potentials: Application to the unfolding of the GCN4 leucine zipper. <i>Proteins: Structure, Function and Bioinformatics</i> , 1999, 35, 447-452.	1.5	30
63	De Novo Simulations of the Folding Thermodynamics of the GCN4 Leucine Zipper. <i>Biophysical Journal</i> , 1999, 77, 54-69.	0.2	31
64	Dynamics of peptide folding. , 1998, , .		0
65	Kinetics of peptide folding: computer simulations of SYPFDV and peptide variants in water 1 Edited by G. von Heijne. <i>Journal of Molecular Biology</i> , 1997, 272, 423-442.	2.0	69
66	Chain folding and A:T pairing in human telomeric DNA: a model-building and molecular dynamics study. <i>Biophysical Journal</i> , 1995, 69, 1046-1067.	0.2	21
67	Conformational polymorphism in telomeric structures: Loop orientation and interloop pairing in d(G4TnG4). <i>Biopolymers</i> , 1994, 34, 1187-1211.	1.2	23
68	Conformational polymorphism in G-tetraplex structures: strand reversal by base flipover or sugar flipover. <i>Nucleic Acids Research</i> , 1993, 21, 1767-1774.	6.5	35
69	Hairpin and parallel quartet structures for telomeric sequences. <i>Nucleic Acids Research</i> , 1992, 20, 4061-4067.	6.5	396
70	DNA Polymorphism and Local Variation in Base-Pair Orientation: A Theoretical Rationale. <i>Journal of Biomolecular Structure and Dynamics</i> , 1991, 9, 127-142.	2.0	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