Thirumal Kumar D

List of Publications by Year in Descending Order

85 papers	1,154 citations	21 h-index	29 g-index
91 ext. papers	1,442 ext. citations	4.7 avg, IF	5.21 L-index

#	Paper	IF	Citations
85	Understanding the activating mechanism of the immune system against COVID-19 by Traditional Indian Medicine: Network pharmacology approach.. *Advances in Protein Chemistry and Structural Biology*, **2022**, 129, 275-379	5.3	1
84	Accumulation of betacyanin in Hylocereus undatus rind: Pigment stability analysis and its role in xanthine oxidase inhibition. *Phytomedicine Plus*, **2022**, 2, 100197		0
83	Siddha Medicine and Computer Modeling: A Treasure for SARS-CoV-2 Treatment. *Studies in Systems, Decision and Control*, **2022**, 521-541	0.8	
82	Computational structural assessment of BReast CAncer type 1 susceptibility protein (BRCA1) and BRCA1-Associated Ring Domain protein 1 (BARD1) mutations on the protein-protein interface.. *Advances in Protein Chemistry and Structural Biology*, **2022**, 130, 375-397	5.3	4
81	Mixed azo dyes degradation by an intracellular azoreductase enzyme from alkaliphilic Bacillus subtilis: a molecular docking study. *Archives of Microbiology*, **2021**, 203, 3033-3044	3	6
80	A review of novel coronavirus disease (COVID-19): based on genomic structure, phylogeny, current shreds of evidence, candidate vaccines, and drug repurposing. *3 Biotech*, **2021**, 11, 198	2.8	8
79	In Silico Identification of Multi-target Anti-SARS-CoV-2 Peptides from Quinoa Seed Proteins. *International Journal of Peptide Research and Therapeutics*, **2021**, 27, 1-11	2.1	6
78	Structure-Based Virtual Screening to Identify Novel Potential Compound as an Alternative to Remdesivir to Overcome the RdRp Protein Mutations in SARS-CoV-2. *Frontiers in Molecular Biosciences*, **2021**, 8, 645216	5.6	10
77	Inhibition of MMP2-PEX by a novel ester of dihydroxy cinnamic and linoleic acid from the seagrass Cymodocea serrulata. *Scientific Reports*, **2021**, 11, 11451	4.9	
76	Effective utilisation of influence maximization technique for the identification of significant nodes in breast cancer gene networks. *Computers in Biology and Medicine*, **2021**, 133, 104378	7	1
75	Plant Bioactive Peptides: Current Status and Prospects Towards Use on Human Health. *Protein and Peptide Letters*, **2021**, 28, 623-642	1.9	3
74	Integrated approach in LDPE degradation - An application using Winogradsky column, computational modeling, and pathway prediction. *Journal of Hazardous Materials*, **2021**, 412, 125336	12.8	2
73	Comparison of potential inhibitors and targeting fat mass and obesity-associated protein causing diabesity through docking and molecular dynamics strategies. *Journal of Cellular Biochemistry*, **2021** , 122, 1625-1638	4.7	3
72	Molecular dynamics simulations to decipher the structural and functional consequences of pathogenic missense mutations in the galactosylceramidase (GALC) protein causing Krabbe's disease. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 1795-1810	3.6	5
71	Investigating mutations at the hotspot position of the ERBB2 and screening for the novel lead compound to treat breast cancer - a computational approach. *Advances in Protein Chemistry and Structural Biology*, **2021**, 123, 49-71	5.3	6
70	Network analysis of transcriptomics data for the prediction and prioritization of membrane-associated biomarkers for idiopathic pulmonary fibrosis (IPF) by bioinformatics approach. *Advances in Protein Chemistry and Structural Biology*, **2021**, 123, 241-273	5.3	22
69	Prediction and characterization of influenza virus polymerase inhibitors through blind docking and ligand based virtual screening. *Journal of Molecular Liquids*, **2021**, 321, 114784	6	2

68	Identification of potential inhibitors against pathogenic missense mutations of PMM2 using a structure-based virtual screening approach. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 171-187	3.6	10
67	A systemic approach to explore the mechanisms of drug resistance and altered signaling cascades in extensively drug-resistant tuberculosis. *Advances in Protein Chemistry and Structural Biology*, **2021**, 127, 343-364	5.3	23
66	An integrative analysis to distinguish between emphysema (EML) and alpha-1 antitrypsin deficiency-related emphysema (ADL)-A systems biology approach. *Advances in Protein Chemistry and Structural Biology*, **2021**, 127, 315-342	5.3	14
65	Integrated approach on azo dyes degradation using laccase enzyme and CuI nanoparticle. *SN Applied Sciences*, **2021**, 3, 1	1.8	4
64	Molecular dynamics, residue network analysis, and cross-correlation matrix to characterize the deleterious missense mutations in GALE causing galactosemia III. *Cell Biochemistry and Biophysics*, **2021**, 79, 201-219	3.2	11
63	3-Hydroxypropane-1,2-Diyl Dipalmitoleate-A Natural Compound with Dual Roles (CB1 Agonist/FAAH1 Blocker) in Inhibiting Ovarian Cancer Cell Line. *Pharmaceuticals*, **2021**, 14,	5.2	1
62	Investigation of nonsynonymous mutations in the spike protein of SARS-CoV-2 and its interaction with the ACE2 receptor by molecular docking and MM/GBSA approach. *Computers in Biology and Medicine*, **2021**, 135, 104654	7	6
61	Effect of shape and anthocyanin capping on antibacterial activity of CuI particles. *Environmental Research*, **2021**, 200, 111759	7.9	3
60	Analysis and effective separation of toxic pollutants from water resources using MBBR: Pathway prediction using alkaliphilic P. mendocina. *Science of the Total Environment*, **2021**, 797, 149135	10.2	4
59	A computational overview on phylogenetic characterization, pathogenic mutations, and drug targets for Ebola virus disease. *Current Opinion in Pharmacology*, **2021**, 61, 28-35	5.1	
58	Investigating the structural impacts of a novel missense variant identified with whole exome sequencing in an Egyptian patient with propionic acidemia. *Molecular Genetics and Metabolism Reports*, **2020**, 25, 100645	1.8	2
57	Deciphering the Role of Filamin B Calponin-Homology Domain in Causing the Larsen Syndrome, Boomerang Dysplasia, and Atelosteogenesis Type I Spectrum Disorders via a Computational Approach. *Molecules*, **2020**, 25,	4.8	7
56	Comprehensive in silico screening and molecular dynamics studies of missense mutations in Sjogren-Larsson syndrome associated with the ALDH3A2 gene. *Advances in Protein Chemistry and Structural Biology*, **2020**, 120, 349-377	5.3	15
55	Kerala, India's Front Runner in Novel Coronavirus Disease (COVID-19). *Frontiers in Medicine*, **2020**, 7, 355	4.9	9
54	Dysregulation of Signaling Pathways Due to Differentially Expressed Genes From the B-Cell Transcriptomes of Systemic Lupus Erythematosus Patients - A Bioinformatics Approach. *Frontiers in Bioengineering and Biotechnology*, **2020**, 8, 276	5.8	42
53	The Rise and Impact of COVID-19 in India. *Frontiers in Medicine*, **2020**, 7, 250	4.9	59
52	Computational model to analyze and characterize the functional mutations of NOD2 protein causing inflammatory disorder - Blau syndrome. *Advances in Protein Chemistry and Structural Biology*, **2020**, 120, 379-408	5.3	6
51	First hybrid complete genome of reveals chromosome-mediated novel structural variant from a human clinical sample. *Access Microbiology*, **2020**, 2, acmi000103	1	4

50	An extensive computational approach to analyze and characterize the functional mutations in the galactose-1-phosphate uridyl transferase (GALT) protein responsible for classical galactosemia. *Computers in Biology and Medicine*, **2020**, 117, 103583	7	17
49	Mutational landscape of K-Ras substitutions at 12th position-a systematic molecular dynamics approach. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-15	3.6	11
48	Analysis of Differentially Expressed Genes and Molecular Pathways in Familial Hypercholesterolemia Involved in Atherosclerosis: A Systematic and Bioinformatics Approach. *Frontiers in Genetics*, **2020**, 11, 734	4.5	57
47	Involvement of Essential Signaling Cascades and Analysis of Gene Networks in Diabesity. *Genes*, **2020**, 11,	4.2	26
46	An integrative bioinformatics pipeline to demonstrate the alteration of the interaction between the ALDH2*2 allele with NAD and Disulfiram. *Journal of Cellular Biochemistry*, **2019**, 120, 17030-17041	4.7	
45	Enhanced mosquitocidal efficacy of colloidal dispersion of pyrethroid nanometric emulsion with benignity towards non-target species. *Ecotoxicology and Environmental Safety*, **2019**, 176, 258-269	7	11
44	Bioinformatics classification of mutations in patients with Mucopolysaccharidosis IIIA. *Metabolic Brain Disease*, **2019**, 34, 1577-1594	3.9	12
43	A computational approach for investigating the mutational landscape of RAC-alpha serine/threonine-protein kinase (AKT1) and screening inhibitors against the oncogenic E17K mutation causing breast cancer. *Computers in Biology and Medicine*, **2019**, 115, 103513	7	9
42	Inhibition of the ATPase Domain of Human Topoisomerase IIa on HepG2 Cells by 1, 2-benzenedicarboxylic Acid, Mono (2-ethylhexyl) Ester: Molecular Docking and Dynamics Simulations. *Current Cancer Drug Targets*, **2019**, 19, 495-503	2.8	8
41	Integrative Bioinformatics Approaches to Map Potential Novel Genes and Pathways Involved in Ovarian Cancer. *Frontiers in Bioengineering and Biotechnology*, **2019**, 7, 391	5.8	50
40	A computational model to predict the structural and functional consequences of missense mutations in O-methylguanine DNA methyltransferase. *Advances in Protein Chemistry and Structural Biology*, **2019**, 115, 351-369	5.3	5
39	Computational and modeling approaches to understand the impact of the Fabry's disease causing mutation (D92Y) on the interaction with pharmacological chaperone 1-deoxygalactonojirimycin (DGJ). *Advances in Protein Chemistry and Structural Biology*, **2019**, 114, 341-407	5.3	9
38	Elucidating the role of interacting residues of the MSH2-MSH6 complex in DNA repair mechanism: A computational approach. *Advances in Protein Chemistry and Structural Biology*, **2019**, 115, 325-350	5.3	7
37	A comparative computational approach toward pharmacological chaperones (NN-DNJ and ambroxol) on N370S and L444P mutations causing Gaucher's disease. *Advances in Protein Chemistry and Structural Biology*, **2019**, 114, 315-339	5.3	14
36	A computational method to characterize the missense mutations in the catalytic domain of GAA protein causing Pompe disease. *Journal of Cellular Biochemistry*, **2019**, 120, 3491-3505	4.7	11
35	Glandular hair constituents of Mallotus philippinensis Muell. fruit act as tyrosinase inhibitors: Insights from enzyme kinetics and simulation study. *International Journal of Biological Macromolecules*, **2018**, 107, 1675-1682	7.9	11
34	Computational approach to unravel the impact of missense mutations of proteins (D2HGDH and IDH2) causing D-2-hydroxyglutaric aciduria 2. *Metabolic Brain Disease*, **2018**, 33, 1699-1710	3.9	34
33	Computational modelling approaches as a potential platform to understand the molecular genetics association between Parkinson's and Gaucher diseases. *Metabolic Brain Disease*, **2018**, 33, 1835-1847	3.9	26

32	Impact of missense mutations in survival motor neuron protein (SMN1) leading to Spinal Muscular Atrophy (SMA): A computational approach. *Metabolic Brain Disease*, **2018**, 33, 1823-1834	3.9	11
31	Structural analysis of missense mutations in galactokinase 1 (GALK1) leading to galactosemia type-2. *Journal of Cellular Biochemistry*, **2018**, 119, 7585-7598	4.7	24
30	Investigating the Influence of Hotspot Mutations in Protein-Protein Interaction of IDH1 Homodimer Protein: A Computational Approach. *Advances in Protein Chemistry and Structural Biology*, **2018**, 111, 243-261	5.3	6
29	Comparative analysis of the two extremes of -mutated autosomal dominant disease spectrum: from clinical phenotypes to cellular and molecular findings. *American Journal of Translational Research (discontinued)*, **2018**, 10, 1400-1412	3	4
28	and activity of ceftolozane/tazobactam against pseudomonas aeruginosa collected across Indian hospitals. *Indian Journal of Medical Microbiology*, **2018**, 36, 127-130	1.3	1
27	Significance of catalase-peroxidase (KatG) mutations in mediating isoniazid resistance in clinical strains of Mycobacterium tuberculosis. *Journal of Global Antimicrobial Resistance*, **2018**, 15, 111-120	3.4	1
26	Probing the Protein-Protein Interaction Network of Proteins Causing Maturity Onset Diabetes of the Young. *Advances in Protein Chemistry and Structural Biology*, **2018**, 110, 167-202	5.3	5
25	Influence of V54M mutation in giant muscle protein titin: a computational screening and molecular dynamics approach. *Journal of Biomolecular Structure and Dynamics*, **2017**, 35, 917-928	3.6	41
24	Unraveling the inhibition mechanism of cyanidin-3-sophoroside on polyphenol oxidase and its effect on enzymatic browning of apples. *Food Chemistry*, **2017**, 227, 102-110	8.5	36
23	Structural Analysis of G1691S Variant in the Human Filamin B Gene Responsible for Larsen Syndrome: A Comparative Computational Approach. *Journal of Cellular Biochemistry*, **2017**, 118, 1900-1910	4.7	33
22	A Molecular Docking and Dynamics Approach to Screen Potent Inhibitors Against Fosfomycin Resistant Enzyme in Clinical Klebsiella pneumoniae. *Journal of Cellular Biochemistry*, **2017**, 118, 4088-4094	4.7	17
21	Genotype-phenotype correlation in patients with isovaleric acidaemia: comparative structural modelling and computational analysis of novel variants. *Human Molecular Genetics*, **2017**, 26, 3105-3115	5.6	25
20	Exploring the interaction between iron oxide nanoparticles (IONPs) and Human serum albumin (HSA): Spectroscopic and docking studies. *Journal of Molecular Liquids*, **2017**, 241, 793-800	6	29
19	Determining the role of missense mutations in the POU domain of HNF1A that reduce the DNA-binding affinity: A computational approach. *PLoS ONE*, **2017**, 12, e0174953	3.7	31
18	A Computational Approach to Identify the Biophysical and Structural Aspects of Methylenetetrahydrofolate Reductase (MTHFR) Mutations (A222V, E429A, and R594Q) Leading to Schizophrenia. *Advances in Protein Chemistry and Structural Biology*, **2017**, 108, 105-125	5.3	10
17	Analysis of interactions of clinical mutants of catalase-peroxidase (KatG) responsible for isoniazid resistance in Mycobacterium tuberculosis with derivatives of isoniazid. *Journal of Global Antimicrobial Resistance*, **2017**, 11, 57-67	3.4	8
16	In vitro efficacy and in silico analysis of cefixime-ofloxacin combination for Salmonella Typhi from bloodstream infection. *Journal of Applied Microbiology*, **2017**, 123, 615-624	4.7	4
15	Role of E542 and E545 missense mutations of PIK3CA in breast cancer: a comparative computational approach. *Journal of Biomolecular Structure and Dynamics*, **2017**, 35, 2745-2757	3.6	27

14	Assessing reproductive toxicity and antioxidant enzymes on beta asarone induced male Wistar albino rats: In vivo and computational analysis. *Life Sciences*, **2017**, 173, 150-160	6.8	7
13	Analyzing the Effect of V66M Mutation in BDNF in Causing Mood Disorders: A Computational Approach. *Advances in Protein Chemistry and Structural Biology*, **2017**, 108, 85-103	5.3	4
12	Deciphering the impact of somatic mutations in exon 20 and exon 9 of PIK3CA gene in breast tumors among Indian women through molecular dynamics approach. *Journal of Biomolecular Structure and Dynamics*, **2016**, 34, 29-41	3.6	25
11	Mechanism of artemisinin resistance for malaria PfATP6 L263 mutations and discovering potential antimalarials: An integrated computational approach. *Scientific Reports*, **2016**, 6, 30106	4.9	21
10	Investigating the Inhibitory Effect of Wortmannin in the Hotspot Mutation at Codon 1047 of PIK3CA Kinase Domain: A Molecular Docking and Molecular Dynamics Approach. *Advances in Protein Chemistry and Structural Biology*, **2016**, 102, 267-97	5.3	30
9	Induction of apoptosis by apocarotenoids in B16 melanoma cells through ROS-mediated mitochondrial-dependent pathway. *Journal of Functional Foods*, **2016**, 20, 346-357	5.1	21
8	Functionality study of santalin as tyrosinase inhibitor: A potential depigmentation agent. *International Journal of Biological Macromolecules*, **2016**, 86, 383-9	7.9	43
7	Binding and molecular dynamic studies of sesquiterpenes (2R-acetoxymethyl-1,3,3-trimethyl-4t-(3-methyl-2-buten-1-yl)-1t-cyclohexanol) derived from marine Streptomyces sp. VITJS8 as potential anticancer agent. *Applied Microbiology and Biotechnology*, **2016**, 100, 2869-82	5.7	24
6	DNA Repair Gene (XRCC1) Polymorphism (Arg399Gln) Associated with Schizophrenia in South Indian Population: A Genotypic and Molecular Dynamics Study. *PLoS ONE*, **2016**, 11, e0147348	3.7	14
5	CoagVDb: a comprehensive database for coagulation factors and their associated SAPs. *Biological Research*, **2015**, 48, 35	7.6	3
4	Computational approaches and resources in single amino acid substitutions analysis toward clinical research. *Advances in Protein Chemistry and Structural Biology*, **2014**, 94, 365-423	5.3	19
3	Application of evolutionary based in silico methods to predict the impact of single amino acid substitutions in vitelliform macular dystrophy. *Advances in Protein Chemistry and Structural Biology*, **2014**, 94, 177-267	5.3	10
2	First hybrid complete genome ofAeromonas veroniireveals chromosome-mediated novel structural variantmcr-3.19from human clinical specimen		1
1	Integrated Approach On Degaradtion Of Azo Dyes Using Laccase Enzyme And Nanoparticle With Its Interaction By In Silco Analysis		1