PROFILE

Dr. J. JEYAKANTHAN
Senior Professor and Head
Department of Bioinformatics Alagappa University
Karaikudi - 630004
Tamil Nadu, India

Dr. J. JEYAKANTHAN M.Sc., M.Phil., Ph.D., D.Sc.
Senior Professor and Head
Department of Bioinformatics

#402, 4th Floor, Science Block
Alagappa University
Karaikudi-630004
Tamil Nadu, India

Phone : +91-4565 - 230725
Mobile : +91-9789809245
Fax : +91-4565 - 225202
E-mail : jjkanthan@gmail.com
jjeyakanthan@alagappauniversity.ac.in
Website : www.jjkanthan.org
www.alagappauniversity.ac.in

TEACHING AND RESEARCH EXPERIENCE

Position	Institute/University	Period
Senior Professor and Head	Department of Bioinformatics	March 2020 - Till date*
Professor and Head	Department of Bioinformatics	March 2010 - March 2020
Research Scientist	National Synchrotron Radiation Research Centre, Taiwan, Beamline, Spring-8, Japan	May 2007 - March 2010
Research Associate	RIKEN Harima Institute, SPring-8, Japan	June 2003 - May 2007
PDF	Indian Institute of Science, Bangalore	January 2000 – May 2003

ACADEMIC COMPETENCE

Year of Passing	Degree/Diploma	University/Institution
2022	D.Sc (Bioinformatics)	Alagappa University
2000	Ph.D. (Crystallography and Biophysics)	University of Madras
1999	P.G.D.C.A	MIT, Anna University
1995	M. Phil. (Physics)	M. K. University
1993	M.Sc. (Physics)	M. K. University

RESPONSIBILITIES - AUTHORITY

2024 - *	Member	Syndicate of Alagappa University (Nominated by Hon'ble Governor of Tamil Nadu)
2024 - *	Member	Finance Committee, Alagappa University
2016 - 19	Member	Syndicate of Alagappa University (Nominated by Hon'ble Governor of Tamil Nadu)
2010 - *	Member	Senate of Alagappa University

ACADEMIC RESPONSIBILITIES - ALAGAPPA UNIVERSITY

2023 - 26	Dean, Faculty of Science	All Science Departments, Alagappa University
2023 - *	Project Coordinator	DBT-BIC & NNP
2022 - 23	Project Coordinator	Higher Education Best Practice Cell, Alagappa University
2022 - *	Project Coordinator	DBT-Bioinformatics and Computational Biology Center, Department of Bioinformatics
2022 - *	Ambassador	The Association of Commonwealth Universities (ACU), Alagappa University
2022 - *	Member	Project Monitoring Unit Academic Core Committee of RUSA 2.0
2021 - *	Member	Learning Outcome Based Curriculum Framework (LOCF)
2021 - *	Member	Guru Dakshata – UGC Quality Mandates
2021 - *	Member	Paramarsh - UGC Quality Mandates
2021 - *	Member	CARE/STRIDE - UGC Quality Mandates
2019 (Mar– Nov)	Head of the Department	Department of Botany, Alagappa University
2017 - *	Project Coordinator	DST-PURSE Program (Phase-II) – All Science Departments, Alagappa University
2017 - *	Project Coordinator	DST-FIST Program (Level-I), Department of Bioinformatics, Alagappa University
2017 - *	Project Coordinator	DST-FIST (Phase-II).
2017 - *	Project Coordinator	DST-FIST (Level-I).
2016 - *	Member	Research Advisory Committee (RAC), Alagappa University
2016 - *	Academic Staff	Anti-Ragging Committee, Alagappa University
2015 - *	Chairperson	School of Biological Sciences, Alagappa University
2013 - *	Project Coordinator	UGC Innovative Program (PG diploma)
2013 - *	Project Coordinator	UGC Innovative Program (PG Diploma), Department of Bioinformatics, Alagappa University
2012 - 13	Coordinator	Career Guidance & Counselling Cell, Alagappa University
2012 - 15	Member	Research Advisory Committee, Alagappa University
2010 - *	Member	Website Maintenance Committee, Alagappa University
2010 - *	Member	Standing Committee on Academic Affairs, Alagappa University
2010 - *	Member	Member of the Senate

2010 - *	Chairman	Board of Studies of Bioinformatics, Alagappa University
2010 - *	Head of the Department	Department of Bioinformatics, Alagappa University

ADMINISTRATIVE RESPONSIBILITIES

2019 - *	Director	Alagappa University Ranking Cell (AURC)
2015 - 17	Director	Directorate of Collaborative Programmes, Alagappa University
2012 - 16	Director	Centre for International Relations, Alagappa University
2018 -*	Project Coordinator	Tamil Nadu State University Rating Framework (TANSURF), Alagappa University
2017 - 19	Project Coordinator	National Institutional Ranking Framework Cell
2022 - 24	Member	Internal Quality Assurance Cell (IQAC)
2019 - 21	Member	Center for Internal Quality Assurance Committee, Directorate of Online Programmes, Alagappa University
2018 - 20	Member	Internal Quality Assurance Committee, Directorate of Distance Education (DDE), Alagappa University
2018 - 20	Member	Sports Advisory Board
2018 - 19	Member	Governing Council for DDE, Alagappa University
2018 - 19	Member	Board of Governors of RUSA 2.0, Alagappa University
2016 - 19	Member	Purchase Committee of Alagappa University
2010 - 16	Member	Internal Quality Assurance Cell (IQAC)

ACADEMIC RESPONSIBILITIES - OTHER UNIVERSITY/ INSTITUTES

2026 - *	Member	Board of Studies, Bishop Heber College, Tiruchirapalli.
2026 - *	Member	Alagappa Model Higher Secondary School, Karaikudi.
2025 - *	Member of Academic Council	Avinashilingam Institute for Home Science and Higher Education for Women, Coimbatore.
2025 - *	Member	PG Board of studies in Bioinformatics & Computational Biology and B.Sc (Honors) in Bioinformatics, Pondicherry University.

2025 - *	Member	Board of Studies, Department of Biotechnology, Central University of Tamil Nadu, Thiruvarur.
2025 - *	Member	Ph.D Horticulture Programme, Central University of Tamil Nadu, Thiruvarur.
2025 - *	Member	Research Advisory Council (RAC), Central University of Tamil Nadu, Thiruvarur
2025 - *	Member	Board of Studies in Department of Epidemiology & Public Health, Central University of Tamil Nadu.
2025 - *	Chairperson	Human Ethics Review Board, Central University of Tamil Nadu, Thiruvarur.
2022 - *	Distinguished Adjunct Faculty	Karpagam Academy of Higher Education, Coimbatore
2019 - 25	Member	Research Advisory Committee, Karpagam Academy of Higher Education, Coimbatore
2019 - 21	Member	Local Program Planning & Management Committee (LPPMC), Bharathiar University, Coimbatore
2018 - 21	Member	Research Committee, Bharathidasan University, Trichy
2017 - 19	Member	Academic Council, Thassim Beevi Abdul Kader College for Women, Ramanathapuram
2015 - 20	UGC Nominee	SAP implementation and governance of in Department of Physics, Punjab University, Chandigarh
2015 - 18	Member	Standing Committee on Academic Affairs, Bharathidasan University, Trichy.

RESPONSIBILITIES IN CURRICULUM DEVELOPMENT- OTHER UNIVERSITY/ INSTITUTES

2025- 28	Chairperson	Institutional Human Ethics Review Board (IHERB), Central University of Tamil Nadu (CUTN)
2022 - *	Member	Board of Studies in Department of Bioinformatics, Bishop Heber College, Bharathidasan University, Trichy.
2022 - *	Member	Board of Studies in Department of Bioinformatics, Bharathidasan University, Trichy.
2022 - *	Member	Board of Studies in Department of Bioinformatics, University of Madras.
2020 - *	Member	Board of Studies in Department of Bioinformatics, School of Chemical and Biotechnology, SASTRA Deemed University,Thanjavur.
2018 - *	Member	Board of Studies in Bioinformatics, Bharathiar University, Coimbatore.
2019 (Mar - Nov)	Chairman	Board of Studies of Botany, Alagappa University.
2018 - 21	Member	Board of Studies in Environmental Biotechnology, Bharathidasan University, Trichy.

2015 - 18	Member	Board of Studies in Bioinformatics and Information Technology, Thiruvalluvar University, Vellorarche.
2015 -18	Chairman	Board of Studies in Bioinformatics (UG, PG & PG Diploma), Bharathidasan University, Trichy.
2015 - 17	Member	Board of Studies in Bioinformatics, Bharathiar University, Coimbatore.
2014 -17	Member	Board of Studies in Faculty of Bio and Chemical Engineering, Sathyabama University, Chennai.
2013 - 16	University Representative	Board of Studies of Bioinformatics (Bharathidasan University), Holy Cross College, Trichy.
2012 - 15	Member	Board of Studies of Bioinformatics, Periyar University, Salem.
2012 - 15	Member	Board of Studies of Physics, V.H.N.S.N. College, Virudhunagar.

MEMBERSHIP IN SCIENTIFIC SOCIETIES

S. No	Position	Affiliation/Society/Body
1.	Member	American Crystallographic Association
2.	Vice-President & Life Member	Bioinformatics and Drug Discovery Society (BIDDS)
3.	Member	British Crystallographic Association
4.	Executive Committee Member & Life Member	Indian Crystallographic Association
5.	Life Member	Indian Science Congress Association
6.		Chemical Research Society of India
7.		Society of Biological Chemists, India
8.		Biotech Research Society, India
9.	Member	World Directory of Crystallographers

RESEARCH PROFILE

Broad Subject : Structural Biology and Bio-Computing

Area of Specialization : Small and Macro Molecule X-ray Crystallography

Current Research Focus

Two areas of research that I am currently working on include Structural Biology, Computer Aided Drug Design and Bio-Computing. My primary research interest is in the field of Structural and Functional aspects of model organisms namely *Thermus thermophilus* HB8 and *Pyrococcus horikoshii* OT3 that share similarity to the human genome. I seek to better understand the structure, mechanism of action and disease processes associated with therapeutic protein targets (Pak1, SIRT4, nsP2 Protease, STAT2, lysine biosynthesis proteins, *Plasmodium falciparum* and ViralRdRp and Spike proteins) in various pathogens and human disorders. My twenty-nine years of research expertise involves mixed methodology of computational, biochemical and structural biological approaches to identify potent protein drug targets to treat Diabetes, Chikungunya, Dengue, Filariasis, Malaria, Covid-19 and Nosocomial Infections (caused by ESKAPE and Nocardia Pathogens).

FUNDS RECEIVED

TOTAL FUNDS RECEIVED FOR VARIOUS RESEARCH SCHEMES, PROJECTS, FELLOWSHIPS AND ORGANIZING CONFERENCES: Rs. 2,280.132 Lakhs.

RESEARCH PROJECTS

FUNDS RECEIVED: Rs. 1197.21 Lakhs

S. No.	Ongoing Research Projects	Position	Funding agency	Amount (Rs in Lakhs)	Period	Status
1.	Targeting Acetate Kinase in *Mycobacterium tuberculosis*: Peptide-Based Inhibitor Developed and Structural Insights	Co-PI	CSIR	11.28	2025 - *	Ongoing
2.	Whole Genome Sequencing and Deposition of NGS Data from Cultivated Microbial Isolates Acquired from Farmed Shrimp Varieties.	PI	US-FDA	64,221 USD	2024 - *	Ongoing
3.	Deciphering the Microbiomes Role in Breast Cancer Progression: A Metagenomic and Bioinformatics Approach to Identifying Biomarkers and Therapeutic Targets.	PI	ICMR	50.07	2024 - *	Ongoing
4.	Understanding the Mechanism of SARS-CoV-2 RNA Replication Initiation and Proofreading for Therapeutics	PI	MoE-STARS	91.00	2024 - *	Ongoing
5.	DBT-NNP (National Network Project)	Coordinator & PI	DBT	144.56	2023 -*	Ongoing
6.	DBT-BIC (Bioinformatics and Computational Biology Center)	Coordinator & PI	DBT	183.8	2022 -*	Ongoing
7.	Molecular Insight and *In vitro* validation of Novel lead molecules against Sh3bp2 and kit protein	Co-PI	ICMR	24.48	2023 -*	Ongoing

S. No.	Completed Research Project	Position	Funding agency	Amount (Rs.in Lakh)	Period	Status
1.	Computational and functional characterization of peptide inhibitors disrupting LIMK2-cofilin interaction as a novel therapeutic target towards	Co-PI	ICMR	15.80	2022 - 24	Completed

	Glaucoma.					
2.	Translational Health Research for Human Animal and Plant systems (TBRP)	PI	RUSA 2.0 (Phase -II)	15.63	2022 -23	Completed
3.	Structural and functional insights of potential anti-malarial drug targets of G6PD and 6PGD from *Plasmodium falciparum*(3D7)	PI	DST INDO-TAIWAN	73.72	2020 - 24	Completed
4.	Structural and functional characterization of phospeotransacetylase (PTA) and Acetate Kinase (ACKA) from Mycobacterium tuberculosis H3R7Rv using *in silico* and *in vitro* studies.	PI	TANSCHE	29.80	2021- 24	Completed
5.	Translational Health Research for Human Animal and Plant systems (TBRP)	PI	RUSA 2.0 (Phase -I)	18.14	2019- 21	Completed
6.	Design, Synthesis and *in vitro* anticancer activity of novel and potent signaling influences therapeutic outcome in pancreatic cancer vated kinase 1 (Pak1) inhibitors	PI	DAE-BRNS	30.33	2018- 21	Completed
7.	Structural insights of SIRT4 protein from *Homo sapiens* to identify inhibitors for the treatment of Type-II diabetes	PI	ICMR	33.34	2017- 20	Completed
8.	Identification of Potential Anti-Filiarial drug targeted enzymes Wbm0441, Wbm0042 from Wolbachia endosymbiont *Brugia malayi*	PI	DST-SERB	69.38	2016- 19	Completed
9.	Structural and Functional Insights of potential therapeutic dengue fever target STAT2 protein from *Homo Sapiens*	PI	UGC-RA	37.8	2016- 18	Completed
10.	Development of Web Based Search Engines for the Analyses of Protein interactions with Nucleotides, Fatty Acids and Buffers	PI	DBT	13.81	2015- 18	Completed
11.	Identification of novel drug…. of the pathogen (TWIN Program)	Co-PI	DBT-Twin	73.69	2014- 17	Completed
12.	Structural and Functional Studies of Purine Biosynthesis complex from *Pyrococcus horikoshii* OT3	PI	DST	48.98	2013- 16	Completed

13.	Structural and Functional Studies of Translation Initiation factors from *Pyrococcus horikoshii* OT3	PI	DBT-Twin	77.00	2013- 16	Completed
14.	Structure determination of CPS and ATCase of *Thermus thermophilus* HB8 and identification of potential inhibitors	PI	DBT	32.16	2012- 15	Completed
15.	Structural and Functional analysis Of Orotate Phosphoribosyl transferase (TTHA1742) and Dihydroorotate Dehydrogenase (TTHA0779) from *Thermus thermophilus* HB8	PI	DBT	50.25	2012- 15	Completed
16.	Structure and functional studies on PH0140 protein from *Pyrococcus horikoshii* OT3	PI	UGC	12.903	2012- 15	Completed

GRANTS GENERATED FOR VARIOUS RESEARCH SCHEMES/SUPPORTING PROGRAMMES

FUNDS RECEIVED: **Rs. 816 Lakhs**

S. No.	Title	Position	Funding agency	Amount (Rs in Lakhs)	Period	Status
1.	DST-FIST (Fund for Improvement of S&T Infrastructure in Universities and Higher Educational Institutions) Level – I	Coordinator	DST	62.0	2018-*	Ongoing
2.	DST-PURSE Programme (Phase 2) – All Science Departments	Coordinator	DST	700	2017-*	Ongoing
3.	UGC Innovative Programme – PG Diploma in Structural Pharmacogenomics (Post M.Sc. – One year Course)	Coordinator	UGC	54.0 + 2 Assistant Professor Salary for 5 yrs	2013-18	Completed

PRINCIPAL INVESTIGATOR FOR STUDENT FUNDED PROJECTS

FUNDS RECEIVED: **Rs. 197.042 Lakhs**

S. No.	Title	Position	Funding agency	Amount (Rs in Lakhs)	Period	Status
1.	Targeting Acetate Kinase in *Mycobacterium tuberculosis*: Peptide-Based Inhibitor Developed and Structural Insights	Research Mentor	CSIR-Direct SRF	11.28	2025 - 28	Ongoing
1.	Deciphering the Microbiomes Role in Breast Cancer Progression: A Metagenomic and Bioinformatics Approach to Identifying Biomarkers and Therapeutic Targets	Research Mentor	ICMR-Women Scientist	50.07	2024- 27	Ongoing
2.	Investigation of potential inhibitors for alpha linolenic acid (ALA) metabolism in the human malaria parasite	Research Mentor	UGC Kothari Fellow	20.96	2022 -24	Completed
3.	Computational and Experimental Characterization of Therapeutic Protein Targets in *Acinetobacter baumanniii*	Research Mentor	ICMR (SRF)	9.55	2022- 24	Completed
4.	Structural studies on polyamine biosynthesis enzymes	Research Mentor	ICMR (SRF)	9.55	2022- 24	Completed
5.	Three-dimensional structure determination of Bacterial DNA Adenine Methyltransferase from Acinetobacter baumannii to be used as drug targets for designing antibiotics	Research Mentor	ICMR (RA)	13.2	2022 -24	Completed
6.	Structural & Functional Insights of Vancomycin Resistant Protein VanR from Enterococcus faecium using In vitro and in silico Approach	Research Mentor	ICMR (RA)	13.2	2022 -24	Completed
7.	Structural and Functional Insights on Anti-Filarial	Research Mentor	ICMR			

	Drug targeted enzymes using *in silico* and *in vitro* approach		(SRF)	4.77	2022- 23	Completed
8.	Experimental and Computational studies on Proteins involved in Peptidoglycan biosynthesis pathway from *Wolbachia* Endosymbiont of *Brugia malayi*	Research Mentor	ICMR (SRF)	9.472	2020- 22	Completed
9.	Structural insights mechanism of type II diabetes proteins from *home sapiens* to identify potential inhibitors computational and biochemical studies	Research Mentor	ICMR (SRF)	8.80	2019- 21	Completed
10.	Structural and functional elucidation and inhibitors identification for SMATase from *Serratia marcescens* to overcome antibiotic resistance	Research Mentor	ICMR (SRF)	8.97	2018- 20	Completed
11.	Transcriptional Regulation by p21-Activating kinase-1 with an Agonist RUNX3 and Antagonist peptides modulating Pancreatic Cancer: A Structural and Computational approach	Research Mentor	UGC (OBC)	19.06	2016- 21	Completed
12.	Structural and functional studies on Transcriptional regulatory proteins from *Thermus thermophilus* HB8 and p*yrococcus horikoshii* OT3 - *In silico* and *in vitro* studies	Research Mentor	UGC (MANF)	18.16	2014- 19	Completed

GRANTS GENERATED FOR ORGANIZING CONFERENCES

FUNDS RECEIVED : Rs. 69.88 Lakhs

S. No.	Title	Position	(Rs in Lakhs)			
			Funding Sources		Industrial Sponsors	Total
1.	International Conference on Recent	Convener	DBT-BIC &	3.50		**12.05**

	Trends in Structural Bioinformatics and Computer-Aided Drug Design **(ICSBCADD'2025)**	And Organizing Secretary	NNP		0.55	
			CSIR	0.50		
			DBT-CTEP	3.00		
			DST-ANRF	3.00		
			ALU	1.50		
2.	Three Days Skill Training Workshop on Structural Bioinformatics and Computer Aided Drug Design **(WSBCADD'2025)**	Organizing Secretary	RUSA 2.0	2.70	-	**2.70**
3.	International Conference on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design **(ICSBCADD'2022)**	Convener	DST-SERB	3.50	1.73	**11.63**
			DBT-CTEP	1.50		
			DBT-BIC	4.90		
4.	International Conference on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design **(ICSBCADD'2019)**	Convener	DBT	1.50	2.25	**12.50**
			DST	2.00		
			CSIR	1.00		
			TNSCST	0.25		
			INSA	0.50		
			AU-RUSA	5.00		
5.	11th National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design **(SBCADD'2019)**	Convener	DST	1.50	0.50	**5.75**
			AU-RUSA	3.75		
6.	10th National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (**SBCADD'2018**)	Organizing Secretary	DBT	1.00	1.75	**6.05**
			DST	1.50		
			ICMR	0.40		
			CSIR	0.50		
			AU	0.90		
7.	9th National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design **(SBCADD'2017)**	Convener	DBT	0.50	0.70	**1.85**
			ICMR	0.40		
			TNSCST	0.25		
8.	8th National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (**SBCADD'2016**)	Convener	DBT	1.00	0.70	**2.70**
			AU	1.00		
9.	7th National Symposium cum Workshop on Recent Trends in	Organizing Secretary	DBT	0.50	0.90	**3.65**
			DST	1.50		

	Structural Bioinformatics and Computer Aided Drug Design (**SBCADD'2015**)		TNSCST	0.25		
10.	6th National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (**SBCADD'2014**)	Convener	DBT CSIR UGC	1.00 0.25 1.00	0.75	**3.0**
11.	5th National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (**SBCADD'2013**)	Convener	DBT DST	2.00 1.00	0.50	**3.50**
12.	4th National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (**SBCADD'2012**)	Convener	DBT TNSCST	2.00 0.25	0.30	**2.55**
13.	3rd National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (**SBCADD'2010**)	Organizing Secretary	DBT TNSCST AU	0.75 0.20 1	-	**1.95**

RESEARCH GUIDANCE: AWARDED - 16 UNDER GUIDENCE - 09

S. No	Name of the candidate	Title	Year of Registration	Year of Completion
1.	K. Surekha	Structural and Functional Studies on Pyrimidine Biosynthetic enzymes from hyperthermophile *Thermus thermophilus* HB8	2011	May, 2018
2.	M. Nachiappan	Structural and Functional Characterization of Aminoacyl tRNA Synthetases using *in vitro* and *in silico* Approaches	2011	May, 2019
3	D. Prabhu	Structural and Functional Characterization of Streptomycin Adenylyltransferase using *in silico*and *in vitro* approaches.	2012	July, 2020
4.	Sanjay Kumar Choubey	Structural and Functional Studies of Notch Signaling Crosstalk Pathway Proteins from *Homo Sapiens*	2013	August, 2019
5.	R. Santhosh	Web based computing servers for the analysis of Biological Macromolecules	2013	October, 2020
6.	R. Guru Raj Rao	Structural and functional studies on Purine Biosynthesis enzymes from *Pyrococcus horikoshii* OT3: An *Insilico* and *Invitro* Apporach	2014	September, 2021

7.	M. Richard	Structural and Functional Studies on Transcriptional Regulatory proteins from *Thermus thermophilus* HB8 and *Pyrococcus horikoshii* OT3 – *In silico* and *In vitro* approaches	2014	November. 2021
8.	Jayashree Biswal	Structure based design and Biological Validation of Inhibitors for Selected Activated Kinases	2014	December, 2021
9.	J. Prajisha	Structural Insights mechanism of Kinase proteins from *Homo sapiens* to identify type 2 diabetes inhibitors using Computational approaches	2015	August 2022
10.	R. Raghu	d Discovery of Potential Kinase Inhibitors	2015	September 2024
11.	M. Veerapandiyan	Structural Studies on Polyamine Biosynthesis Enzymes	2016	September 2024
12.	P. Saritha	Experimental and computational studies on protein involved in peptidoglycan biosynthesis pathway from pathogens	2018	September 2023
13.	M. Amala	Structural and Functional Insights on Anti-Filarial Drug targeted enzymes using *in silico* and *in vitro* approach	2018	September 2023
14.	S. Madhumathi	Web based server for protein sequences and structures through data mining and Computational approaches	2019	September 2024
15.	N. Hemavathy	Insilico conformational analysis and design of inhibitors targeting LIM kinases	2019	August 2025
16.	R. Raji	Computational and Experimental Characterization of Therapeutic Protein Targets in *Acinetobacter baumannii*	2020	April 2026
17.	S. Sneha	Structural and Functional Characterization of enzymes involved in central metabolism pathway from *Mycobacterium tuberculosis* using *Insilco* and *Invitro* studies	2021	April 2026
18.	A. Karthika	Structural and Functional Exploration of Multi-Drug Resistant Efflux Pump Proteins from *Acinetobacter baumannii* towards Inhibitors Identification	2021	August 2025
19.	N. Shaslinah	Computational and Characterization of Therapeutic Potent Targets from *Nocardia farcinica*.	2022	Ongoing
20.	N. Bhuvaneswari	Characterization of Novel Drug Targets in *Pseudomonas aeruginosa* using Subtractive Genomics Approach	2022	Ongoing
21.	K. Heyram	Investigaing the Transcriptome of the Medicinal plants to identify lead molecules for Antibacterial against ESKAPE pathogens	2023	Ongoing
22.	Pradeep Kumar S	Computational and Experimental Characterization of Therapeutic Protein Targets from *Enterococcus faecium*	2024	Ongoing

23.	Maharaja M. S	Identification of Potent Therapeutic Protein Targets from Pathogenic Strains of *Nocardia asteriodes* using Computational Approaches	2024	Ongoing
24.	R. Veena	Identification of Potential Drug Targets in Human pathogenic *Nocardia cyriacigeorgica* using Computational Approaches	2024	Ongoing
25.	N Maheswari	Identification of Novel Drug Targets and Vaccine Candidates in *Leptospira interrogans* through Subtractive Genomics and Reverse Vaccinology	2024	Ongoing

Dissertation Supervision				
Degree	**Ongoing**		**Completed**	
M. Phil	**-**		**Alagappa:** 8	**Other:** -
M.Sc/ M.Tech	**Alagappa:** 5	**Other:** 1	**Alagappa:** 17	**Other:** 12
Others	**Alagappa:** -	**Other:** -	**Alagappa:** 13	**Other:** 7
Project Fellows	-	12		

POST DOCTORAL FELLOWS/RESEARCH ASSOCIATE

S. No	Name of the candidate	Title of the Project	Period	Status
1.	Dr. S. Rajamanikandan	RUSA 2.0 - Experimental and Computational Drug Discovery Studied for Life Threatening Disease	2019 - 2021	Completed
2.	Dr. V. M. Manikandamathavan	RUSA 2.0 - Experimental and Computational Drug Discovery Studied for Life Threatening Disease	2019 - 2021	Completed
3.	Dr. Balajee Ramachandran	RUSA 2.0 - Experimental and Computational Drug Discovery Studied for Life Threatening Disease	2019-2021	Completed
4.	Dr. M. Nachiappan	RUSA 2.0 - Experimental and Computational Drug Discovery Studied for Life Threatening Disease	2019 - 2021	Completed
5.	Dr. Vishwanathan Vijayan	Three-dimensional structure determination of Bacterial DNA Adenine Methyltransferase from Acinetobacter baumannii to be used as drug targets for designing antibiotics	2022 - 2023	Completed
6.	Dr. M. Ahila	Structural and Functional Insights of Vancomycin Resistant Protein VanR from Enterococcus faecium using In vitro and in silico Approach	2022 - 2024	Completed

7.	Dr. C.N. Rahul	Investigation of potential inhibitors for alpha linolenic acid (ALA) metabolism in the human malaria parasite	2021 - 2024	Completed
8.	Dr. J. Manikandan	Identification of potent drug for life threatening disease	2022 - *	Ongoing
9.	Dr. B. Thiyonila	Deciphering the Microbiomes Role in Breast Cancer Progression: A Metagenomic and Bioinformatics Approach to Identifying Biomarkers and Therapeutic Targets	2024 - *	Ongoing

AWARDS & HONORS

Fellowships

S. No	Fellowship	Funding agency	Period
1.	Post- Doctoral Fellowship	IRPHA	January 2000 - May 2003
2.		DST	
3.		DBT	
4.	Senior Research Fellowship	CSIR	December 1997– December 2000

National Awards

S. No	Award	Funding agency	Year
1.	IITM-Nurturing Future Leadership Program (IITM-NFLP)	Indian Institute of Technology, Madras	2026
2.	Academic and Research Excellence Award	Alagappa University, Karaikudi, India.	2025
3.	Senior Scientist Award (Dr Niranjalii Devaraj Award)	The Academy of Science (ACS), Chennai	2024
4.	Outstanding Academic and Researcher Award	Alagappa University, Karaikudi	2024
5.	Outstanding Academic and Researcher Award		2023
6.	Outstanding Researcher Award		2022
7.	Leadership Development for the Dean of Faculty and head of the Department of Universities	National Institute of Educational Planning and Administration (NIEPA), New Delhi, India. Ministry of Education (MoE)	2024
8.	Tamil Nadu Scientist Award (TANSA-2018)	Tamil Nadu State Council for Science and Technology	2018

9.	MHRD –Leadership for Academicians Programme (LEAP)	NIT-Trichy, IIIT-Sri City& NTU-Singapore	2019
10.	Research Award (with 2 years' salary)	UGC	2016
11.	Elected Fellow (FASCh.)	Academy of Sciences, Chennai	2015
12.	Young Scientist Travel Grant	DST, Government of India	1999
13.	Senior Research Fellow (SRF)	CSIR, Government of India	1997

International Awards

S. No	Award	Funding agency	Year
1.	Fellow Royal Society of Chemistry, UK	RSC	2025
2.	Fellow Royal Society of Biology, UK	RSB	2025
3.	Who's Who Scientific Directory	'Marquis'	2007
4.	Young Scientist Travel Grant	UNESCO	1999
5.	Young Scientist Fellow	IUCr	1999

INTERNATIONAL VISIT FOR ACADEMIC/ RESEARCH PURPOSE

S. No	Name of the University	Country	Purpose	Duration
1.	Binary University of Management and Entrepreneurship	Malaysia	Academic and Research Collaborations	29th-31st January, 2019
2.	Open University of Malaysia			
3.	Tangshan Polytechnic College	China		8th – 10th April, 2019
4.	Tianjin University			
5.	Nanyang Technological University	Singapore		11th – 12th April, 2019

INTERNATIONAL VISITS AS VISITING SCIENTIST/RESEARCHER

S. No	Institute	Period
1.	National Synchrotron Radiation Research Center, Taiwan	05th-08thDecember, 2017
2.	Osaka University and RIKEN SPring-8, Japan	22nd -30thJune, 2014
3.		02nd -08thDecember, 2012
4.		09th-16thDecember, 2011
5.		22ndMarch- 6thJune, 2010
6.	Abroad Academic Visit/Visiting Scientist - USA, UK, Australia, Japan, Italy, China, South Korea, Singapore, Germany Taiwan, Hawaii, and Malaysia etc...	1999 - *

MOU EXECUTED WITH INSTITUTES & UNIVERSITIES

International

S. No	Institute	Purpose	Period	Status

1.	National Synchrotron Radiation Research Centre (NSRRC), Taiwan	Joint Research and Academic Programmes	2022-27	Ongoing
2.		Joint Research and Academic Programmes	2017-20	Completed
3.		Joint Research and Academic Programmes	2014-17	Completed
4.	School of Science, Osaka University, Japan	Academic and Student Exchange Program	2010-15	Completed
5.	Institute for Protein Research (IPR), Japan	Collaborative Research	2010-15	Completed
6.	RIKEN, Kanagawa, Japan	Collaborative Research	2010-15	Completed
7.	Bio-Metal Science Lab, RIKEN, Spring-8, Japan	Material Transfer Agreement	2010-15	Completed

National

S. No	Institute	Purpose	Period	Status
1.	Vellamal Medical College Hospital and Research Institute, Madurai	Collaborative Research	2024-29	Ongoing
2.	Sri Ramachandra Institute of Higher Edcation and Research, Chennai	Collaborative Research	2024-29	Ongoing
3.	ICAR- National Research Centre for Bannana, Tiruchirappalli	Collaborative Research	2023 - 28	Ongoing
4.	Karpagam Academy of Higher Education, Coimbatore	Collaborative Research	2023 - 28	Ongoing
5.	Sri Ramachandra University, Chennai	Collaborative Research	2023-28	Ongoing
6.	Orbito Asia Diagnostics, Coimbatore	Collaborative Research	2022 - 27	Ongoing
7.	Sree Balaji Medical College and Hospital (Biher) Medical College, Chennai.	Collaborative Research	2021 - 26	Ongoing
8.	Vision Research Foundation, Chennai	Collaborative Research	2021- 24	Ongoing
9.	CSIR-Institute of Genomics & Integrative Biology, Delhi	Collaborative Research	2020 - 25	Ongoing
10.	Bishop Heber College (Autonomous, Tiruchirappalli)	Joint Research and Academic Programmes	2018 - 23	Completed
11.	Indian Institute of Technology-Madras, Chennai	Joint Research and Academic Programmes	2017 - 22	Completed

12.	GE Healthcare Pvt. Ltd., Karnataka	Academia and Industry training towards application on Protein related studies	2017 - 19	Completed
13.	Sri Ramachandra University, Chennai	Joint Research and Academic Programmes	2016 - 21	Ongoing

ACADEMIC/ RESEARCH EVENTS ORGANIZED IN LEAD ROLES

S. No	Position	Event Title	Date
1.	Convenor and Organizing Secretary	3rd International Conference on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (ICSBCADD'2025)	17th – 19th Dec, 2025
2.	Convener	2nd International Conference on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (ICSBCADD'2022)	21st - 25th Nov, 2022
3.	Convener	E-Learning Program on "Bioinformatics as cartographic tool in drug discovery"	19th - 30th May, 2020
4.	Convener	1st InternationalConference on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (ICSBCADD'2019)	11th - 13th Dec, 2019
5.	Convener	International Conference on Innovative and Emerging Trends in Botany (ICIETB-2019)	6th - 7th Nov, 2019
6.	Convener	11th National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (SBCADD'2019)	12th - 15th Feb, 2019
7.	Organizing Secretary	10th National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (SBCADD'2018)	20th - 23rd Feb, 2018
8.	Convener	9th National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (SBCADD'2017)	14th - 17th Feb, 2017
9.	Organizing Secretary	Fire and Safety Awareness Camp for our University Students and Staff members	19th Oct, 2016
10.	Organizing Secretary	Eye Camp for Faculty members, Administrative Staffs and Students of our University	5th Oct, 2016
11.	Convener	World Habitat Day Celebration	3rd Oct, 2016
12.	Co-Convener	International Conference on Recent Trends in Biosciences-2016 (ICRTB-2016)	07th - 09th Apr, 2016
13.	Convener	8th National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (SBCADD'2016)	16th - 19th Feb, 2016
14.	Convener	World Habitat Day Celebration	15th Oct, 2015
15.	Organizing Secretary	7th National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (SBCADD'2015)	24th - 27th Feb, 2015
16.	Convener	World Creativity Day celebration	21st Apr, 2014

17.	Convener	6th National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (SBCADD'2014)	18th - 21st Feb, 2014
18.	Convener	5th National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (SBCADD'2013)	19th - 22nd Feb, 2013
19.	Convener	4th National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (SBCADD'2012)	20th - 23rd Feb, 2012
20.	Convener	Nation Youth Day celebration	12th Jan, 2012
21.	Convener	World Water Day celebration	22nd Mar, 2011
22.	Organizing Secretary	3rd National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (SBCADD'2010)	20th - 22nd Dec, 2010

DETAILS OF PATENT, IMPACT FACTOR, CITATIONS and H-INDEX and

Patent	:	**2**
Cumulative Impact Factor	:	**958.77**
H-index	:	**34**
i10 index	:	**116**
Total Citations	**:**	**4786**

PATENT - 2

S.No.	Title of Patent / Tech.Transfer / Product / Process	Author(s)	Patent Number	Date	Status (Filed/ Published / Granted)
1.	A Process of Extraction of Copper Oxide Nanoparticles Using Green Synthesis	Dr. A. Sivaranjini, Dr. R. Subashkumar, Dr. P. Boomi, Dr. S. Santhosh Baboo, Dr. B. L Shivakumar, A. Aswini, **Dr. J. Jeyakanthan,** Dr. H. Gurumallesh Prabhu, Dr. P. Sagadevan	202141049992	December, 2021	Published
2.	Synergistic formulation for preventing antibiotic resistance effect ofserratia marcescens	Dr.Dhamodharan prabhu, Dr.Sundarraj rajamanikandan, Ramasamy palaniappan, **Dr. Jeyaraman Jeyakanthan**	202241057508 A	December, 2022	Published

RESEARCH PUBLICATIONS IN SCIENTIFIC JOURNALS

Total number of papers published: 272

S. No	Author details and Title of Paper	Journal, Issue No. and Page, etc	Impact Factor	Citations
272	Decoding PCOS pathogenesis: deleterious mutations in PEPD and ZNF572 uncovered by transcriptomics and molecular dynamics Harshini Senthilkumar, Tamil Barathi Palanisamy, **Jeyakanthan Jeyaraman**, Chun-Jung Chen & Mohanapriya Arumugam	Network Modeling Analysis in Health Informatics and Bioinformatics 15,117 (2026)	2.0	Nil
271	Subtractive proteomics-driven identification of AgrA and structure-guided discovery of phytochemical and marine natural products as novel anti-quorum sensing therapeutic leads against *Enterococcus faecium* Pradeep Kumar Sriram, Manikandan Jayaraman, Maharaja Muthuvairam Subbulakshmi, Shaslinah Nathar, Dhamodharan Prabhu, **Jeyakanthan Jeyaraman**	Molecular Diversity (2026)	3.8	Nil
270	Pradeep Kumar Sriram, Manikandan Jayaraman, Prabu Dhamodharan, Maharaja Muthuvairam Subbulakshmi, **Jeyakanthan Jeyaraman,** Multi-Tier Virtual Screening Driven Discovery of Marine Natural Products as Potential DltA Inhibitors in Drug-Resistant Enterococcus faecium	Journal of Pharmaceurical Innovation 21(393) (2026)	2.7	Nil
269	Maharaja Muthuvairam Subbulakshmi, Manikandan Jayaraman, **Jeyakanthan Jeyaraman,** Advancing digital mental healthcare: the role of artificial intelligence and natural language processing in powering medical chatbots for future healthcare interventions	Expert Review of Medical Devices 1-13 (2026)	2.7	Nil
268	Veena Radhakrishnan, Lalitha Prajna, Bharanidharan Devarajan, **Jeyakanthan Jeyaraman,** Whole-genome sequencing and analysis of Nocardia veterana isolates from keratitis patients	Molecular Genetics and Genomics 301,76 (2026)	2.1	Nil
267	Shanthini Karuppiah, Manikandan Jayaraman, Maharaja Muthuvairam Subbulakshmi, **Jeyakanthan Jeyaraman,** Komalavalli Narayanaswamy Structure-Guided Discovery of Phytochemical Leads Targeting the Glucocorticoid Receptor (NR3C1) for Anti-Stress Activity: Computational Insights from Multi-Tier Virtual Screening and Structural Dynamics	Journal of Pharmaceutical Innovation 21,251 (2026)	2.7	1
266	Maheswari Narthanareeswaran, Hemavathy Nagarajan, Sneha Subramaniyan, Bhuvaneswari Narthanareeswaran, Sampathkumar Ranganathan, **Jeyakanthan Jeyaraman,** Probing the conserved catalytic mechanism of ThiL protein in pathogenic Leptospira species: An in silico strategy for inhibitor discovery to combat leptospirosis	Computers in Biology and Medicine 111540 (2026)	-	Nil
265	Maharaja Muthuvairam Subbulakshmi, Manikandan Jayaraman, Prabhu Dhamodharan, **Jeyakanthan Jeyaraman,** Structural and functional insights into glycosyltransferase from Nocardia asteroides NCTC11293 and structure-guided discovery of marine and phytochemical leads through pharmacokinetic	Journal of Molecular Graphics and Modelling 144, 109317 (2026)	3.0	Nil

	screening and molecular dynamics studies			
264	Richard Mariadasse, Mohammed Ahmad, Ravi Kant Pal, Kohila Gurunathan, Sneha Subramaniyan, Bichitra K Biswal, Suresh Kumar Muthuvel, Stalin Thambusamy, **Jeyakanthan Jeyaraman** Crystal structure of PH0140: Exogenous Amino Acids Induce Open Octameric Assembly Enables PromoterTTTT Binding for Transcription Regulation	Journal of Molecular Biology 169664 (2026)	4.5	Nil
263	Sangavi Pandi, Hemavathy Nagarajan, Sneha Subramaniyan, **Jeyakanthan Jeyaraman**, Sampathkumar Ranganathan, Langeswaran Kulanthaivel Targeting hORAI1-Mediated Calcium Influx in Triple-Negative Breast Cancer: A Computational Drug Discovery Approach	The Journal of Membrane Biology 259, 1 (2026)	2.9	Nil
262	Manikandan Jayaraman, Vijayakumar Gosu, Maharaja Muthuvairam Subbulakshmi, Rajalakshmi Kumar, Donghyun Shin, **Jeyaraman Jeyakanthan** Investigating Marine Natural Products as Potential Antivirals of Mpox Virus Replication by Targeting Thymidylate Kinase	ACS Omega (2026)	4.3	Nil
261	Yu-Hung Chen, Yen-Chieh Huang, R Guru Raj Rao, Hao-Chin Chang, Yu-Hsuan Lan, Atsushi Nakagawa, **Jeyakanthan Jeyaraman**, Chun-Jung Chen Structural insights into substrate binding, domain swapping and heat resistance of a hyperthermostable archaeal AIR synthetase	International Journal of Biological Macromolecules Volume 344, Part 1, 150493 (2026)	8.5	Nil
260	Santhiya Panchalingam, Govindaraju Kasivelu, Manikandan Jayaraman, **Jeyakanthan Jeyaraman** Machine learning guided structural dynamics identifies translation elongation factor 1 (EEF1A1) as an immunological biomarker and marine natural products as therapeutic leads for rheumatoid arthritis with major depressive disorder	Computers in Biology and Medicine 203, 11480 (2026)	-	Nil
259	Ponnuchamy Kumar, Gunasowmiya Velsamy, Velu Manikandan, Duraisamy Elango, Sundarraj Manikandan, **Jeyakanthan Jeyaraman** Biogenic Synthesis of Blue Luminescent Carbon Quantum Dots From *Gymnema sylvestre* for Anticancer Studies	ChemistrySelect 11, no. 1 (2026)	2.0	Nil
258	Targeting TetR-family transcription regulators for combating tetracycline resistance in resilient *Acinetobacter baumannii*: in silico identification of potent inhibitors Karthika Alagesan, Hemavathy Nagarajan, Balajee Ramachandran, Umashankar Vetrivel, Chitra Jeyaraj Pandian, **Jeyakanthan Jeyaraman**	Journal of Biomolecular Structure and Dynamics 44,4 (2025)	2.4	4
257	Nagarajan Hemavathy, Sampathkumar Ranganathan, Vetrivel Umashankar, **Jeyakanthan J** Rational design and structural Bioinformatics-Driven discovery of tetrapeptide inhibitors for LIMK-Targeted cancer therapy	Medical Oncology 43, 2, 83 (2025)	3.5	Nil
256	Gopalakrishnan Shankari, Dhamodharan Prabhu, Muthusamy Sureshan, **Jeyakanthan J**, Sundararaj Rajamanikandan A Review of ARID1A's Role in Breast Cancer Progression: Context-Dependent Mechanisms and Therapeutic Implications	Cancers 18, 1, 142 (2025)	4.4	Nil

255	Janaranjani Murugesan, Hemamalini Vedagiri, Premkumar Kumpati, **Jeyakanthan J,** Network pharmacology analysis of Simarouba glauca bioactive molecules reveals potential therapeutic targets and mechanistic insights into cancer	Natural Products 10, 100475 (2025)	-	Nil
254	M Muthuvairam Subbulakshmi, H Nagarajan, S Pandi, S Subramaniyan, T Berchmans, **Jeyakanthan J**, Computational identification of potential PAK1 inhibitors for anti-cancer therapy: an e-pharmacophore guided virtual screening study	SAR and QSAR in Environmental Research (P:1-28), (2025)	2.4	Nil
253	Zeeshan Hyderi, Hemavathy Nagarajan, Kiruthika Saravanan, Sathiyaraj Ganesan, **Jeyakanthan Jeyaraman**, Sampathkumar Ranganathan, Arumugam Veera Ravi Inhibition of MMP-2/MMP-9 and biofilm formation by 4, 5, 7-trihydroxyflavanone (THF): a promising therapeutic approach against Enterococcus gallinarum endocarditis	Archives of Microbiology 208 (1) P-36 (2025)	2.8	Nil
252	Manikandan Jayaraman, Vijayakumar Gosu, Maharaja Muthuvairam Subbulakshmi, Jeong Woong Park, **Jeyakanthan Jeyaraman**, Donghyun Shin. Binding modes and interaction mechanism of bisphenol A and its analogs in constitutive androstane receptor	Scientific Reports (2025)	3.9	Nil
251	Mariadasse Richard, Sneha Subramaniyan, Hemavathy Nagarajan, Sanjay Kumar Choubey, Mohini Singla, Bichitra K Biswal, **Jeyakanthan J**, Targeting Catalytic Residues of TKTL1: A Multi-Approach Study With Thiamine Analogs Combining QSAR, Pharmacophore Modeling, DFT, and Molecular Dynamics	Chemistry Select (10, 46), (2025)	2.0	Nil
250	Shaslinah Nathar, Hemavathy Nagarajan, Bhuvaneswari Narthanareeswaran, Chitra Jeyaraj Pandian, Berchmans Thiyonila, **Jeyakanthan J**, In silico identification of novel alpha/beta hydrolase fold domain-containing protein associated with virulence and antibiotic resistance in Nocardia farcinica (Strain: JJSBBCNF_01)	Molecular Diversity (2025)	3.8	Nil
249	Zeeshan Hyderi, Hemavathy Nagarajan, Kiruthika Saravanan, Sathiyaraj Ganesan, **Jeyakanthan J**, Sampathkumar Ranganathan, Arumugam Veera Ravi Inhibition of MMP-2/MMP-9 and biofilm formation by 4, 5, 7-trihydroxyflavanone (THF): a promising therapeutic approach against Enterococcus gallinarum endocarditis	Archives of Microbiology, 208, (36) (2025)	2.6	Nil
248	Nagarajan Hemavathy, Sneha Subramaniyan, Saritha Poopandi, Sampathkumar Ranganathan, Vetrivel Umashankar, **Jeyakanthan J** Structure-Guided Design of Isoform-Selective LIMK1 Inhibitors: A Peptidomimetic Screening Approach with Molecular Dynamics and Quantum Mechanical Characterization	Journal of Computational Biophysics and Chemistry (2650032) (2025)	2.3	Nil
247	Maharaja M S, Sneha S, Hemavathy N, **Jeyakanthan J** Computational Identification of FDA-Approved Drugs as Potential BMX Inhibitors: An Integrated Virtual Screening, Pharmacokinetics and Molecular Dynamics Study	Chemistry Select (10, 41)	2.0	1
246	Raji Rajmichael, Nagarajan Hemavathy, Sangavi Pandi, Saritha Poopandi, mashankar Vetrivel **J. Jeyakanthan** Unraveling the Bifunctional HisIE Enzyme in Acinetobacter baumannii JJAB01: A Novel Therapeutic Target for Combating Antimicrobial	Journal of Pthology, Microbiology and Immunology (133,10) (2025)	2.6	Nil

	Resistance			
245	Heyram Krishnakumar, Saranya nallusamy, Raji Rajmaichael, Ahila Mathimaran, Chitra Jeyaraj Pandian, GomathinayagamSubramaniyan **J.Jeyakanthan** Transcri ptomic profiling to investigate the therapeutic potential and medicinal properties of Momordica cymbalaria.	Scientific Reports, 33882 (2025)	3.9	Nil
244	Heyram Krishnakumar, manikandan Jayaraman, Prabhu Dhamodharan, **J. Jeyakanthan** Structure-guided discovery of marine natural products as glucokinase activators for type 2 diabetes mellitus: A computational perspective	Journal of Molecular Graphics and Modelling, (142, 109181), (2025)	3.0	Nil
243	Bhuvaneswari Narthanareeswaran, Nagarajan Hemavathy, Sampathkumar Ranganathan, Shaslinah Nathar, Chitra Jeyaraj Pandian **J. Jeyakanthan** Integrative genomics and structural bioinformatics uncovers AMR-associated drug targets and pqsH inhibitors in multidrug-resistant Pseudomonas aeruginosa JJPA01	Molecular Diversity (2025)	3.8	Nil
242	D. Prabhu, M. Sureshan, S. Rajamanikandan, **J. Jeyakanthan** Harnessing the potential of phytochemicals to design anti-filarial molecules targeting the MurE enzyme of Brugia malayi: a hierarchical virtual screening and molecular dynamics simulation study	SAR and QSAR (753-773), (2025)	2.4	Nil
241	Bhuvaneswari Narthanareeswaran, Maheswari Narthanareeswaran, Sampathkumar Ranganathan, Chitra Jeyaraj Pandian, **Jeyakanthan, J.,** Exploration of hypothetical proteins and reverse vaccinology approach for novel multi-epitope vaccine design against multidrug-resistant clinical isolate Pseudomonas aeruginosa JJPA01	Computers in Biology and Medicine, 197, 111045. (2025)	6.3	Nil
240	Sneha Subramaniyan, Hemavathy Nagarajan, Richard Mariadasse, Umashankar Vetrivel, **Jeyakanthan, J.,** Strategic targeting of AckA in Mycobacterium tuberculosis using peptide inhibitors	Archives of Microbiology, 207, 235 (2025)	2.6	Nil
239	Sankar Muthumanickam, Murugesan Manikandan, Boomi Pandi, Balajee Ramachandran, Sonamuthu Jegatheswaran,Mangaiyarkarasi Rajkumar, **Jeyakanthan Jeyaraman.,** In Silico Design and Evaluation of a Hydrophobic-Hydrophilic Combinatorial Drug Systems for Targeted Breast Cancer Therapy	Biochemical and Biophysical Research Communications, 781, 152499 (2025)	2.2	Nil
238	Shaslinah N., Hemavathy N., Bhuvaneswari N., Sneha S., and **Jeyakanthan, J.,** Integrated Subtractive Genomics and Inhibitor Identification of Novel FAD-dependent Monooxygenase in Nocardia farcinica JJSBBCNF_01	Biochemical and Biophysical Research Communications, 781, 152502 (2025)	2.2	Nil
237	Maharaja, M S., Manikandan, J., Hemavathy, N., Pradeep Kumar, S., and **Jeyakanthan, J.,** In-silico structural and functional annotation of hypothetical proteins from Nocardia asteroides NCTC11293: A computational approach for novel drug target identification and therapeutic development	Computers in Biology and Medicine, 196, 110936. (2025)	6.3	2
236	Perinbaraj, S., Jayaraman, M., **Jeyaraman, J**., & Girija, K. R. (2025). Designing Novel Potent Oxindole Derivatives as VEGFR2 Inhibitors for Cancer Therapy:	J. Mol. Graph. Model, 109049	2.7	Nil

	Computational Insights from Molecular Docking, Drug-likeness, DFT, and Structural Dynamics Studies. Journal of Molecular Graphics and Modelling, 109049**.**			
235	Alagesan, K., Nagarajan, H., Mathimaran, A., Vetrivel, U., Malaisamy, V., Chen, C. J., & **Jeyaraman, J**. (2025). A Promising Strategy to Disrupt Plasmodium falciparum Metabolic Resilience by Targeting G6PD: Virtual Screening for Potential Inhibitors Against Malaria. *Computational Biology and Chemistry*, 108495.	*Comput. Biol. Chem.* 108495. (2025).	2.6	Nil
234	Muthumanickam, S., Ramachandran, B., **Jeyakanthan, J**., Jegatheswaran, S., & Pandi, B. (2025). Designing a novel drug–drug conjugate as a prodrug for breast cancer therapy: in silico insights.	*Molecular Diversity*, *29*(2), 991-1007.	3.8	1
233	Jayaraman, M., Gosu, V., Kumar, R., **Jeyaraman, J**., Lee, H. K., & Shin, D. (2025). Exploring Marine natural products as potential Quorum sensing inhibitors by targeting the PqsR in Pseudomonas aeruginosa: Virtual screening assisted structural dynamics study.	*PloS one*, *20*(3), e0319352	2.9	Nil
232	Subramaniyan, S., Jayaraman, M., & **Jeyaraman, J**. (2025). Exploring Phytochemicals and Marine Natural Products as Alternative Therapeutic Agents Targeting Phosphotransacetylase (PTA) in Mycobacterium tuberculosis: An Underexplored Drug Target.	J. Mol. Graph. Model, 109025	2.7	Nil
231	Gnanavelou, R., Jayaraman, M., **Jeyaraman, J**., & Girija, K. R. (2025). Computational Design and Structural Insights into Quinazoline-Based Lead Molecules for Targeting PARP10 in Cancer Therapy.	J. Mol. Graph. Model, 109005	2.7	Nil
230	Hemavathy, N., Ranganathan, S., Umashankar, V., & **Jeyakanthan, J**. (2025). Computational Development of Allosteric Peptide Inhibitors Targeting LIM Kinases as a Novel Therapeutic Intervention.	Cell Biochem. Biophys, 1-13	1.8	Nil
229	Heyram, K., Manikandan, J., Prabhu, D., & **Jeyakanthan, J.** Computational insights into marine natural products as potential antidiabetic agents targeting the SIK2 protein kinase domain.	*SAR and QSAR in Env. Res.35*(12), 1129-1154. (2024).	2.3	Nil
228	Hemavathy, N., Umashankar, V., & **Jeyakanthan, J**. Unveiling novel type 1 inhibitors for targeting LIM kinase 2 (LIMK2) for cancer therapeutics: An integrative pharmacoinformatics approach.	*Comput. Bio. Chem*, *115*, 108289. (2025)	2.6	Nil
227	Shankari, G., Raji, R., Prabhu, D., **Jeyakanthan, J.,** & Gopinath, S. C. Progressive Dynamics of Cancer Stem Cells in Oral Squamous Cell Carcinoma.	*Curr. Cancer. Drug Targets*, *25*(2), 113-117. (2025).	2.91	Nil
226	Rajmichael, R., Hemavathy, N., Mathimaran, A., Pandian, C. J., Kingsley, J. D., Subramanian, G., &**Jeyakanthan, J.** Whole Genome Sequencing, Characterization and Comparative Genome Analysis of Acinetobacter baumannii JJAB01: A Comprehensive Insights on Antimicrobial Resistance and Virulence Genotype.	*Microb. Pathog*, 107224. (2024).	3.3	Nil

225	Sangavi, P., Nagarajan, H., Subramaniyan, S., **Jeyaraman, J.,** & Langeswaran, K.. Unveiling the oncological inhibition of bioactive compounds from Adansonia digitata via in silico analysis by targeting γ-butyrobetaine dioxygenase 1 against triple negative breast cancer.	*J. Biomol. Struct. Dyn.* 1-24. (2024)	2.7	Nil
224	Nagarajan. H., Samdani, A., Umashankar, V., **Jeyakanthan, J.** Deciphering the conformational transitions of LIMK2 active and inactive states to ponder specific druggable states through microsecond scale molecular dynamics simulation.	*J Comput Aided Mol Des.* 6(6):459-482. (2022)	4.17	1
223	Roy, J., Hemavathy, N., Saravanan, R., Gopinath, P., Pugazh, P., **Jeyaraman, J.,** Venkatraman, G., Rayala, S.K. Spatio-temporal localization of P21-activated kinase in endometrial cancer.	*Biotechnol Appl Biochem.* 2024 Nov 6.	3.2	Nil
222	Prabhu, D., Shankari, G., Rajamanikandan, S., **Jeyakanthan, J.,** Velusamy, P., Gopinath, S. C., & Pattabi, S. Designing potential lead compounds targeting aminoglycoside N (6′)-acetyltransferase in Serratia marcescens: A drug discovery strategy.	*Int J Biol Macromol*, (2024). 136976.	7.7	Nil
221	Kumar, P., Ravichandran, A., Durgadevi, S., Manikandan, V., Song, K. S., Prabhu, D., **Jeyaraman, J.,** & Muthusamy, G.. Microwave-Assisted Green Synthesis of CQDs from Mesosphaerum suaveolens Extract: Photocatalytic Degradation and Anticancer Activity.	*Waste Biomass Valorization*. (2024)*15*(11), 6539-6552.	2.6	Nil
220	Arumugam, M. P., Vetrivel, U., **Jeyaraman, J.,**Chauhan, S. C., & Mannu, J. Interaction and dynamics of biological molecules.	*Front. Phy. 12*, 1439802. (2024).	3.1	Nil
219	Panchalingam, S., Jayaraman, M., **Jeyaraman, J.,** & Kasivelu, G. Harnessing Marine Natural Products to Inhibit PAD4 Triple Mutant: A Structure-Based Virtual Screening Approach for Rheumatoid Arthritis Therapy.	*Arch. Biochem. Bioph*. 110164. (2024).	3.8	Nil
218	Alagesan, K., Nagarajan, H., & **Jeyakanthan, J**. Repurposing FDA-approved drugs for combating tigecycline resistance in Acinetobacter baumannii: in silico screening against BaeR protein.	*Mol. Div.* 1-22. (2024).	3.8	Nil
217	Sanjeevi, M., Rajendran, S., **Jeyaraman, J.,** & Sekar, K. MIPDS: a comprehensive database on the molecular interactions in protein dimer structures.	*J. Appl. Crystallogr. 57* (5). (2024).	4.86	Nil
216	Sanjeevi, M., Mohan, A., Ramachandran,D., **Jeyaraman, J.,** & Sekar, K. CSSP-2.0: A refined Consensus method for accurate protein secondary structure prediction.	*Comput. Biol. Chem.* 108065 (2024).	2.6	Nil

215	Rangaswamy, R., Sneha, S., Hemavathy, N., Umashankar, V., & **Jeyakanthan, J.** Computational discovery of AKT serine/threonine kinase 1 inhibitors through shape screening for rheumatoid arthritis intervention.	*Mol. Div.*, 1-17. (2024).	3.8	Nil
214	Mathimaran, A., Nagarajan, H., Mathimaran, A., Huang, Y. C., Chen, C. J., Vetrivel, U., & **Jeyaraman, J**. Deciphering the pH-dependent oligomerization of aspartate semialdehyde dehydrogenase from Wolbachia endosymbiont of Brugia malayi: An in vitro and in silico approaches.	*Int J Biol Macromol*, 133977. (2024)	8.2	Nil
213	Mathimaran, A., Pandian, C. J., Sappanimuthu, P., Kirshnakumar, H., Amala, M., Veerapandiyan, M., & **Jeyaraman, J.** Synthesis of multifunctional Silver oxide, Zinc oxide, Copper oxide and Gold nanoparticles for enhanced Antibacterial activity against ESKAPE Pathogens and Antioxidant, Anticancer activities using Momordica cymbalaria seed extract.	*Mater. Today Commun.* 108838. (2024).	3.662	Nil
212	Jayaraman, M., Kumar, R., Panchalingam, S., & **Jeyaraman, J.** Mechanistic Insights into the Conformational Changes and Alterations in Residual Communications Due to the Mutations in the pncA Gene of Mycobacterium tuberculosis: A Computational Perspective for Effective Therapeutic Solutions.	*Comput. Biol. Chem.* 108065. (2024).	3.737	Nil
211	Amala, M., Nagarajan, H., Ahila, M., Nachiappan, M., Veerapandiyan, M., Vetrivel, U., & **Jeyakanthan, J.** Unveiling the intricacies of allosteric regulation in aspartate kinase from the Wolbachia endosymbiont of Brugia Malayi: Mechanistic and therapeutic insights.	*Int J Biol Macromol*, 131326. (2024).	8.2	Nil
210	Loganathan, L., **Jeyaraman, J.,** & Muthusamy, K. HTNpedia: A Knowledge Base for Hypertension Research.	*Comb Chem High T Scr, 27*(5), 745-753. (2024).	1.8	Nil
209	Meiyazhagan, G., Devaraj, M., Biswal, J., Manogaran, P., **Jayaraman, J.,** & Kreedapathy, G. E. Silver nanoparticle interaction with ergosterol induces cell death and inhibits Trichosporon asahii cell proliferation.	Europe PMC (2024).	2.478	Nil
208	Priya, M. G. R., Solomon, V. R., Hemavathy, N., **Jeyakanthan, J.,** Kumar, D., & Mahesh, J. Design, synthesis, in silico, and pharmacological evaluation of novel quinoline derivatives containing substituted piperazine moieties as potential anti-breast cancer agents.	*Results. Chem.* 101359. (2024).	2.3	Nil

207	Malaisamy, V., Alagesan, K., Nagarajan, H., Jayaraman, M., Vetrivel, U., & **Jeyaraman, J.** Biochemical and biophysical characterization of biosynthetic arginine decarboxylase from *Thermus thermophilus*. *Journal of biomolecular structure & dynamics*, 1–18. Advance online publication.	*J. Biomol. Struct. Dyn.* (2024).	4.4	Nil
206	Nathar, S., Rajmichael, R., Jeyaraj Pandian, C., Nagarajan, H., Mathimaran, A., Kingsley, J. D., & **Jeyaraman, J.** Exploring Nocardia's ecological spectrum and novel therapeutic frontiers through whole-genome sequencing: unraveling drug resistance and virulence factors.	*Arch. Microbiol, 206*(2), 76. (2024).	2.667	Nil
205	Aiswarya, N., Rahul, C. N., Kothandan, G., Kurup, M. P., Manoj, E., Chandrasekaran, P., **Jeyakanthan J** & Sekar, K. Crystal structure of 1-(E)-[(5-bromo-2-hydroxybenzylidene amino) pyrrolidin-2-one]: Design, synthesis and computational evaluation of a novel racetam congener for epilepsy.	*J. Mol. Struct*, 1300, 137219. (2024).	3.196	Nil
204	Hyderi, Z., Nagarajan, H., Priya, S. J., **Jeyakanthan, J.,** & Veera Ravi, A. Exploring the antimicrobial potential of 4, 5, 7-trihydroxyflavanone (THF) against vancomycin-resistant Enterococcus gallinarum infections: in vitro and in silico investigations.	*J. Biomol. Struct. Dyn.* 1-15. (2023).	4.4	Nil
203	Rangaswamy, R., Hemavathy, N., Subramaniyan, S., Vetrivel, U., & **Jeyakanthan, J.** Harnessing allosteric inhibition: prioritizing LIMK2 inhibitors for targeted cancer therapy through pharmacophore-based virtual screening and essential molecular dynamics.	*J. Biomol. Struct. Dyn.* 1-18. (2023).	4.4	Nil
202	Jayaraman, M., Gosu, V., Kumar, R., & **Jeyaraman, J.** Computational Insights into Potential Marine Natural Products as Selective Inhibitors of Mycobacterium tuberculosis InhA: A Structure-Based Virtual Screening Study.	*Comput. Biol. Chem.* 107991 (2023).	3.737	Nil
201	Veerapandian, M., Hemavathy, N., Karthika, A., Manikandan, J., Vetrivel, U., & **Jeyakanthan, J.** pH-Dependent conformational stability of SpeB from Thermus thermophilus HB8: insights from molecular dynamics simulation.	*Mol. Simul.* 1-17. (2023).	2.346	Nil
200	Ahmad, M., Jha, B., Bose, S., Tiwari, S., Dwivedy, A., Kar, D., Pal, R., Mariadasse, R., Parish, T., **Jeyakanthan, J.,** Vinothkumar, K. R., & Biswal, B. K. Structural snapshots of Mycobacterium tuberculosis enolase reveal dual mode of 2PG binding and its implication in enzyme catalysis.	*IUCrJ.* (2023)	5.588	Nil

199	Madhumathi, S., Santhosh, R., Dhanalakshmi, R., Rahul, C.N., **Jeyakanthan, J.,** & Sekar, K. A novel search engine for the proteins involved in the Notch crosstalk signaling pathways.	*J. Biosci.* (2023)	2.795	Nil
198	Subramaniyan, S., Nagarajan, H., Vetrivel, U., & **Jeyaraman, J.** Multilayer precision-based screening of potential inhibitors targeting Mycobacterium tuberculosis acetate kinase using in silico approaches.	*Comput. Biol. Chem.* (2023). *107*, 107942.	3.737	Nil
197	Vinita, N. M., Devan, U., Durgadevi, S., Anitha, S., Govarthanan, M., Antony Joseph Velanganni, A., **Jeyaraman, J.** & Kumar, P. Impact of Surface Charge-Tailored Gold Nanorods for Selective Targeting of Mitochondria in Breast Cancer Cells Using Photodynamic Therapy.	*ACS Omega*. (2023).	4.132	Nil
196	Karthika, A., Hemavathy, N., Amala, M., Rajamanikandan, S., Veerapandian, M., Prabhu, D., Umashankar V., Chen CJ., Chitra JP., & **Jeyakanthan, J.** Structural and functional characterization of 6-phosphogluconate dehydrogenase in Plasmodium falciparum (3D7) and identification of its potent inhibitors.	*J. Biomol. Struct. Dyn.* 1-17. (2023).	5.235	Nil
195	Panchalingam, S., Govindaraju, K., Jayaraman, M., Kumar, R., Kalimuthu, S., & **Jeyaraman, J.** Differential gene expression analysis combined with molecular dynamics simulation study to elucidate the novel potential biomarker involved in pulmonary TB.	*Microb. Pathog*., 1- 06266. (2023).	3.84	Nil
194	Jayaprakash, P., Biswal, J., Pandian, C. J., Kingsley, J., & **Jeyakanthan, J.** Investigation of translation initiation factor through protein–protein interactions and molecular dynamics approaches.	*Mol. Simul.*, 1-13. (2023)	2.346	Nil
193	Nallasamy, P., shafreen Rajamohamed, B., **Jeyaraman, J.,** Kathirvel, B., & Natarajan, S. Regenerative marine waste towards CaCO3 nanoformulation for Alzheimer's therapy.	*Environ. Res.*, *225*, 115631. (2023)	8.431	Nil
192	Muthumanickam, S., Ramachandran, B., Boomi, P., **Jeyakanthan, J.,** Prabu, H. G., Jegatheswaran, S., & Premkumar, K. Combination of bendamustine-azacitidine against Syk target of breast cancer: an in silico study.	*J. Biomol. Struct. Dyn.* (2023)	5.235	Nil

191	Chitra Jeyaraj Pandian, N Arul Murugan, SM Rajendren & **Jeyakanthan Jeyaraman.** Computer-Aided vaccine design for selected positive-sense single stranded RNA viruses	*Indian J. Biochem. & Biophy.* Vol. 60, pp. 281-296. (2023)	1.476	Nil
190	Sruthi, S., Saritha, P., Yen- Chieh, H., Amala, M., **Jeyakanthan, J.,** Chen, CJ. Purification, crystallization and X-ray diffraction analysis of succinyl-diaminopimelate desuccinylase from Wolbachia endosymbiont of *Brugia malayi.*	*J Chin Chem Soc. (*2023)	1.74	Nil
189	Ramachandran, B., Muthupandian, S., **Jeyaraman, J.,** & Lopes, B. S. Computational exploration of molecular flexibility and interaction of meropenem analogs with the active site of oxacillinase-23 in Acinetobacter baumannii.	*Front. Che. 11* (2023).	5.545	Nil
188	Javali, P. S., **Jeyakanthan, J.,** Chen, C. J., & Arumugam, M. An integrated bioinformatics approach to identify candidate biomarkers and the evaluation of drugs for pheochromocytoma.	*bioRxiv*, (2023).	Peer review	Nil
187	Vinita, NM., Devan, U., Durgadevi, S., Anitha, S., Prabhu, D., Rajamanikandan, S., Govarthanan, M., Ananthanarayanan Yuvaraj, A., Biruntha, M., Joseph Velanganni, AA., **Jeyakanthan, J.,** Arul Prakash, P., Mohamed Jaabir, MS & Kumar. P**.** Triphenylphosphonium conjugated gold nanotriangles impact Pi3K/AKT pathway in breast cancer cells: a photodynamic therapy approach.	*Sci. Rep.* (2023)	4.996	1
186	Rahul, CN., Aiswarya, N., **Jeyakanthan, J.,** Sekar, K. Computational Analysis of RNA Sequencing Dataset Reveals Novel Associations in Response to Artemisinin-Resistant Malaria: Implications in Drug Discovery and Design.	*J Appl Bioinforma Comput Biol.* (2022) 11:7.	1.04	Nil
185	Prabhu, D., Rajamanikandan, S., Amala, M., Saritha, P., **Jeyakanthan, J.,** & Ramasamy, P. Functional Characterization, Mechanism, and Mode of Action of Putative Streptomycin Adenylyltransferase from Serratia marcescens.	*J. Antibiot.11*(12) 1722. (2022)	4.94	Nil
184	Arul Murugan, N, Chitra, J, **Jeyakanthan , J**, Rajendren, SM. Multi-level scoring approach to discover multi-targeting potency of medicinal plant phytochemicals against protein targets in SARS-CoV-2 and human ACE-2 receptor	*Indian J. Biochem. Biophys*. (2022)	1.918	3

183	Sindhu, T., Rajamanikandan, S., **Jeyakanthan, J.,** & Pal, D. Investigation of protein-ligand binding motions through protein conformational morphing and clustering of cytochrome bc1-aa3 super complex.	*J Mol Graph Model*. *118*, 108347. (2022)	2.518	Nil
182	Yuvaraj, I., Chaudhary, S. K., **Jeyakanthan, J.,** & Sekar, K. Structure of the hypothetical protein TTHA1873 from Thermus thermophilus.	*Acta Crystallogr. F:Struct. Biol. Commun. 78*(9). (2022).	1.004	Nil
181	Jeyaraj Pandian, C., **Jeyaraman, J.,** & SM, R. Post-acute sequelae of SARS-CoV-2 Delta variant infection: A report of three cases in a single family.	*Indian J. Biochem. Biophys*. (2022)	1.918	2
180	Balu, R., Ramachandran, S. S., Mathimaran, A., **Jeyaraman, J.,** & Paramasivam, S. G. Functional significance of mouse seminal vesicle sulfhydryl oxidase on sperm capacitation in vitro.	*Mol. Hum. Reprod.*(2022).	4.518	Nil
179	Tomar, A., Sahoo, S., Aathi, M., Kuila, S., Khan, M. A., Ravi, G. R. R., **Jeyaraman, J.,** Mehta, J.L., Varughese, K.I. and Arockiasamy, A. Exploring the druggability of oxidized low-density lipoprotein (ox-LDL) receptor, LOX-1, a proatherogenic drug target involved in atherosclerosis.	*Biochem. Biophys. Res. Commun*. (2022).	3.575	Nil
178	Jayaprakash, P., Biswal, J., Rangaswamy, R., & **Jeyakanthan, J.** Designing of potent anti-diabetic molecules by targeting SIK2 using computational approaches.	*Mol. Divers.* (2022)	2.943	Nil
177	Nagarajan, H., Samdani, A., Umashankar, V., & **Jeyakanthan, J.** Deciphering the conformational transitions of LIMK2 active and inactive states to ponder specific druggable states through microsecond scale molecular dynamics simulation.	*J. Comput. Aided Mol. Des.* (2022)	3.686	Nil
176	Muthusamy, S., Sundarraj, R., Srikanth, S., Dhamodharan, P., **Jeyaraman, J.,** Kadhirvel, S. Designing specific inhibitors against dihydrofolate reductase of W. bancrofti towards drug discovery for lymphatic filariasis.	*Struct. Chem.* (2022)	1.494	2
175	Nirusimhan, V., Andrew Gideon, D., Parashar, A., Jeyachandran, S., **Jeyaraman, J.,** Subbaraj, G., & Kulanthaivel, L. Structural Modeling of Drosophila melanogaster Gut Cytochrome P450s and Docking Comparison of Fruit Fly Gut and Human Cytochrome P450s.	*Curr. Drug Metab.* (2022)	3.731	Nil
174	Ramachandran, B., Jeyarajpandian, C., Jeyaseelan, J. M., Prabhu, D., Rajamanikandan, S., Boomi, P., & **Jeyakanthan, J.** Quercetin-induced apoptosis in HepG2 cells and identification of quercetin derivatives as potent inhibitors for Caspase-3 through computational methods.	*Struct. Chem.* (2022)	1.494	5

173	Alexpandi, R., Gendrot, M., Abirami, G., Delandre, O., Fonta, I., Mosnier, J., Mariadasse R., **Jeyakanthan, J.,** & Veera Ravi, A. Repurposing of doxycycline to hinder the viral replication of SARS-CoV-2: From in silico to in vitro validation.	*Front. Microbiol.* (2022)	5.64	3
172	Sureshan, M., Rajamanikandan, S., Srimari, S., Prabhu, D., **Jeyakanthan, J.,** & Saraboji, K. Designing specific inhibitors against dihydrofolate reductase of W. bancrofti towards drug discovery for lymphatic filariasis. 1-13.	*Struct. Chem.* (2022)	1.494	1
171	Murugan, N. A., Javali, P. S., Pandian, C. J., Ali, M. A., Srivastava, V., & **Jeyaraman, J.** Computational investigation of the increased virulence and pathogenesis of SARS-CoV-2 lineage B.1.1.7.	*Phys. Chem. Chem. Phys. 24*(34), 20371–20380. (2022).	3.676	9
170	Ramachandran, S. S., Balu, R., Vilwanathan, R., **Jeyaraman, J.,** & Paramasivam, S. G. A mouse testis serine protease, TESP1, as the potential SPINK3 receptor protein on mouse sperm acrosome.	*Mol Hum Reprod*. (2021).	4.025	2
169	Poopandi, S., Sundaraj, R., Rajmichael, R., Thangaraj, S., Dhamodharan, P., Biswal, J., Malaisamy, V., Jeyaraj Pandian, C., & **Jeyaraman, J.** Computational screening of potential inhibitors targeting MurF of Brugia malayi Wolbachia through multi-scale molecular docking, molecular dynamics and MM-GBSA analysis.	*Mol. Biochem. Parasito. 246*, 111427 (2021)	1.759	3
168	Dwivedy, A., Mariadasse, R., Ahmad, M., Chakraborty, S., Kar, D., Tiwari, S., Bhattacharyya, S., Sonar, S., Mani, S., Tailor, P., Majumdar, T., **Jeyakanthan, J.,** & Biswal, B. K.. Characterization of the NiRAN domain from RNA-dependent RNA polymerase provides insights into a potential therapeutic target against SARS-CoV-2.	*PloS. Comput. Biol*. *17*(9), e1009384 (2021)	4.475	15
167	Biswal, J., Jayaprakash, P., Rayala, S. K., Venkatraman, G., Rangaswamy, R., & **Jeyaraman, J.** WaterMap and Molecular Dynamic Simulation-Guided Discovery of Potential PAK1 Inhibitors Using Repurposing Approaches.	*ACS Omega*. *6*(41), 26829–26845 (2021)	3.512	3
166	Murugan, N. A., Pandian, C. J., & **Jeyakanthan, J.** Computational investigation on *Andrographis paniculata* phytochemicals to evaluate their potency against SARS-CoV-2 in comparison to known antiviral compounds in drug trials.	*J Biomol Struct Dyn*. *39*(12), 4415–4426 (2021)	3.392	102
165	Karthika, A., Ramachandran, B., Chitra, J., Prabhu, D., Rajamanikandan, S., Veerapandiyan, M., & **Jeyakanthan, J.** Molecular dynamics simulation of Toxin-Antitoxin (TA) system in *Acinetobacter baumannii* to explore the novel mechanism for inhibition of cell wall biosynthesis: Zeta Toxin as an effective therapeutic target.	*J Cell Biochem* (2021)	4.429	3

164	Mohanrasu, K., Guru Raj Rao, R., Dinesh, G. H., Zhang, K., Sudhakar, M., Pugazhendhi, A., **Jeyakanthan, J.,** Ponnuchamy, K., Govarthanan, M., & Arun, A. Production and characterization of biodegradable polyhydroxybutyrate by Micrococcus luteus isolated from marine environment	*Int J Biol Macromol.186*, 125–134 (2021)	6.953	4
163	Kanumuri, R., Chelluboyina, A. K., Biswal, J., Vignesh, R., Pandian, J., Venu, A., Vaishnavi, B., Leena, D. J., **Jeyaraman, J.,** Ganesan, K., Aradhyam, G. K., Venkatraman, G., & Rayala, S. K. Small peptide inhibitor from the sequence of RUNX3 disrupts PAK1-RUNX3 interaction and abrogates its phosphorylation-dependent oncogenic function.	*Oncogene*. 40(34):5327-5341 (2021)	9.867	2
162	Sankar, M., Ramachandran, B., Pandi, B., Mutharasappan, N., Ramasamy, V., Prabu, P. G., Shanmugaraj, G., Wang, Y., Muniyandai, B., Rathinasamy, S., Chandrasekaran, B., Bayan, M. F., **Jeyaraman, J.,** Halliah, G. P., & Ebenezer, S. K. *In silico* Screening of Natural Phytocompounds Towards Identification of Potential Lead Compounds to Treat COVID-19.	*Front Mol Biosci*. *8*, 637122 (2021)	5.246	13
161	Mariadasse, R., Rajmichael, R., Dwivedy, A., Amala, M., Ahmad, M., Mutharasappan, N., Biswal, B. K., &**Jeyakanthan, J.** Characterization of putative transcriptional regulator (PH0140) and its distal homologue.	*Cell Signal*. *84*, 110031 (2021)	4.315	Nil
160	Prabhu, D., Rajamanikandan, S., Sureshan, M., **Jeyakanthan, J.,** & Saraboji, K. Modelling studies reveal the importance of the C-terminal inter motif loop of NSP1 as a promising target site for drug discovery and screening of potential phytochemicals to combat SARS-CoV-2.	*J Mol Graph Model*. *106*, 107920 (2021)	2.518	8
159	Biswal, J., Jayaprakash, P., Rayala, S. K., Venkatraman, G., Rangasamy, R., Poopandi, S., & **Jeyakanthan, J.** Water Mapping and Scoring approaches to predict the role of Hydration sites in Binding Affinity of PAK1 inhibitors.	*Comb Chem High Throughput Screen*. 10.2174/1386207324666210308110646 (2021)	1.339	3
158	M, R. K., Gideon, D. A., Mariadasse, R., Nirusimhan, V., A, S. R., Edward, J. C., **Jeyaraman, J.,** & Dhayabaran, V., 5th *Insilico* evaluation of isatin-based derivatives with RNA-dependent RNA polymerase of the novel coronavirus SARS-CoV-2.	*J Biomol Struct Dyn*. 1–16 (2021)	3.392	4
157	Rajamanikandan, S., Soundarya, S., Paramasivam, A., Prabhu, D., **Jeyakanthan, J.,** & Ramasamy, V. Computational identification of potential lead molecules targeting rho receptor of *Neisseria gonorrhoeae*.	*J Biomol Struct Dyn*. 1–11 (2021)	3.392	3
156	Ahmad, M., Dwivedy, A., Mariadasse, R., Tiwari, S., Kar, D., **Jeyakanthan, J.,** & Biswal, B. K. Prediction of small molecule inhibitors targeting the severe acute respiratory syndrome coronavirus-2 RNA-dependent RNA polymerase.	*ACS omega*, *5*(29), (2020). 18356-18366.	4.132	18
155	Kanagarajan, S., Dhamodharan, P., Mutharasappan, N., Choubey, S. K., Jayaprakash, P., Biswal, J., &	*J Biomol Struct Dyn*. *39*(9),	3.392	2

	Jeyaraman, J. Structural insights on binding mechanism of CAD complexes (CPSase, ATCase and DHOase).	3144–3157. (2021).		
154	Premnath, N., Mohanrasu, K., Guru Raj Rao, R., Dinesh, G. H., Siva Prakash, G., Pugazhendhi, A., **Jeyakanthan, J.,** Govarthanan, M., Kumar, P., & Arun, A. Effect of C/N substrates for enhanced extracellular polymeric substances (EPS) production and Poly Cyclic Aromatic Hydrocarbons (PAHs) degradation.	*Environ Pollut. 275*, 116035 (2021)	8.071	42
153	Ramachandran, B., Srinivasadesikan, V., Chou, T. M., **Jeyakanthan, J.,** & Lee, S. L. Atomistic simulation on flavonoids derivatives as potential inhibitors of bacterial gyrase of *Staphylococcus aureus*.	*J Biomol Struct Dyn*. 1–14 (2020)	3.392	13
152	Prajisha, J., Biswal, J., & **Jeyakanthan, J.** Discovery of potent Camkk1 kinase inhibitors through e-pharmacophore and molecular screening approaches.	*J Biomol Struct Dyn*. 1–17 (2020)	3.392	3
151	Amala, M., Richard, M., Saritha, P., Prabhu, D., Veerapandiyan, M., Surekha, K., & **Jeyakanthan, J.** Molecular evolution, binding site interpretation and functional divergence of aspartate semialdehyde dehydrogenase.	*J Biomol Struct Dyn*. 1–19 (2020)	3.392	1
150	Joseph Sahayarayan, J., Soundar Rajan, K., Nachiappan, M., Prabhu, D., Guru Raj Rao, R., **Jeyakanthan, J.,** Hossam Mahmoud, A., Mohammed, O. B., & Morgan, A. Identification of potential drug target in malarial disease using molecular docking analysis.	*Saudi J Biol Sci*. *27*(12), 3327–3333 (2020)	4.219	7
149	Lokesh, R., **Jeyakanthan, J.,** & Kannabiran, K Targeting VEGFR2 protein by marine Streptomyces globosus VITLGK011-derived compound BECA: An in vitro and in silico analysis.	*J Basic Microbiol*. *60*(11-12), 983–993 (2020)	2.281	Nil
148	Murugan, N. A., Kumar, S., **Jeyakanthan, J.,** & Srivastava, V. Searching for target-specific and multi-targeting organics for Covid-19 in the Drugbank database with a double scoring approach.	*.Sci Rep*. *10*(1), 19125. (2020).	5.133	51
147	Murugan, N. A., Muvva, C., Jeyarajpandian, C., **Jeyakanthan, J.,** & Subramanian, V. Performance of Force-Field- and Machine Learning-Based Scoring Functions in Ranking MAO-B Protein-Inhibitor Complexes in Relevance to Developing Parkinson's Therapeutics.	*Int J Mol Sci*. . *21*(20), 7648. (2020).	5.923	6
146	Chaudhary, S. K., Elayappan, M., **Jeyakanthan, J.,** & Kanagaraj, S. Structural and functional characterization of oligomeric states of proteins in RecFOR pathway.	*Int J Biol. Macromol.163*, 943-953. (2020).	6.953	1
145	Muthumanickam, S., Indhumathi, T., Boomi, P., Balajee, R., **Jeyakanthan, J.,** Anand, K., Ravikumar, S., Kumar, P., Sudha, A., & Jiang, Z. *In silico* approach of naringin as potent phosphatase and tensin homolog (PTEN) protein agonist against prostate cancer.	*J Biomol Struct Dyn*. 1–10. (2020).	3.392	16
144	Boomi, P., Ganesan, R., Prabu Poorani, G., Jegatheeswaran, S., Balakumar, C., Gurumallesh Prabu, H., Anand, K., Marimuthu Prabhu, N., **Jeyakanthan, J.,** & Saravanan, M. Phyto-Engineered Gold	*Int J Nanomedicine. 15*, 7553–7568. (2020).	6.400	64

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143	Prabhu, D., Rajamanikandan, S., Saritha, P., & **Jeyakanthan, J.** Evolutionary significance and functional characterization of streptomycin adenylyltransferase from *Serratia marcescens*.	*J Biomol Struct Dyn.* 38(15):4418-4431.(2020).	3.392	10
142	Vanajothi, R., Hemamalini, V., **Jeyakanthan, J.,** & Premkumar, K. Ligand-based pharmacophore mapping and virtual screening for identification of potential discoidin domain receptor 1 inhibitors.	*J Biomol Struct Dyn.38*(9), 2800–2808. (2020).	3.392	20
141	Chitra, J., Rajendran, S. M., Mercy, J. J., & **Jeyakanthan, J.** Impact of COVID-19 lockdown in Tamil Nadu: Benefits and challenges on environment perspective.	*Indian J. Biochem. Biophys.,*57, 370-381(2020).	1.66	11
140	Choubey, S. K., Nachiappan, M., Richard, M., Chitra, J. P., & **Jeyakanthan, J.** Structural and functional insights of STAT2-NS5 interaction for the identification of NS5 antagonist - An approach for restoring interferon signaling.	*Comput Biol Chem*. *88*, 107332. (2020).	2.877	2
139	Ahmad, M., Dwivedy, A., Mariadasse, R., Tiwari, S., Kar, D., **Jeyakanthan, J.,** & Biswal, B. K. Prediction of Small Molecule Inhibitors Targeting the Severe Acute Respiratory Syndrome Coronavirus-2 RNA-dependent RNA Polymerase.	*ACS Omega*, *5*(29), 18356–18366. (2020).	3.512	17
138	Ramachandran, B., **Jeyakanthan, J.,** & Lopes, B. S. Molecular docking, dynamics and free energy analyses of *Acinetobacter baumannii* OXA class enzymes with carbapenems investigating their hydrolytic mechanisms.	*J Med Microbiol*. *69*(8), 1062–1078. (2020).	2.35	7
137	Prabhu, D., Rajamanikandan, S., Anusha, S. B., Chowdary, M. S., Veerapandiyan, M., & **Jeyakanthan, J.** In silico Functional Annotation and Characterization of Hypothetical Proteins from *Serratia marcescens* FGI94.	*Biol Bull Russ Acad Sci*. *47*(4), 319–331.(2020).	1.818	16
136	Prabhu, D., Rajamanikandan, S., Saritha, P., & **Jeyakanthan, J.** Evolutionary significance and functional characterization of streptomycin adenylyltransferase from Serratia marcescens.	*J Biomol Struct Dyn*. *38*(15), 4418-4431.(2020).	3.01	10
135	K. Mohanrasu, R. Guru Raj Rao, G.H. Dinesh, Kunyu Zhan, Siva Prakash, Dong-Po Song, Sudhakar Muniyasamy, Arivalagan Pugazhendh, **J.Jeyakanthan,** A. Arun. Optimization of media components and culture conditions for polyhydroxyalkanoates production by Bacillus megaterium.	*Fuel*, *271*, 117522. (2020).	6.609	45
134	Sundarraj, R., Mohanty, N. N., Yogisharadhya, R., **Jeyakanthan, J.,** Prajapati, A., Chanda, M. M., & Shivachandra, S. B. Comparative sequence, structure and functional analysis of Skp protein, a molecular chaperone among members of Pasteurellaceae and its homologues in Gram-negative bacteria.	*Meta Gene,* 24, 100680, (2020).	0.536	1
133	Santhosh, R., Bankoti, N., Gurudarshan, M., **Jeyakanthan, J.,**& Sekar, K. IMRPS: Inserted and Modified Residues in Protein Structures. A database. .	*J Appl. Cryst., 53*(2), 569-573(2020).	3.304	1

132	Nachiappan, M., Jain, V., Sharma, A., Manickam, Y., & **Jeyakanthan, J.** Conformational changes in glutaminyl-tRNA synthetases upon binding of the substrates and analogs using molecular docking and molecular dynamics approaches.	*J Biomol Struct Dyn*. *38*(6), 1575–1589.(2020).	3.392	6
131	Sundarrajan, S., Nandakumar, M. P., Prabhu, D., **Jeyaraman, J.,** & Arumugam, M. Conformational insights into the inhibitory mechanism of phyto-compounds against Src kinase family members implicated in psoriasis.	*J Biomol Struct Dyn*. *38*(5), 1398–1414. (2020).	3.392	6
130	Nanda, H., Ponnusamy, N., Odumpatta, R., **Jeyakanthan, J.,** & Mohanapriya, A. Exploring genetic targets of psoriasis using genome wide association studies (GWAS) for drug repurposing.	*Biotech*.*10*(2), 43. (2020).	2.4	3
129	Mariadasse, R., Choubey, S. K., & **Jeyakanthan,** J. Insights into Exogenous Tryptophan-Mediated Allosteric Communication and Helical Transition of TRP Protein for Transcription Regulation.	*J Chem Inf Model*. *60*(1), 175–191. (2020).	4.956	10
128	**Jeyakanthan J**, Parimal P, Raju G & Rama SD. Technology Enhanced Learning in Higher Education status and Strategies.	*IJHER,* 9(2), 142-150, 2020.	5.425	Nil
127	Biswal, J., Jayaprakash, P., Suresh Kumar, R., Venkatraman, G., Poopandi, S., Rangasamy, R., & **Jeyaraman, J.** Identification of Pak1 inhibitors using water thermodynamic analysis.	*J Biomol Struct Dyn*. *38*(1), 13–31. (2020).	3.392	10
126	Gowri, M., Jayashree, B., **Jeyakanthan, J.,** & Girija, E. K. Sertraline as a promising antifungal agent: inhibition of growth and biofilm of Candida auris with special focus on the mechanism of action in vitro.	*J Appl Microbiol*. *128*(2), 426–437. (2020).	3.772	38
125	Sekar Vijayakumar., Baskaralingam Vaseeharan., Raja Sudhakaran., **Jeyaraman Jeyakandan.,** Palaniappan Ramasamy., Avinash Sonawane., Avinash Padhi., Palaniyandi Velusamy., Periyasamy Anbu &Caterina Faggio. Bioinspired zinc oxide nanoparticles using Lycopersicon esculentum for antimicrobial and anticancer applications.	*J Cluster Sci., 30*(6), 1465-1479. (2019).	3.061	37
124	Langeswaran, K., **Jeyaraman, J.,** R, J. B., Biswas, A., & Dhurgadevi, K. R. Identifying dual leucine zipper kinase (DLK) inhibitors using e-pharamacophore screening and molecular docking.	*J Recept Signal Transduct Res*. *39*(2), 99–105.(2019).	2.09	3
123	Santhosh, R., Bankoti, N., Padmashri, A. M., Michael, D., **Jeyakanthan, J.,**& Sekar, K. MRPC (Missing Regions in Polypeptide Chains): a knowledgebase. *Journal of Applied Crystallography*,	*J Appl. Cryst., 52*(6), 1422-1426.(2019).	3.304	2
122	Santhosh, R., Chandrasekaran, P., Michael, D., Rangachari, K., Bankoti, N., **Jeyakanthan, J.,** & Sekar, K. ACMS: a database of alternate conformations found in the atoms of main and side chains of protein structures.	*J. Appl. Cryst., 52*(4), 910-913..(2019).	3.304	3
121	Boomi, P., Poorani, G. P., Palanisamy, S., Selvam, S., Ramanathan, G., Ravikumar, S., Barabadi H., Prabu, H.G., **Jeyakanthan, J.,** Saravanan, M. Evaluation of antibacterial and anticancer potential of polyaniline-bimetal nanocomposites synthesized from chemical	*J Cluster Sci, 30*(3), 715-726. (2019).	3.061	61

	reduction method.			
120	Imran, H., Manikandan, P. N., Prabhu, D., Dharuman, V., **Jeyakanthan, J.,** & Hahn, J. H. Ultra selective label free electrochemical detection of cancer prognostic p53-antibody at DNA functionalized graphene.	*Sens Bio Res. 23*, 100261. (2019).	4.124	13
119	Boomi, P., Ganesan, R. M., Poorani, G., Gurumallesh Prabu, H., Ravikumar, S., & **Jeyakanthan, J.** Biological synergy of greener gold nanoparticles by using Coleus aromaticus leaf extract.	*Mater Sci Eng C Mater Biol Appl*. *99*, 202–210. (2019).	7.328	69
118	Santhosh, R., Velayudham, E., Michael, D., Bankoti, N., Chandrasekaran, P., Karthikeyan, D., Pavithra, S., Gurusaran, M., Nisha, K.P.R., Satheesh, S.N., Rangachari, K., **Jeyakanthan, J.,** Sekar. Diffraction precision index of macromolecular structures: a web based database.	*RJLBPCS,*Vol 5(2), 126-133. (2019).	*Peer Reviewed*	Nil
117	Jayaprakash, P., Biswal, J., Kanagarajan, S., Prabhu, D., Gogoi, P., Prasad Kanaujia, S., & **Jeyakanthan, J.** Design of novel *Ph*MTNA inhibitors, targeting neurological disorder through homology modeling, molecular docking, and dynamics approaches.	*J Recept Signal Transduct Res*. ;39(1):28-38. (2019).	2.09	5
116	Ravi, G., Biswal, J., Kanagarajan, S., & **Jeyakanthan, J.** Exploration of N5-CAIR Mutase Novel Inhibitors from *Pyrococcus horikoshii* OT3: A Computational Study.	*J Comput Biol*. *26*(5), 457–472. (2019).	1.479	3
115	Chaudhary, S. K., Iyyappan, Y., Elayappan, M., **Jeyakanthan, J.,**& Sekar, K. Insights into product release dynamics through structural analyses of thymidylate kinase.	*Int J Biol Macromol*. *123*, 637–647. (2019).	6.953	5
114	Amala, M., Rajamanikandan, S., Prabhu, D., Surekha, K., & **Jeyakanthan,** J. Identification of anti-filarial leads against aspartate semialdehyde dehydrogenase of Wolbachia endosymbiont of Brugia malayi: combined molecular docking and molecular dynamics approaches.	*J Biomol Struct Dyn*. *37*(2), 394–410. (2019).	3.392	25
113	Nachiappan, M., Jain, V., Sharma, A., Yogavel, M., & **Jeyakanthan, J.** Structural and functional analysis of Glutaminyl-tRNA synthetase (TtGlnRS) from Thermus thermophilus HB8 and its complexes.	*J Biol Macromol.120*(Pt B), 1379–1386. (2018).	6.953	11
112	Sindhu, T., Venkatesan, T., Prabhu, D., **Jeyakanthan, J.,** Gracy, G. R., Jalali, S. K., & Rai, A. Insecticide-resistance mechanism of Plutella xylostella (L.) associated with amino acid substitutions in acetylcholinesterase-1: A molecular docking and molecular dynamics investigation.	*Comput Biol Chem*.*77*, 240–250. (2018).	2.877	14
111	Kulanthaivel, L., **Jeyaraman, J.,** Biswas, A., Subbaraj, G. K., & Santhoshkumar, S. Identification of potential inhibitors for Penicillinbinding protein (PBP) from Staphylococcus aureus.	*Bioinformation*. *14*(9), 471–476. (2018).	6.937	3

110	Thulasinathan, B., Kulanthaisamy, M. R., Nagarajan, A., Soorangkattan, S., Muthuramalingam, J. B., **Jeyaraman, J.,** & Arun, A. Studies on the diversity of macrofungus in Kodaikanal region of Western Ghats, Tamil Nadu, India.	*Biodiversitas, 19*(6), 2283-2293.(2018).	1.046	4
109	Choubey, S. K., & **Jeyakanthan, J.** Molecular dynamics and quantum chemistry-based approaches to identify isoform selective HDAC2 inhibitor - a novel target to prevent Alzheimer's disease.	*J Recept Signal Transduct Res*. *38*(3), 266–278.(2018).	2.09	12
108	Langeswaran, K., **Jeyaraman, J.,** Mariadasse, R., & Soorangkattan, S. Insights from the Molecular modeling, docking analysis of illicit drugs and Bomb Compounds with Honey Bee Odorant Binding Proteins (OBPs).	*Bioinformation.14*(5), 219–231. (2018).	6.937	7
107	Sahana, J. J., Sriraghav, S., Vijeth, T. A., Nagarushyanth, T., Santhosh, R., Michael, D., Sameer Ahmed, Z., Nisha, K.P.R., **Jeyakanthan, J.,**& Sekar, K. PlaneFinder: a methodology to find the best plane for a set of atoms involved in the metal coordination in protein structures.	*J ApplCrys*, *51*(4), 1251-1256.(2018).	3.304	Nil
106	Chaudhary, S. K., **Jeyakanthan, J.,** & Sekar, K. Structural and functional roles of dynamically correlated residues in thymidylate kinase.	*Acta Crystallogr D Struct Biol*. *74*(Pt 4), 341–354. (2018).	7.652	6
105	Boomi, P., Anandha Raj, J., Palaniappan, S. P., Poorani, G., Selvam, S., Gurumallesh Prabu, H., Manisankar, P., **Jeyakanthan, J.,** & Langeswaran, V. K. Improved conductivity and antibacterial activity of poly(2-aminothiophenol)-silver nanocomposite against human pathogens.	*J Photochem Photobiol B. 178*, 323–329. (2018).	6.252	14
104	Maniyazagan, M., Mariadasse, R., Nachiappan, M., **Jeyakanthan, J.,** Lokanath, N. K., Naveen, S., Sivaraman, G., Muthurasa, P.,Manisankar, P., & Stalin, T. Synthesis of rhodamine based organic nanorods for efficient chemosensor probe for Al (III) ions and its biological applications.	*Sens Actuator B: Chemical. 254*, 795-804. (2018).	7.335	57
103	Singal, B., Balakrishna, A. M., Nartey, W., Manimekalai, M., **Jeyakanthan, J.,** & Grüber, G. Crystallographic and solution structure of the N-terminal domain of the Rel protein from Mycobacterium tuberculosis.	*FEBS Lett, 591*(15), 2323–2337. (2017).	4.124	28
102	Sudha, A., **Jeyakanthan, J.,** & Srinivasan, P. Green synthesis of silver nanoparticles using Lippia nodiflora aerial extract and evaluation of their antioxidant, antibacterial and cytotoxic effects.	*ResEffiTech, 3*(4), 506-515. . (2017).	*Peer Reviewed*	151
101	Biswas, A., Shukla, A., Chaudhary, S. K., Santhosh, R., **Jeyakanthan, J.,** & Sekar, K. Structural studies of a hyperthermophilic thymidylate kinase enzyme reveal conformational substates along the reaction coordinate.	*FEBS J284*(15), 2527–2544. (2017).	5.542	6

100	Choubey, S. K., Prabhu, D., Nachiappan, M., Biswal, J., & **Jeyakanthan, J.** Molecular modeling, dynamics studies and density functional theory approaches to identify potential inhibitors of SIRT4 protein from Homo sapiens : a novel target for the treatment of type 2 diabetes.	*J Biomol Struct Dyn*. *35*(15), 3316–3329. (2017).	3.392	48
99	Biswas, A., Shukla, A., Vijayan, R., **Jeyakanthan, J.,** & Sekar, K. Crystal structures of an archaeal thymidylate kinase from Sulfolobus tokodaii provide insights into the role of a conserved active site Arginine residue.	*J Struct Biol*.*197*(3), 236–249. (2017).	2.867	16
98	Rajamanikandan, S., **Jeyakanthan, J.,** & Srinivasan, P. Binding mode exploration of LuxR-thiazolidinedione analogues, e-pharmacophore-based virtual screening in the designing of LuxR inhibitors and its biological evaluation.	*J Biomol Struct Dyn*., *35*(4), 897–916. (2017).	3.392	20
97	Maniyazagan, M., Rameshwaran, C., Mariadasse, R., **Jeyakanthan, J.,** Premkumar, K., & Stalin, T. Fluorescence Sensor for Hg2+ and Fe3+ ions using 3, 3′–Dihydroxybenzidine: α–Cyclodextrin Supramolecular Complex: Characterization, in-silico and Cell Imaging Study.	*Sens Actuators B Chem*., Vol 242, PP: 1227–1238, (2017).	7.335	18
96	**Jeyakanthan, J.** Unravelling the Importance of Multidrug Efflux Transporter Protein from Thermus thermophilus HB8-an in silico approach.	*RJMAS*, Vol 1; Issue 1, (2017).	*Peer Reviewed*	Nil
95	Prabhu, D., Vidhyavathi, R., & **Jeyakanthan, J.** Computational identification of potent inhibitors for Streptomycin 3″-adenylyltransferase of Serratia marcescens.	*Microb Pathog*.*103*, 94–106. (2017).	3.738	16
94	Rajamanikandan, S., **Jeyakanthan, J.,** & Srinivasan, P. Discovery of potent inhibitors targeting Vibrio harveyi LuxR through shape and e-pharmacophore based virtual screening and its biological evaluation.	*Microb Pathog*., *103*, 40–56. (2017).	3.738	25
93	Rajamanikandan, S., **Jeyakanthan, J.,** & Srinivasan, P. Molecular Docking, Molecular Dynamics Simulations, Computational Screening to Design Quorum Sensing Inhibitors Targeting LuxP of Vibrio harveyi and Its Biological Evaluation.	*Appl Biochem Biotechnol*.*181*(1), 192–218.(2017).	2.926	33
92	Maniyazagan, M., Mariadasse, R., **Jeyakanthan, J.,** Lokanath, N. K., Naveen, S., Premkumar, K., ... & Stalin, T. Rhodamine based "turn–on" molecular switch FRET–sensor for cadmium and sulfide ions and live cell imaging study.	*Sens Actuators B Chem*., , *238*, 565-577. (2017).	7.335	58
91	Surekha, K., Nachiappan, M., Prabhu, D., Choubey, S. K., Biswal, J., & **Jeyakanthan, J.** Identification of potential inhibitors for oncogenic target of dihydroorotate dehydrogenase using in silico approaches.	*J Mol Struct. 1127*, 675-688. (2017).	3.196	11
90	Sasikala, D., **Jeyakanthan, J.,**& Srinivasan, P. Structure-based virtual screening and biological evaluation of LuxT inhibitors for targeting quorum sensing through an in vitro biofilm formation.	*J Mol Struct. 1127*, 322-336. (2017).	3.196	7

89	Biswas, A., Jasti, S., **Jeyakanthan, J**., & Sekar, K. Role of sequence evolution and conformational dynamics in the substrate specificity and oligomerization mode of thymidylate kinases.	*J Biomol Struct Dyn*. *35*(10), 2136–2154. (2017).	3.392	3
88	Choubey, S. K., & **Jeyaraman, J.** A mechanistic approach to explore novel HDAC1 inhibitor using pharmacophore modeling, 3D- QSAR analysis, molecular docking, density functional and molecular dynamics simulation study.	*J Mol Graph Model*.*70*, 54–69., (2016).	2.518	30
87	Choubey, S. K., Mariadasse, R., Rajendran, S., & **Jeyaraman, J.** Identification of novel histone deacetylase 1 inhibitors by combined pharmacophore modeling, 3D-QSAR analysis, in silico screening and Density Functional Theory (DFT) approaches.	*J Mol Struct*.,*1125*, 391-404. (2016).	3.196	17
86	Sudha, A., **Jeyakanthan, J.,** & Srinivasan, P. Protective effect of 5-hydroxy-3′, 4′, 7-trimethoxyflavone against inflammation induced by lipopolysaccharide in RAW 264.7 macrophage: in vitro study and in silico validation.	*Med Chem Res*. *25*(9), 1754-1767.(2016).	1.965	4
85	Rao, R. G., Biswal, J., Dhamodharan, P., Kanagarajan, S., & **Jeyaraman, J.** Identification of potential inhibitors for AIRS from de novo purine biosynthesis pathway through molecular modeling studies - a computational approach.	*J Biomol Struct Dyn*.*34*(10), 2199–2213. (2016).	3.392	14
84	Jagadeeshan, S., Subramanian, A., Tentu, S., Beesetti, S., Singhal, M., Raghavan, S., Surabhi, R. P., Mavuluri, J., Bhoopalan, H., Biswal, J., Pitani, R. S., Chidambaram, S., Sundaram, S., Malathi, R., **Jeyaraman, J.,** Nair, A. S., Venkatraman, G., & Rayala, S. K. P21-activated kinase 1 (Pak1) signaling influences therapeutic outcome in pancreatic cancer.	*Ann Oncol*.*27*(8), 1546–1556. (2016).	32.976	42
83	Santhosh, R., Satheesh, S. N., Gurusaran, M., Michael, D., Sekar, K., & **Jeyakanthan, J.** NIMS: a database on nucleobase compounds and their interactions in macromolecular structures.	*J ApplCrystallogr*., *49*(3), 1093-1098. (2016).	3.304	2
82	Sasikala, D., **Jeyakanthan, J.,** & Srinivasan, P. Structural insights on identification of potential lead compounds targeting WbpP in Vibrio vulnificus through structure-based approaches.	*J Recept Signal Transduct Res*.*36*(5), 515–530. (2016).	2.09	5
81	Surekha, K., Prabhu, D., Richard, M., Nachiappan, M., Biswal, J., & **Jeyakanthan, J.** Investigation of vital pathogenic target orotate phosphoribosyltransferases (OPRTase) from Thermus thermophilus HB8: Phylogenetic and molecular modeling approach.	*Gene*.583(2). PP: *583*(2), 102–111. (2016).	2.984	24
80	Mariadasse, R., Biswal, J., Jayaprakash, P., Rao, G. R., Choubey, S. K., Rajendran, S., & **Jeyakanthan, J.** Mechanical insights of oxythiamine compound as potent inhibitor for human transketolase-like protein 1 (TKTL1 protein).	*J Recept Signal Transduct Res*. *36*(3), 233–242.(2016).	1.78	17

79	Gowri, M., Sofi Beaula, W., Biswal, J., Dhamodharan, P., Saiharish, R., Rohan prasad, S., Pitani, R., Kandaswamy, D., Raghunathan, R., **Jeyakanthan, J.,** Rayala, S. K., & Venkatraman, G. β-lactam substituted polycyclic fused pyrrolidine/pyrrolizidine derivatives eradicate C. albicans in an ex vivo human dentinal tubule model by inhibiting sterol 14-α demethylase and cAMP pathway.	*Biochim Biophys Acta*.*1860*(4), 636–647. (2016).	3.77	12
78	Gogoi, P., Srivastava, A., Jayaprakash, P., **Jeyakanthan, J.,** & Kanaujia, S. P. In silico analysis suggests that PH0702 and PH0208 encode for methylthioribose-1-phosphate isomerase and ribose-1,5-bisphosphate isomerase, respectively, rather than aIF2Bβ and aIF2Bδ.	*Gene*. *575*(1), 118–126. (2016).	3.688	6
77	Ravi, M., Tentu, S., Baskar, G., Rohan Prasad, S., Raghavan, S., Jayaprakash, P., **Jeyakanthan, J.,** Rayala, S. K., & Venkatraman, G. Molecular mechanism of anti-cancer activity of phycocyanin in triple-negative breast cancer cells.	*BMC Cancer*.*15*, 768. (2015).	4.430	Nil
76	Meiyazhagan, G., Raju, R., Winfred, S. B., Mannivanan, B., Bhoopalan, H., Shankar, V., Sekar, S., Venkatachalam, D. P., Pitani, R., Nagendrababu, V., Thaiman, M., Devivanayagam, K., **Jayaraman, J.,** Ragavachary, R., & Venkatraman, G. Bioactivity Studies of β-Lactam Derived Polycyclic Fused Pyrroli-Dine/Pyrrolizidine Derivatives in Dentistry: In Vitro, In Vivo and In Silico Studies.	*PLoS One*. *10*(7), e0131433.. (2015).	3.24	6
75	Manjunath, K., **Jeyakanthan, J.,** & Sekar, K. Catalytic pathway, substrate binding and stability in SAICAR synthetase: A structure and molecular dynamics study.	*J Struct Biol*. *191*(1), 22–31. (2015).	2.867	9
74	Devi, S. K., Chichili, V. P., **Jeyakanthan, J.,** Velmurugan, D., & Sivaraman, J. Structural basis for the hydrolysis of ATP by a nucleotide binding subunit of an amino acid ABC transporter from Thermus thermophilus.	*J Struct Biol*. *190*(3), 367–372. (2015).	2.867	6
73	Kanagarajan, S., Mutharasappan, N., Dhamodharan, P., Jeyaraman, M., Ramadas, K., & **Jeyaraman, J.** Exploring the structural features of Aspartate Trans Carbamoylase (TtATCase) from Thermus thermophilus HB8 through in silico approaches: a potential drug target for inborn error of pyrimidine metabolism.	*J Biomol Struct Dyn*. *32*(4), 591–601. (2014).	3.392	5
72	Karthik, L., Nachiappan, M., Velmurugan, D., **Jeyakanthan, J.,** & Gunasekaran, K. Crystal structure analysis of L-fuculose-1-phosphate aldolase from Thermus thermophilus HB8 and its catalytic action: as explained through in silico.	*J Struct Funct Genomics*. *14*(2), 59–70. (2013).	0.48	3
71	Balakrishnan, T., Ramamurthi, K., **Jeyakanthan, J.,** & Thamotharan, S. catena-Poly[aqua-(glycine-κO)lithium]-μ-glycine-κ(2) O:O'] bromide].	*Acta Crystallogr Sect E Struct Rep. 69*(Pt 1), m60–m61. (2013).	0.517	17

70	Chaudhary, S. K., **Jeyakanthan, J.,** & Sekar, K. Cloning, expression, purification, crystallization and preliminary X-ray crystallographic study of thymidylate kinase (TTHA1607) from Thermus thermophilus HB8.	*Acta Crystallogr Sect F Struct Biol Cryst Commun.69*(Pt 2), 118–121. (2013).	1.056	5
69	Manjunath, K., Kanaujia, S. P., Kanagaraj, S., **Jeyakanthan, J.,** & Sekar, K. Structure of SAICAR synthetase from Pyrococcus horikoshii OT3: insights into thermal stability.	*Int J Biol Macromol*. *53*, 7–19. (2013).	6.953	6
68	Uthayakumar, M., Benazir, B., Patra, S., Vaishnavi, M. K., Gurusaran, M., Sureka, K., **Jeyakanthan, J.,** & Sekar, K. Homepeptide repeats: implications for protein structure, function and evolution.	*Genomics Proteomics Bioinformatics*. 10(4), *10*(4), 217–225. (2012).	7.691	9
67	Grover, A., Katiyar, S. P., **Jeyakanthan, J.,** Dubey, V. K., & Sundar, D. Mechanistic insights into the dual inhibition strategy for checking Leishmaniasis.	*J Biomol Struct Dyn*.30(4), *30*(4),474–487. (2012).	3.392	6
66	Saranya, N., **Jeyakanthan, J.,** & Selvaraj, S. Impact of protein binding cavity volume (PCV) and ligand volume (LV) in rigid and flexible docking of protein-ligand complexes.	*Bioorg Med Chem Lett.22*(24), 7593–7597. (2012).	2.823	3
65	Grover, A., Katiyar, S. P., **Jeyakanthan, J.,** Dubey, V. K., & Sundar, D. Blocking protein kinase C signaling pathway: mechanistic insights into the anti-leishmanial activity of prospective herbal drugs from Withania somnifera.	*BMC Genomics*, *13 Suppl 7*(Suppl 7), S20.. (2012).	3.969	39
64	Chacko, A. R., **Jeyakanthan, J.,** Ueno, G., Sekar, K., Rao, C. D., Dodson, E. J., Suguna, K., & Read, R. J. A new pentameric structure of rotavirus NSP4 revealed by molecular replacement.	*Acta Crystallogr D Biol Crystallogr.68*(Pt 1), 57–61. (2012).	7.652	13
63	Singh, K., Kirubakaran, P., Nagarajan, S., Sakkiah, S., Muthusamy, K., Velmurgan, D., & **Jeyakanthan, J**. Homology modeling, molecular dynamics, e-pharmacophore mapping and docking study of Chikungunya virus nsP2 protease.	*J Mol Model*. *18*(1), 39–51. (2012).	1.810	94
62	Srinivasan, P., Kumar, S. P., Karthikeyan, M., **Jeyakanthan, J.,** Jasrai, Y. T., Pandya, H. A., Rawal, R. M., & Patel, S. K. Epitope-based immunoinformatics and molecular docking studies of nucleocapsid protein and ovarian tumor domain of crimean-congo hemorrhagic Fever virus.	*Front Genet*. *2*, 72. (2011).	4.274	20
61	Kojiro Mimura, Shinya Hosokawa, Naohisa Happo, Wen Hu, Kouichi Hayashi, Kazuki Wakita, Hirofumi Ishii, Masato Yoshimura, **Jeyaraman Jeyakanthan,** Nazim Mamedov. Three Dimensional Atomic Image of TlInSe2 by X-ray Fluorescence Holography.	*e-J. Surf. Sci. Nanotech*. *9*, 273-276. (2011).	1.940	4

60	Muthukumaran, J., Manivel, P., Kannan, M., **Jeyakanthan, J.,** & Krishna, R. Advancement in computational analysis methods of plant antifreeze proteins (AFPs): An application towards classification and gene expression studies of leucine rich repeat (LRR) and ice-recrystallization inhibition domain (IRI) containing AFPs.	*J Comput Biol Bioinform Res.*, *3*(6), 63-82. (2011).	1.479	3
59	Chacko, A. R., Arifullah, M., Sastri, N. P., **Jeyakanthan, J.,** Ueno, G., Sekar, K., Read, R. J., Dodson, E. J., Rao, D. C., & Suguna, K. Novel pentameric structure of the diarrhea-inducing region of the rotavirus enterotoxigenic protein NSP4.	*J Virol*. *85*(23), 12721–12732.. (2011).	5.013	28
58	Muthukumaran, J., Manivel, P., Kannan, M., **Jeyakanthan, J.,** & Krishna, R. A framework for classification of antifreeze proteins in over wintering plants based on their sequence and structural features.	*JBSA*. *3*(4), 70-88.. (2011).	1.122	17
57	Muthukumaran, J., Nachiappan, M., Chitra, S., Manisankar, P., Bhattacharya, S., Muthusubramanian, S., Krishna, R.,& **Jeyakanthan, J. J**1-(2-Naphthyl)-3-phenyl-3-(4, 5, 6, 7-tetrahydro-1, 2, 3-benzoselenadiazol-4-yl) propan-1-one.	*Acta Cryst.* *67*(8), o2010-o2011.. (2011).	0.517	3
56	Muthukumaran, J., Nishandhini, M., Chitra, S., Manisankar, P., Bhattacharya, S., Muthusubramanian, S., Krishna, R.,& **Jeyakanthan, J.** 3-(4-Methylphenyl)-1-phenyl-3-(4, 5, 6, 7-tetrahydro-1, 2, 3-benzoselenadiazol-4-yl) propan-1-one.	*Acta Cryst.* *67*(7), o1660-o1661. (2011).	0.517	3
55	Hosokawa, S., Happo, N., Hayashi, K., Mimura, K., Wakita, K., Hu, W., Ishii, H., Yosimura, M., **Jeyakanthan J** & Mamedov, N. Three-Dimensional Atomic Images of TlInSe2 Thermoelectric Material Obtained by X-ray Fluorescence Holography.	*Jpn. J. Appl. Phys. 50*(5S2), 05FC06. (2011).	1.480	8
54	Muthukumaran, J., Nishandhini, M., Chitra, S., Muthusubramanian, S., Manisankar, P., Bhattacharya, S., Krishna, R.,& **Jeyakanthan, J.** 4-{(4-Chlorophenyl)[4-(4-methylphenyl)-1, 2, 3-selenadiazol-5-yl] methyl}-4, 5, 6, 7-tetrahydro-1, 2, 3-benzoselenadiazole.	*Acta Cryst* *67*(6), o1421-o1422. (2011).	5.469	1
53	Manimekalai, M. S. S., Kumar, A., **Jeyakanthan, J.,** & Grüber, G. The transition-like state and Pi entrance into the catalytic a subunit of the biological engine A-ATP synthase.	*J.Mol.Biol*. *408*(4), 736-754. (2011).	4.00	11
52	Kanaujia, S. P., **Jeyakanthan, J.,** Shinkai, A., Kuramitsu, S., Yokoyama, S., & Sekar, K. Crystal structures, dynamics and functional implications of molybdenum-cofactor biosynthesis protein MogA from two thermophilic organisms.	*Acta Crystallogr Sect F Struct Biol Cryst Commun.67*(Pt 1), 2–16. (2011).	1.056	4
51	Kanaujia, S. P., **Jeyakanthan, J.,** Nakagawa, N., Balasubramaniam, S., Shinkai, A., Kuramitsu, S., Yokoyama, S., & Sekar, K. Structures of apo and GTP-bound molybdenum cofactor biosynthesis protein MoaC from Thermus thermophilus HB8.	*Acta Crystallogr D Biol Crystallogr*. *66*(Pt 7), 821–833. (2010).	7.652	23

50	Kumar, A., Manimekalai, M. S., Balakrishna, A. M., Priya, R., Biuković, G., **Jeyakanthan, J.,** & Grüber, G. The critical roles of residues P235 and F236 of subunit A of the motor protein A-ATP synthase in P-loop formation and nucleotide binding.	*J. Mol. Biol*. *401*(5), 892–905. (2010).	5.469	9
49	Balakrishna, A. M., Manimekalai, M. S., Hunke, C., Gayen, S., Rössle, M., **Jeyakanthan, J.,** & Grüber, G. Crystal and solution structure of the C-terminal part of the Methanocaldococcus jannaschii A1AO ATP synthase subunit E revealed by X-ray diffraction and small-angle X-ray scattering.	*J Bioenerg Biomembr*. *42*(4), 311–320.. (2010).	2.945	7
48	**Jeyakanthan, J.,** Kanaujia, S. P., Nishida, Y., Nakagawa, N., Praveen, S., Shinkai, A., Kuramitsu, S., Yokoyama, S., & Sekar, K. Free and ATP-bound structures of Ap4A hydrolase from Aquifex aeolicus V5.	*Acta Crystallogr D Biol Crystallogr*. *66*(Pt 2), 116–124. (2010).	7.652	7
47	Alikhajeh, J., Khajeh, K., Ranjbar, B., Naderi-Manesh, H., Lin, Y. H., Liu, E., Guan, H. H., Hsieh, Y. C., Chuankhayan, P., Huang, Y. C., **Jeyaraman, J.,** Liu, M. Y., & Chen, C. J. Structure of Bacillus amyloliquefaciens alpha-amylase at high resolution: implications for thermal stability.	*Acta Crystallogr Sect F Struct Biol Cryst Commun*.*66*(Pt 2), 121–129. (2010).	1.056	64
46	**Jeyakanthan, J.,** Drevland, R. M., Gayathri, D. R., Velmurugan, D., Shinkai, A., Kuramitsu, S., Yokoyama, S., & Graham, D. E. Substrate specificity determinants of the methanogen homoaconitase enzyme: structure and function of the small subunit.	*Biochemistry*. *49*(12), 2687–2696. (2010).	3.162	16
45	Grüber, A., Manimekalai, M. S., Balakrishna, A. M., Hunke, C., **Jeyakanthan, J.,** Preiser, P. R., & Grüber, G. Structural determination of functional units of the nucleotide binding domain (NBD94) of the reticulocyte binding protein Py235 of Plasmodium yoelii.	*PLoS One*.*5*(2), e9146. (2010).	3.240	10
44	Gupta, V., Prakash, N. A., Lakshmi, V., Boopathy, R., **Jeyakanthan, J.,** Velmurugan, D., & Sekar, K. Recognition of active and inactive catalytic triads: A template based approach.	*Int J Biol Macromol*. *46*(3), 317–323.(2010).	6.953	9
43	**Jeyakanthan, J.,** Thamotharan, S., Panjikar, S., Kitamura, Y., Nakagawa, N., Shinkai, A., Kuramitsu, S., & Yokoyama, S. Expression, purification and X-ray analysis of 1,3-propanediol dehydrogenase (Aq_1145) from Aquifex aeolicus VF5.	*Acta Crystallogr Sect F Struct Biol Cryst Commun. 66*(Pt 2), 184–186. (2010).	1.056	5
42	Manjunath, K., **Jeyakanthan, J.,** Nakagawa, N., Shinkai, A., Yoshimura, M., Kuramitsu, S., Yokoyama, S., & Sekar, K. Cloning, expression, purification, crystallization and preliminary X-ray crystallographic study of the putative SAICAR synthetase (PH0239) from Pyrococcus horikoshii OT3.	*Acta Crystallogr Sect F Struct Biol Cryst Commun*. *66*(Pt 2), 180–183.(2010).	1.056	3
41	Kumar, A., Manimekalai, M. S., Balakrishna, A. M., **Jeyakanthan, J.,** & Grüber, G. Nucleotide binding states of subunit A of the A-ATP synthase and the implication of P-loop switch in evolution.	*J. Mol.Biol. 396*(2), 301–320. (2010).	5.469	33
40	Hemavathi, K., Kalaivani, M., Udayakumar, A., Sowmiya, G., **Jeyakanthan, J.,** & Sekar, K. MIPS: metal interactions in protein structures.	*JAppl cryst*. *43*(1), 196-199.. (2010).	3.304	29

39	Guan, H. H., Goh, K. S., Davamani, F., Wu, P. L., Huang, Y. W., **Jeyakanthan, J.,** Wu, W. G., & Chen, C. J. Structures of two elapid snake venom metalloproteases with distinct activities highlight the disulfide patterns in the D domain of ADAMalysin family proteins.	*J Struct Biol*. *169*(3), 294–303. (2010).	2.867	56
38	**Jeyakanthan, J.,** Takada, K., Sawano, M., Ogasahara, K., Mizutani, H., Kunishima, N., Yokoyama, S., & Yutani, K. Crystal Structural and Functional Analysis of the Putative Dipeptidase from Pyrococcus horikoshii OT3.	*J Biophys*. 434038. (2009).	Peer Reviewed	16
37	Chiang, Y. L., Hsieh, Y. C., Fang, J. Y., Liu, E. H., Huang, Y. C., Chuankhayan, P., **Jeyakanthan, J.,** Liu, M. Y., Chan, S. I., & Chen, C. J. Crystal structure of Adenylylsulfate reductase from Desulfovibrio gigas suggests a potential self-regulation mechanism involving the C terminus of the beta-subunit.	*J. Bacteriol*, *191*(24), 7597–7608. (2009).	3.49	31
36	**Jeyakanthan, J.,** Thamotharan, S., Velmurugan, D., Rao, V. S., Nagarajan, S., Shinkai, A., Kuramitsu, S., & Yokoyama, S. New structural insights and molecular-modelling studies of 4-methyl-5-beta-hydroxyethylthiazole kinase from Pyrococcus horikoshii OT3 (PhThiK).	*Acta Crystallogr Sect F Struct Biol Cryst Commun*.*65*(Pt 10), 978–986. (2009).	1.056	4
35	Lee, J. J., Thamotharan, S., **Jeyakanthan, J.,** Bansal, R., & Yadav, R. Structure Determination on Asthmatic Drugs by Synchrotron Powder Diffraction.	*Acta Cryst* (Vol. 65, pp. S324-S324 (2009, January).	2.290	Nil
34	Chen, L. C., Huang, S. C., Chuankhayan, P., Chen, C. D., Huang, Y. C., **Jeyakanthan, J.,** Pang, H. F., Men, L. C., Chen, Y. C., Wang, Y. K., Liu, M. Y., Wu, T. K., & Chen, C. J. Purification, crystallization and preliminary X-ray crystallographic analysis of xylose reductase from Candida tropicalis.	*Acta Crystallogr Sect F Struct Biol Cryst Commun*. *65*(Pt 4), 419–421. (2009).	1.056	7
33	Lee, J. J., Thamotharan, S., **Jeyakanthan, J.,** Bansal, R., & Yadav, R. Structure Determination on Asthmatic Drugs by Synchrotron Powder Diffraction.	*Acta Cryst.* (Vol. 65, pp. S324-S324)., . (2009, January).	2.290	Nil
32	**Jeyakanthan, J.,** Rangarajan, S., Mridula, P., Kanaujia, S. P., Shiro, Y., Kuramitsu, S., Yokoyama, S., & Sekar, K. Observation of a calcium-binding site in the gamma-class carbonic anhydrase from Pyrococcus horikoshii.	*Acta Crystallogr D Biol Crystallogr*..*64*(Pt 10), 1012–1019. (2008).	7.652	60
31	Mizuno, H., Mal, T. K., Wälchli, M., Kikuchi, A., Fukano, T., Ando, R., **Jeyakanthan, J.,** Taka, J., Shiro, Y., Ikura, M., & Miyawaki, A. Light-dependent regulation of structural flexibility in a photochromic fluorescent protein.	*Proc Natl Acad Sci U S A*.*105*(27), 9227–9232. (2008).	11.205	173
30	Rangarajan, S., **Jeyakanthan, J.,** Mridula, P., Sakamoto, K., Kitamura, Y., Agari, Y., Shinkai, A., Ebihara, A., Kuramitsu, S., Yokoyama, S., & Sekar, K. Crystallization and preliminary crystallographic studies of L30e, a ribosomal protein from Methanocaldococcus jannaschii (MJ1044).	*Acta Crystallogr Sect F Struct Biol Cryst Commun*. *64*(Pt 2), 102–104. (2008).	1.056	7

29	Gowri Shankar, B. A., Sarani, R., Michael, D., Mridula, P., Ranjani, C. V., Sowmiya, G., Vasundhar, B., Sudha, P., **Jeyakanthan, J.,** Velmurugan, D., & Sekar, K. Ion pairs in non-redundant protein structures.	*J Biosci*.*32*(4), 693–704.(2007).	1.826	18
28	Kanaujia, S. P., Ranjani, C. V., **Jeyakanthan, J.,** Nishida, M., Kitamura, Y., Baba, S., Ebihara, A., Shimizu, N., Nakagawa, N., Shinkai, A., Yamamoto, M., Kuramitsu, S., Shiro, Y., Sekar, K., & Yokoyama, S. Preliminary X-ray crystallographic study of glucose dehydrogenase from Thermus thermophilus HB8.	*Acta Crystallogr Sect F Struct Biol Cryst Commun.63*(Pt 5), 446–448.(2007).	1.056	3
27	Kanaujia, S. P., Ranjani, C. V., **Jeyakanthan, J.,** Baba, S., Chen, L., Liu, Z. J., Wang, B. C., Nishida, M., Ebihara, A., Shinkai, A., Kuramitsu, S., Shiro, Y., Sekar, K., & Yokoyama, S. Crystallization and preliminary crystallographic analysis of molybdenum-cofactor biosynthesis protein C from Thermus thermophilus.	*Acta Crystallogr Sect F Struct Biol Cryst Commun*. *63*(Pt 1), 27–29.(2007).	1.056	6
26	Kanaujia, S. P., Ranjani, C. V., **Jeyakanthan, J.,** Baba, S., Kuroishi, C., Ebihara, A., Shinkai, A., Kuramitsu, S., Shiro, Y., Sekar, K., & Yokoyama, S. Cloning, expression, purification, crystallization and preliminary X-ray crystallographic study of DHNA synthetase from Geobacillus kaustophilus.	*Acta Crystallogr Sect F Struct Biol Cryst Commun.63*(Pt 2), 103–105.(2007).	1.056	7
25	Kanaujia, S. P., Ranjani, C. V., **Jeyakanthan, J.,** Ohmori, M., Agari, K., Kitamura, Y., Baba, S., Ebihara, A., Shinkai, A., Kuramitsu, S., Shiro, Y., Sekar, K., & Yokoyama, S. Cloning, expression, purification, crystallization and preliminary X-ray crystallographic study of molybdopterin synthase from Thermus thermophilus HB8.	*Acta Crystallogr Sect F Struct Biol Cryst Commun.63*(Pt 4), 324–326.(2007).	1.056	3
24	Sekar, K., Gayathri, D., Velmurugan, D., **Jeyakanthan, J.,** Yamane, T., Poi, M. J., & Tsai, M. D. Third calcium ion found in an inhibitor-bound phospholipase A2.	*Acta Crystallogr D Biol Crystallogr*. *62* (Pt 4), 392–397.(2006).	7.652	4
23	**Jeyakanthan, J.,** Inagaki, E., Kuroishi, C., & Tahirov, T. H. Structure of PIN-domain protein PH0500 from Pyrococcus horikoshii.	*Acta Crystallogr Sect F Struct Biol Cryst Commun*. *61*(Pt 5), 463–468.(2005).	1.056	20
22	Taka, J., Ogasahara, K., **Jeyakanthan, J.,** Kunishima, N., Kuroishi, C., Sugahara, M., Yokoyama, S., & Yutani, K. Stabilization due to dimer formation of phosphoribosyl anthranilate isomerase from Thermus thermophilus HB8: X-ray Analysis and DSC experiments.	*J Biochem*. *137*(5), 569–578.(2005).	3.387	14
21	**Jeyakanthan, J.,** Taka, J., Kikuchi, A., Kuroishi, C., Yutani, K., & Shiro, Y. Purification, crystallization and preliminary X-ray crystallographic study of the L-fuculose-1-phosphate aldolase (FucA) from Thermus thermophilus HB8.	*Acta Crystallogr Sect F Struct Biol Cryst Commun.61*(Pt 12), 1075–1077.(2005).	1.056	11

20	**Jeyakanthan, J.,** Kikuchi, A., Taka, J., Karasawa, S., Miyawaki, A., & Shiro, Y. Crystal Structure of Novel Cyan-emitting Fluorescent Protein from Acropara Stony Coral..	*Acta. Cryst.* Vol. 61, pp. C263-C263. (2005, January).	2.290	Nil
19	Saikrishnan, K., Manjunath, G. P., Singh, P., **Jeyakanthan, J.,** Dauter, Z., Sekar, K., Muniyappa, K., & Vijayan, M. Structure of Mycobacterium smegmatis single-stranded DNA-binding protein and a comparative study involving homologus SSBs: biological implications of structural plasticity and variability in quaternary association.	*Acta Crystallogr D Biol Crystallogr. 61*(Pt 8), 1140–1148.(2005).	7.652	43
18	Saikrishnan, K., **Jeyakanthan, J.,** Venkatesh, J., Acharya, N., Sekar, K., Varshney, U., & Vijayan, M. Structure of Mycobacterium tuberculosis single-stranded DNA-binding protein. Variability in quaternary structure and its implications.	*J Mol Biol*. *331*(2), 385–393.(2003).	5.469	77
17	Rajakannan, V., Yogavel, M., Poi, M. J., Jeyaprakash, A. A., **Jeyakanthan, J.,** Velmurugan, D., Tsai, M. D., & Sekar, K. Observation of additional calcium ion in the crystal structure of the triple mutant K56,120,121M of bovine pancreatic phospholipase A2.	*J. Mol. Biol*. *324*(4), 755–762.(2002).	5.469	20
16	Hussain, A. S., Shanthi, V., Sheik, S. S., **Jeyakanthan, J.,** Selvarani, P., & Sekar, K. PDB Goodies--a web-based GUI to manipulate the Protein Data Bank file.	*Acta CrystD Biol Crystallogr.58*(Pt 8), 1385–1386.(2002).	7.652	25
15	Vijayan, M., **Jeyakanthan, J.,** Venkatesh, J., Acharya, N., Sekar, K., Varshney, U., & Saikrishnan, K. The crystal structure of the single-stranded DNA-binding protein from Mycobacterium tuberculosis.	*Acta Cryst. A*, *58*(Suppl.), c275-c275. (2002).	2.290	Nil
14	Saikrishnan, K., **Jeyakanthan, J.,** Venkatesh, J., Acharya, N., Purnapatre, K., Sekar, K., Varshney, U., & Vijayan, M. Crystallization and preliminary X-ray studies of the single-stranded DNA-binding protein from Mycobacterium tuberculosis.	*Acta Cryst D Biol Crystallogr..58*(Pt 2), 327–329.(2002).	7.652	9
13	Kanthimathi, M., Jebanesan, D., Nair, B. U., &**Jeyakanthan, J.** Effect of molecular association and reactivity on substitution in chromium (III)–salprn complexes.	*Transit Metal Chem*, , *27*(8), 895-901.(2002).	1.588	13
12	**Jeyakanthan, J.,** Yogavel, M., Joseph Rajan, T., Velmurugan, D., & Sekar, K. Crystal and molecular structure of an acridinedione.	*Crys Res Tech.37*(9), 1029-1037.(2002).	1.639	8
11	**Jeyakanthan, J.,** Velmurugan, D., Selvi, S., & Perumal, P. T. 1-(2,4-Dinitrophenyl)-3-(2-hydroxy-5-methylphenyl) pyrazole-4-carboxaldehyde.	*Acta. Cryst. 57*(5), o474-o476.(2001).	0.517	4
10	Kanthimathi, M., Nair, B. U., Ramasami, T., **Jeyakanthan, J.,** & Velmurugan, D. Synthesis, crystal structure and reactivity of trans-diaquo N, N′-ethylenebis-(3-methoxysalicylideneiminato) chromium (III).	*Transit Metal Chem*. *25*(2), 145-149.(2000).	1.588	10

9	**Jeyakanthan, J.,** Shanmuga Sundara Raj, S., Velmurugan, D., Fun, H. K., Rajan, T. J., & Ramakrishnan, V. T. Two benzoylaminoacridinedione derivatives.	*Acta. Cryst.* *56*(9), 1109-1112..(2000).	1.172	11
8	**Jeyakanthan, J.,** Velmurugan, D., Selvi, S., & Perumal, P. T. 1-(2,4-Dinitrophenyl)-3-(2-hydroxyphenyl)-4-methyl-1H-pyrazole.	*Acta. Cryst.* *55*(11), 1926-1928(1999).	1.172	5
7	Shanmuga Sundara Raj, S., **Jeyakanthan, J.,** Selvi, S., Velmurugan, D., Fun, H. K., & Perumal, P. T. 1-(2, 4-Dinitrophenyl)-3-(2-hydroxyphenyl)-1H-pyrazole-4-carbaldehyde.	*Acta. Cryst.* *55*(10), 1667-1669.(1999).	1.172	4
6	**Jeyakanthan, J.,** & Velmurugan, D. The Crystal and Molecular Structure of 1, 8-Dioxo-9-(o-nitrophenyl)-1, 2, 3, 4, 5, 6, 7, 8-octahydroxanthene.	*Crys ResTech*, *34*(10), 1339-1344.(1999).	1.639	10
5	**Jeyakanthan, J.,** Shanmuga Sundara Raj, S., Velmurugan, D., Fun, H. K., & Murugan, P. Two tetramethylxanthenediones.	*Acta Cryst.* *55*(9), 1515-1517.(1999).	1.172	7
4	**Jeyakanthan, J.,** Velmurugan, D., Josephrajan, T. M., & Ramakrishnan, V. T. Water mediated hydrogen bonding network in an acridine carboxamide derivative.	Acta. Cryst. Vol. 55, pp. 384-384. (1999, January).	2.290	Nil
3	**Jeyakanthan, J.,** Velmurugan, D., Panneerselvam, K., Soriano-Garcia, M., Perumal, S., & Chandrasekaran, R. Three diphenyl sulfones.	*Acta. Cryst.* *54*(5), 630-633.(1998).	1.172	6
2	**J. Jeyakanthan** & D. Velmurugan. 4-Chlorophyenyl 2, 6-DimethylphenylSulfone.	*Acta. Cryst.* *C*53, PP: 1344-1345, 1997.	1.172	2
1	**Jeyakanthan, J.,** Saravanan, R., & Mohanlal, S. K. Temperature dependence of core and valence thermal vibrations in germanium.	*Physica Status Solidi* (b. *190*(2), 415-419.(1995).	1.710	Nil

CONTRIBUTION IN BOOK/ CHAPTERS – 21

S. No	Particulars	Publisher and Year
1.	P. Shanmugavel & **J. Jeyakanthan.** Molecular Interactions (ISBN: 8170195116)	Today & Tomorrows Printers and Publishers, 2015
2.	Nachiappan M, Guru R Rao, Richard M, Saritha P, Amala M, Prabhu D, Rajamanikandan S, Chitra JP & **Jeyakanthan J**. Experimental and Computational Methods to Determine Protein Structure and Stability. Frontiers in Protein Structure, Function, and Dynamics (ISBN 978-981-15-5529-9) Pages: 23 - 55.	Springer, USA 2020
3.	Jayashree B, Prajisha J, Raghu R & **Jeyakanthan J.** Synergistic Effects of Hydration Sites in Protein Stability: A Theoretical Water Thermodynamics Approach. Frontiers in Protein Structure, Function, and Dynamics. (ISBN 978-981-15-5529-9) Pages: 187 – 212.	Springer, USA 2020
4.	Balajee R, Saravanan M, **Jeyakanthan J.** Prospects of Covalent approaches in Drug Discovery: An Overview.	Scrivener, USA 2020

5.	Mutharasappan Nachiappan, Ravi Guru Raj Rao, Mariadasse Richard, Dhamodharan Prabhu, Sundarraj Rajamanikandan, Jeyaraj Pandian Chitra and **Jeyaraman Jeyakanthan**. 3D Structural Determination of Macromolecules using X-ray Crystallography Methods. Molecular Docking for Computer-Aided Drug Design.	Elsevier, Netherlands 2020
6.	K. Mohanrasu, R. Guru Raj Rao, M. Sudhakar, Rathinam Raja, **J. Jeyakanthan**, A. Arun. Marine Microbial Pharmacognosy: Prospects and Perspectives. Marine Niche: Applications in Pharmaceutical Sciences	Springer Nature, USA 2020
7.	K. Mohanrasu, R. Guru Raj Rao, V. Ananthi, G. Sivaprakash, G.H. Dinesh, Angelin Swetha, A. Arun & **Jeyakanthan J**. Microbial Bio-Based Polymer Nanocomposite for Food Industry Applications.	Elsevier, Netherlands 2020
8.	Chitra J, Rajendren J, Jeykanthan B, Gopalsamy J, Jeba mercy N, Manikandan, Prasanna Kumari N.K. & **Jeyakanthan J.** Microbes and their products as novel therapeutics in medical applications**,** Bio prospecting of Microbial Diversity. 0020-0255	Elsevier, Netherlands 2020
9.	Mohanrasu K, Guru Raj Rao R, Sivaprakash G, Angelin Swetha T, Abhispa Bora, Balaji P, Arun A. & **Jeyakanthan J.** Bioplastics from Microbial and Agricultural Biomass. Editor: Inamuddin. Applications of Biodegradable Materials and Bioplastics.	John Wiley & Sons, Inc., USA 2021
10.	N. Arul murugan, Chitra Jeyraj Pandian, Jeba Mercy Jeayseelan, S. Muneeswaran, K. Saranraj, K. Muruga Poopathi Raja and **J Jeyaraman.** Computaional Development of Alzheimer's Therapeutics and Diagnostics.	Royal socity of Chemistry, UK 2022
11.	Madhumathi Sanjeevi, Prajna N Hebbar, Natarajan Aiswarya, S Rashmi, Chandrashekar Narayanan Rahul, Ajitha Mohan, **J. Jeyakanthan**, Kanagaraj Sekar. Methods and applications of machine learning in structure-based drug discovery, Advances in Protein Molecular and Structural Biology Methods.	Academic Press, USA 2022
12.	Vijay Nirusimhan, Daniel Andrew Gideon, Abhinav Parashar, Sangavi Jeyachandran, **Jeyakanthan Jeyaraman**, Gowthamkumar Subbaraj and Langeswaran Kulanthaivel. Structural Modelling of *Drosophila melanogaster* Gut Cytochrome P450s and Docking Comparison of fruit fly gut and human cytochrome p450s.	Bentham Science, UAE 2022
13.	Jesucastin Edward, Karthik Sundarsha, **J. Jeyakanthan**, A. Sherlin Rosita, Daniel A. Gideon. Efficacy of synthetic organic molecular inhibitors of TRAF2 and NCK interacting kinase (TNIK) against colorectal cancer	Springer Nature, Singapore 2022
14.	**Jeyaraman Jeyakanthan**, Chitra Jeyraj Pandian, Jeba Mercy Jeayseelan, Sundarraj Rajamanikandan, Dhamodharan prabhu, Ravi Guru Raj Rao, Mutharasappan Nachiappan. An integrative approach to explore potent therapeutic protein targets in multidrug resistant nosocomaial pathogen *Acinetobacter baumannii.* Therapeutic protein targets for drug dicovery and clinical evalution: Bio-crystallography and drug design.	World scientific, 2022

15.	Chitra Jeyraj Pandian, Rajendren Sironmani, **Jeyakanthan Jeyaraman,** Gopal Samy Balakrishnan. Development in Waste Water Treatment Research and Processes. Application of dairy sludge derived products for removal of pollutants from the insustrial effluents: A way to sustainable disposal.	Elsevier, Netherlands 2022
16.	N. Arul murugan, S. Muneeswaran, K. Saranraj, K. Muruga Poopathi Raja and **J Jeyakanthan** Computational Development of Alzheimer's Therapeutics and Diagnostics.	Royal socity of Chemistry, UK, 2022.
17.	Chitra J and **Jeyakanthan J.** Implications of Immuno-oncology in Immunodiagnostics and Immunotherapy. ISBN: 978-93-5528-175-3.	MJP Publication 2023
18.	Nagarajan, H., Ranganathan, S., **Jeyaraman, J.,** & Chitipothu, S. Antimicrobial Peptides and Antibacterial Antibodies for the Elimination of ESKAPE Pathogens. In ESKAPE Pathogens: Detection, Mechanisms and Treatment Strategies (pp. 435-462).	Springer Nature Singapore 2024
19.	Pandian, C. J., Rajendren, S. M., & **Jeyaraman, J.** Probiogenomics and Genome Annotation in Bifidobacteria and Lactobacilli. In *Industrial Microbiology and Biotechnology: An Insight into Current Trends* (pp. 465-491).	Singapore: Springer Nature Singapore 2024
20.	Maharaja M. S, Pradeep Kumar. S, **Jeyakanthan** J & Gamathinayagam S Optimizing Smart Hospitals with IoMT A Deep Dive into the Next-Generation Paradigm for Digital Healthcare Page No: 15-25, eBook ISBN: 9781003476344	Taylor & Francis Group 2025
21.	Maharaja Muthuvairam Subbulakshmi, Manikandan Jayaraman, **Jeyakanthan Jeyaraman** Transforming gastrointestinal tract cancer with applications and advancements of artificial intelligence and machine learning: A next-generation patient care. Page No: 193-208, eBook ISBN: 978-0-443-44121-9	Elsevier Publications 2026

GENBANK DEPOSITIONS – 26

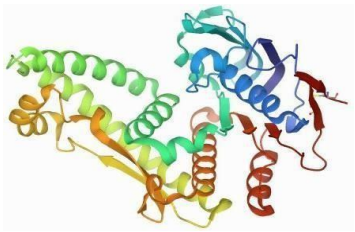
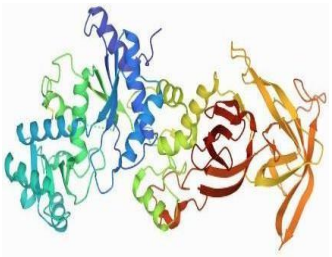
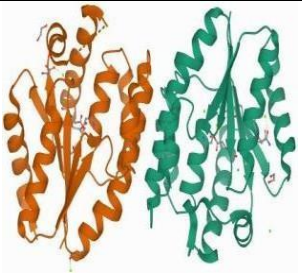
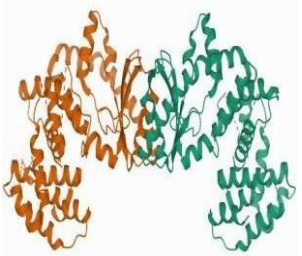
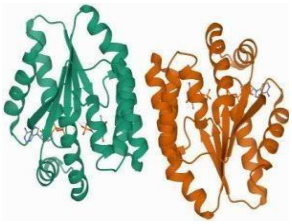
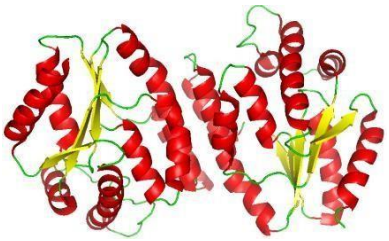
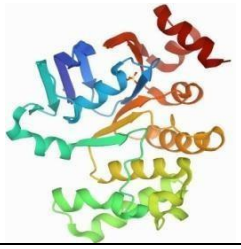
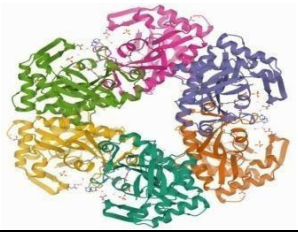
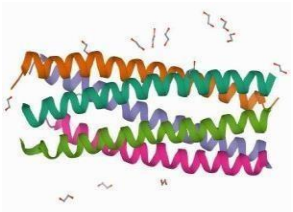
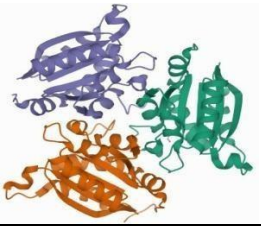
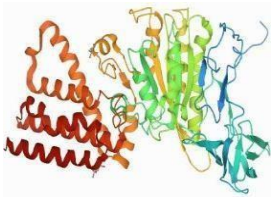
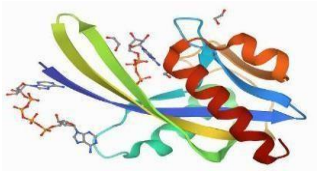
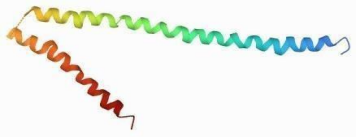
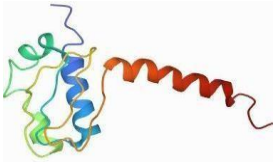
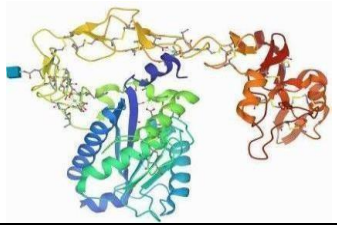
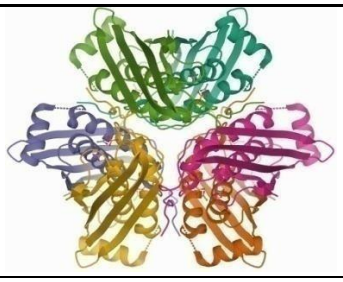
S. No	Accession No.	Details
1.	MN749550.1	*Staphylococcus aureus* strain U190175 16S ribosomal RNA gene, partial sequence
2.	MN749549.1	*Staphylococcus aureus* strain U190172 16S ribosomal RNA gene, partial sequence
3.	MN749548.1	*Shewanella putrefaciens* strain B190208 16S ribosomal RNA gene, partial sequence
4.	MN749541.1	*Proteus vulgaris* strain P190036 16S ribosomal RNA gene, partial sequence
5.	MN749537.1	*Staphylococcus aureus* strain P190067 16S ribosomal RNA gene, partial sequence
6.	MN749534.1	*Staphylococcus aureus* strain O190017 16S ribosomal RNA gene, partial sequence

7.	MN749533.1	*Enterococcus faecalis* strain P190052 16S ribosomal RNA gene, partial sequence
8.	MN749520.1	*Enterococcus faecalis* strain P190052 16S ribosomal RNA gene, partial sequence
9.	MN749519.1	*Acinetobacter baumannii* strain O190037 16S ribosomal RNA gene, partial sequence
10.	MN744697.1	*Morganella morganii* strain ab1 16S ribosomal RNA gene, partial sequence
11.	MN749522.1	*Citrobacter freundii* strain U190042 16S ribosomal RNA gene, partial sequence
12.	MK820067.1	*Impatiens leschenaultii* voucher ALUH_18 maturase K (matK) gene, partial cds; chloroplast
13.	MK820068.1	*Impatiens leschenaultii* voucher ALUH_18 ribulose-1,5-bisphosphate carboxylase/oxygenase large subunit (rbcL) gene, partial cds; chloroplast
14.	MK759659.1	*Drosera indica* voucher ALUH_17 ribulose-1,5-bisphosphate carboxylase/oxygenase large subunit gene, partial cds; chloroplast
15.	MK759658.1	*Drosera burmannii* voucher ALUH_16 ribulose-1,5-bisphosphate carboxylase/oxygenase large subunit gene, partial cds; chloroplast
16.	MT262990.1	*Shigella sonnei* strain O190087 16S ribosomal RNA gene, partial sequence
17.	MT262927.1	*Mycolicibacterium senegalense* strain P190172 16S ribosomal RNA gene, partial sequence
18.	MT261888.1	*Klebsiella sp.* strain P190051 16S ribosomal RNA gene, partial sequence
19.	MT261871.1	*Enterococcus faecalis* strain P190052 16S ribosomal RNA gene, partial sequence
20.	KX022944.1	*Coprinus sterquilinus* isolate JJAA3 internal transcribed spacer 1, partial sequence; 5.8S ribosomal RNA gene and internal transcribed spacer 2, complete sequence; and 28S ribosomal RNA gene, partial sequence
21.	KX022943.1	*Psathyrella candolleana* isolate JJAA2 internal transcribed spacer 1, partial sequence; 5.8S ribosomal RNA gene and internal transcribed spacer 2, complete sequence; and 28S ribosomal RNA gene, partial sequence
22.	KX022942.1	*Psathyrella candolleana* isolate JJAA1 internal transcribed spacer 1, partial sequence; 5.8S ribosomal RNA gene and internal transcribed spacer 2, complete sequence; and 28S ribosomal RNA gene, partial sequence
23.	FJ804147.1	*Candida tropicalis* NAD(P)H-dependent xylose reductase (xyl1) gene, complete cds
24.	JJSBBCNF_01	*Nocardia farcinica* JJSBBCNF_0, Whole genome sequence
25.	GCA_027920125.1	*Acinetobacter baumannii* JJAB01, Whole genome sequence
26.	GCF_027891115.1	*Pseudomonas aeruginosa* JJPA01, Whole genome sequence

PROTEIN DATA BANK CONTRIBUTIONS (PDB's) - More than 153 structures

Protein Data Bank ID: 5ZDK, 5ZDL, 5ZDH ..... etc.,

(**http://www.rcsb.org/pdb/home/home.do**)

			
IJBIOMAC, 2020 **PDB ID - 5ZWU**	**IJBIOMAC, 2019** **PDB ID - 5ZDO**	**Acta D, 2018** **PDB ID - 5XT8**	**FEBS Lett, 2017** **PDB ID - 4S35**
			
FEBS J, 2017 **PDB ID - 2PBR**	**J. Str. Bio, 2017** **PDB ID - 2PLR**	**J. Str. Bio, 2015** **PDB ID - 4O7N**	**J. Str. Bio, 2015** **PDB ID - 4UOO**
			
IJBIOMAC, 2013 **PDB ID - 3U54**	**Acta D, 2012** **PDB ID - 3MIW**	**Acta F, 2011** **PDB ID - 3MCH**	**JMB 2011** **PDB ID - 3P20**
			
Acta D, 2010 **PDB ID - 3I7U**	**Plos, 2010** **PDB ID - 3HGF**	**Biochemistry, 2010** **PDB ID - 2PKP**	**J. Bioe. Biom, 2010** **PDB ID - 3LG8**
			
J. Str. Bio, 2010 **PDB ID - 3K7l**	**Acta D, 2010** **PDB ID - 3JQJ**	**J. Bact., 2009** **PDB ID - 3GYX**	**PNAS, 2008** **PDB ID - 2Z1O**

JOURNAL EDITOR/EDITORIAL MEMBER/ REVIEWER

EDITOR/EDITORIAL MEMBER	
PloS ONE	Current Bioinformatics
Frontiers in Physiology	Frontiers in Molecular Biosciences
Frontiers in Physics	Frontiers in Genetics
Combinatorial Chemistry & High Throughput Screening	
REVIEWER	
Acta Crystallographica Sections	ACS Omega
Computational Biology and Chemistry	Gene
Indian Journal of Biochemistry & Biophysics	International Journal of Bioinformatics Research
International Journal of Bioinformatics Research and Applications	Interdisciplinary Sciences
Journal of Molecular Graphics and Modelling	Journal of Biomolecular Structure & Dynamics
Letters in Drug Design & Discovery	Microbial Pathogenesis
Molecular BioSystems	Molecular Biology Reports
Medicinal Chemistry Research	Progress in Biophysics and Molecular Biology, Etc

EXTERNAL THESIS EXAMNIER / EVALUATED – 59

S. No	Name of the candidate	Title	Degree Awarding Institution	Year
59.	Poorvi Vishwakarma	Structural and Functional Investigation of Glycoside Hydrolase	AIIMS, New Delhi	2026
58.	Chevula Kishan	DESIGN, SYNTHESIS, BIOLOGICAL AND COMPUTATIONAL EVALUATION OF PYRAZOLE TETHERED WITH TRIAZOLES, 4H-CHROMENE, 1,4-DIHYDROPYRIDINE, THIAZOLIDINEDIONE AND RHODANINE	Osmania University	2025
57.	Menaka Priya B	Synergistic Effects of Chamaecostus cuspidatus Leaf Extract and p-Coumaric Acid on Endothelial Dysfunction in Type 2 Diabetes Induced by High-Fat Diet and Low-Dose Streptozotocin: An In-Silico, In-Vitro and InVivo Perspective	Vellore Institute of Technology (VIT), Vellore	2025
56	Adhish Mazumder	Investigating the role of taurine and vitamin b12 in ameliorating the effects of homocysteine-induced osteoporotic	Vellore Institute of Technology (VIT), Vellore	2025

		conditions using *in-silico* and *in-vitro* techniques		
55.	Jyotilipsa Mohanty	Understanding the trafficking and inhibition mechanisms of plant viruses using *in silico* approaches with Sesbania Mosaic Virus as a model system	Pondicherry University	2025
54	Muralikrishna V	Synthesis, biological evaluation and molecular docking studies on novel heterocycles containing meldrum's acid -7-azaindole-1,2,3-triazoles, 7-azaindoleimidazole- 1,2,3-triazoles, pyrimidine-indole- 4*h*-chromenes and pyrimidine-indole-1,4-dihydropyridines	Osmania University	2025
53.	Patnam Nagesh	Molecular Modellling Studies, Synthesis and activity studies based on metabolic pathways for diabetes mellitus	Osmania University	2025
52.	Farah Naz	Structural and Functional Studies of FtsZ cell division protein as a potential drug target against *Salmonella Typhi*	AIIMS, New Delhi	2024
51	Anuja Jain	Gene Expression meta-analysis, lead generation and cellular specificity prediction for Toll like receptors	Jawaharlal Nehru University	2024
50	Satish Tiwari	Targeting an essential metabolic pathway of Mycobacterium tuberculosis to design new anti-TB compounds	National Institute for Immunology	2023
49.	Kimona Kisten	Strategic application of in silico drug discovery approaches to discover novel TB drugs	University of Kwazulu, Natal college of Health Sciences	2023
48	Suchitra Surendran	Computer assisted drug design for *Mycobacterium tuberculosis*	University of Kerala	2023
47	Koyyada praveena	Target identification and multi-target drug designing for *Mycobacterium tuberculosis* H37Rv active infection by Systems Biology approach	University of Hyderabad	2023
46	Mohammed Ahmad	Structural and biochemical studies of enolase from *Mycobacterium tuberculosis*	Jawaharlal Nehru University	2022
45	Rajdeep kaur	Computational studies of inhibitors against Aβ aggregation and β-secretase (BACE1) enzyme in Alzheimer's disease	Department of chemistry, Sri Guru Granth Sahib world university	2022
44	Sambit Dalui	Structural and Functional Characterization of Testis-specific Y encoded-like protein 5: a novel member of NAP histone chaperone superfamily	Jadavpur university	2022
43	Anirban Dasgupta	Molecular Characterization of human histone H2BK120 Ubiquitin Ligase UBR7	Jadavpur university	2022

42.	Indu	Structural and biochemical studies of a membrane protein Rv2903c from *Mycobacterium tuberculosis*	Jawaharlal Nehru University	2022
41.	Shobhan Kuila	Structural and functional studies of chloride intracellular ion channels	Jawaharlal Nehru University	2022
40.	Anirban Dasgupta	Molecular Characterization of human histone H2BK120 Ubiquitin Ligase UBR7	Jadavpur university	2022
39.	Suresh Palanivel	Evaluation of Cytotoxic Effects and Underlying Mechanisms of Phenolic Compounds on Breast Cancer Cell Lines	Tampere University Finland	2022
38.	M. Mathavan	Comprehensive analysis of Zaire ebolavirus-Human Interaction for Understanding of Disease Mechanism and Drug Re-purposing	Pondicherry University	2021
37.	K. Muthuvel Prasath	Development of novel structure based methods, online database and web servers to predict Superfamily for the Annotation of Twilight Zone Protein Sequences	Bharathidasan University	2021
36.	Anam Ashraf	Dissecting the mechanistic properties of HisI (Rv1606) and the dynamics of Histidine Biosynthesis Enzymes in *in-vivo* infection of *Mycobacterium tuberculosis*	National Institute of Immunology	2021
35.	M. K. Hema	Synthesis, Structural and Biological Studies of Metal-Oxygen Coordinated Complexes	University of Mysore	2020
34.	Rama Krishna Munnaluri	*In silico* strategies in developing new inhibitors against molecular targets in HIV and *Mycobacterium tuberculosis*	Osmania University	2019
33.	Dr. Vineet Mohan Samal	Biophysical Characterisation of ATP Sulfurylase protein from *Mycobacterium tuberculosis*	All India Institute of Medical Sciences	2019
32.	Ballu Srilata	Computer Aided Drug Design, Synthesis and Biological Evaluation of Anti-bacterial Agents against Wild and Resistant Strains of *Staphylococcus aureus*	Osmania University	2019
31.	K. N. Chethan Prathap	Crystal and Molecular Studies of Medicinally Important Heterocyclic Compounds	University of Mysore	2018
30.	S.Chandrasekar	Insights on binding mode of ruthenium based anticancer pro-drug like compound with serum albumin and “The catalyst of oxidative protein folding”: A structural prospective	Pondicherry University	2018
29.	Satyaprakash Yadav	Structural and functional of Proliferating Cell Nuclear Antigen from *Leishmania donovani*	All India Institute of Medical Sciences	2018

28.	Ankita Pan	Structural and Functional Characterization of Flavivirus Non-Structural Protein3 (NS3) in solution and atomic and enzymatic insights of vancomycin resistant *Enterococcus faecalis* (V583) alkyl hydroperoxide subunit C	Nanyang Technological University	2018
27	P. Moorthi	Understanding key events involved in Age dependent Brain region specific alterations of alzheimer's diseaese proteins that influence neurodegeneration and dementia: Neuroprotective Role	Bharathidasan University	2018
26.	Arvind Kumar	Structural and Mechanistic Insights into Mycothiol disulfide reuctase, Mycoredoxin-1 and peroxiredoxin alkyl hydroperoxide subunit E of *M. tuberculosis*	Nanyang Technological University	2017
25	P. Perumal	Structural and Bioinformatics Characterization of Quorum Sensing Proteins from the outer membrane Enzymes of *S.typhi*	Bharathiyar University	2017
24.	V. Rajni Swamy	Structure investigation of some novel compounds	Madurai Kamaraj University	2017
23.	Nivedita Rai	Dynamics of multitasking DegP and the role of HpHtrA as a therapeutic target: A computational approach on HtrA family Proteins	Pondicherry University	2017
22.	M. Ajitha	Novel algorithms to predict the structure and functions of uncharacterised proteins	Kalasalingam University	2017
21.	Manish Kumar Thakur	Structural and Functional Studies on PTK6, A kinase involved in cancer	University of Mysore	2017
20.	Hiral Murawala	Evaluation of protein Expression pattern during vertebrate appendage regeneration	Maharaja Sayajirao, University of Baroda	2017
19.	T. Arun Kumar	Studies on Laccase production from Pseudomonas species and its application in degradation of azo enzymes	Sathyabama University	2017
18.	B. Sai Krishna	Insilico Drug design and synthesis of potential antimalarial agents	University college of science	2016
17.	Ms. Jemmy Christy. H	Immunoinformatics approach for the study of HIV-1 isolated from Indian population	Sathyabama University	2016
16.	B.R. Anitha	Crystal and molecular structure studies of some chalcone derivatives in medicinal interests	University of Mysore	2016
15.	Enock Kiage Oirere	Isolation, Structural characterization and Anticancer potential of Bioactive Compounds from Alipina purpurata: An Invitro and Insilco Approach	Karpagam University	2016
14.	Kotapati Kasi Viswanath	Molecular Cloning, Functional Analysis and Structural Prediction of Lipoxygenase from Eleusine coracana seedlings	Pondicherry University	2016

13.	Lavanya P	Investigations on the role of Non-Conventional Hydrogen bonds and its impact on stability and specificity of b-lactamases and Penicillin Binding Protein	Vellore Institute of Technology	2016
12.	Divyani Paul	Characterisation of p73 and Insilico based Drug Design for stabilization of p53 mutants	All India Institute of Medical Sciences	2016
11.	M. Kannan	Ovarian Cancer regulation by ID1 and ARHI Proteins: A structural Perspective	Pondicherry University	2015
10.	S. Kalaiselvi	Elucidating the plausible mechanism for the adriamycin induced lipotoxicity leading to type2 diabetes, cardiomyopathy, and reproductive toxicity: A remedy through Costus pictus supplementation	Bharathidasan University	2015
9.	P. Manoj Kumar	Structural understanding of Protein Function in relation to prophage protein yage	Madurai kamaraj University	2014
8.	K. Bhargavi	New cancer therapeutics- Inhibitors for novel BCl2 mitochondrial protein to initiate apoptosis	Osmania University	2013
7.	L. Yamini	Computer aided drug design and synthesis of DHFR inhibitors	Osmania University	2013
6.	A. Maheswari	*In-silico* assessment of interrelationship between protein folding and protein stability	Bharathidasan University	2013
5.	V. Bhavani Prasad	Computational Analysis of Claudin1 in different pathological conditions: A molecular dynamics approach	Vellore Institute of Technology	2013
4.	C. Rani	In-vitro evaluation and In-silico analysis of Novel Drug leads and targets from sponge associated marine bacteria	Bharathidasan University	2012
3.	C.S. Vinobha	Comparative Analysis on Large Hydrophobic Residues and Small Hydrophobic Residues in different organisms	Bharathidasan University	2012
2.	R. Sathish Kumar	Studies on the effect of isolated and characterised phytochemical compounds of Enicostemma Littorale Blume on the cancer target	Bharathiyar University	2011
1.	K. Ganesan	Structure based in-silico tool development for the annotation of twilight zone protein sequences	Bharathidasan University	2011

CONFERENCE PRESENTATIONS: 230

Presentation in International Level events: 110
Presentation in National Level events: 120

INAUGURAL/VALEDICTORY ADDRESS DELIVERED: 36

S. No	Title of Conference/ Seminar/ Workshop etc.	Organizer, with Place	Date(s)	Role	National / International
1.	Biochemistry Exhibition BYOKEM "X" BIT	Sri Saradha Niketan College for Women, Amaravathipudur	September 09, 2012	Inaugural Address	N
2.	Karpagam University Annual Research Congress KUARC-2014	Department of Biochemistry and Bioinformatics Karpagam University Coimbatore	5th December, 2014	Keynote Speaker	N
3.	National Seminar on Biocheminformatics	Department of Bioinformatics, Bharathiar University, Coimbatore	February 26th – 27th, 2016	Inaugural Address	N
4.	International Workshop on Data Science and Analytics	Department of Computer Science, Alagappa University, Karaikudi	27th September, 2016	Felicitation address	I
5.	National Workshop on Computational Analysis of Molecular Data	School of Bio Sciences and Technology, VIT University, Vellore	17th November, 2016	Keynote Address	N
6.	Winter Schools Organized by National Centre of Excellence (MHRD)	Thiagarajar College, Madurai	21st November, 2016	Inaugural Address	N
7.	Recent Trends in Microbiology (RTM'2016)	Department of Microbiology, Alagappa University, Karaikudi	20th – 21st December, 2016	Inaugural address	I

8.	Two – Day Workshop on ICT Based Innovative Teaching Methods in Business Studies	Department of Commerce and International Business & Higher Education Innovation Cell, Alagappa University, Karaikudi	24th January, 2017	Felicitation address	N
9.	One day Training Program on "LATEX" – A Mathematical Document Preparation Tool	Department of Mathematics &University Business Collaboration Centre, Alagappa University, Karaikudi	10th February, 2017	Special Address	N
10.	Awareness Program on First Aid and Basic Life Support	Alagappa University Health Care Centre & Alagappa University College of Physical Education, Alagappa University, Karaikudi	10th February, 2017	Felicitation address	N
11.	International Conference on Mathematical Modeling and Computational Methods in Science and Engineering	Ramanujan Centre for Higher Mathematics & Department of Mathematics, Alagappa University, Karaikudi	22nd February, 2017	Felicitation address	I
12.	Two-day Workshop on Career Prospects & Developments in Computer Science	University Business Collaboration Centre & Dept. of Computer Science, Alagappa University, Karaikudi	27th February, 2017	Felicitation address	N

13.	Business Oriented Hands-on Training on Analytical Instrumentation (HI-BOAT)	Dept. of Physics & Business Collaboration Centre & Consultancy Cell, Alagappa University, Karaikudi	2nd March, 2017	Felicitation address	N
14.	Two day training Programme on "Campus Interview Skills"	Equal Opportunity and Placement cell, Alagappa University, Karaikudi	2nd March, 2017	Felicitation address	N
15.	Three Days Zonal Level Orientation Training Programme for YRC Volunteers and YRC Programme Officers	Alagappa University & Alagappa Chettiar College of Engineering and Technology	22nd March, 2017	Felicitation address	N
16.	National Conference on Futuristic Materials (NCFM-2017)	Department of Physics, Alagappa University, Karaikudi	27th March, 2017	Felicitation address	N
17.	Three Days Zonal Level Orientation Training Programme for YRC Volunteers and YRC Programme Officers	Youth Red Cross, Alagappa University & Alagappa Chettiar College of Engineering and Technology, Karaikudi	22nd March, 2017	Valedictory address	N
18.	Two-day training Programme on Campus Interview Skills	Equal Opportunity and Placement cell, Alagappa University, Karaikudi	02nd March, 2017	Felicitation address	N
19.	Business Oriented Hands-on Training on Analytical Instrumentation (HI-BOAT)	Dept. of Physics & Business Collaboration Centre & Consultancy Cell, Alagappa University, Karaikudi	02nd March, 2017	Felicitation address	N

20.	Two-day Workshop on Career Prospects & Developments in Computer Science	University Business Collaboration Centre & Dept. of Computer Science, Alagappa University, Karaikudi	27th February, 2017	Felicitation address	N
21.	UGC Sponsored One Day Orientation Programme on "Know Your Rights – Empower Yourself"	Department of History and Alagappa Institute of Skill Development, Alagappa University, Karaikudi	13th September, 2017	Valedictory address	N
22.	National Theme on University – Industry Interface 2017 (NTM U2I-2017)	Industry and Consultancy Cell & Department of Physics	20th September, 2017	Felicitation address	N
23.	World Animal Day Celebration	Department of Animal Health and Management	4th October, 2017	Thematic address	N
24.	Four Days National Workshop Cum Short Term Training Programme on Cultivation of Mushroom and Business Commercialization	Department of Botany and University Business Collaboration Centre	8th January, 2018	Felicitation address	N
25.	Arise Youth Empowerment Programme	National Service Scheme and Swami Vivekananda Centre for Higher Research and Education & Heartfulness Institute, Chennai (Karaikudi Centre)	12th January, 2018	Inaugural address	N
26.	2nd International Conference on Recent Trends in Microbiology (RTM - 2018)	Department of Microbiology, Alagappa University	12th January, 2018	Valedictory address	I

27.	Two-day orientation programme on Marketing Strategies for Business Excellence (MSBE-2018)	Department of Commerce and University Business Collaboration Centre	09th February, 2018	Felicitation address	N
28.	National Trends in Skill Informatics (NCRTI - 2018)	Alagappa Institute of Skill Development	20th March, 2018	Valedictory address	N
29.	National Conference on Conservation and Sustainable Development of Marine Resources (CASDOMAR – 2018	School of Marine Sciences, Department of Oceanography & Coastal Area Studies	22nd March, 2018	Inaugural address	N
30.	Idhayam Merit Excellence Awards-2018	Rotary Club of Karaikudi and Rotary Club of Virudhunagar	24th July, 2018	Motivational Address	N
31.	Inauguration of Life Science Association Bio Cogniza 2K18 &Herbal	Department of Biotechnology & Microbiology, Vidhyaa Giri College of Arts and Science, Puduvayal, Karaikudi	21st August, 2018	Inaugural Address	N
32.	1st two days National Workshop on "indigenous Cow Management and their Value-Added Products"	Department of Animal Health and Management, Alagappa University	18th December, 2018	Felicitation	N
33.	4th Batch of MBA (Logistics Management) Inauguration & Orientation Programme	Department of Logistics Management, Alagappa University	8th July, 2019	Felicitation Address	N
34.	World Habitat Day	Department of Botany, Alagappa University	16th October, 2019	Special Address	N
35.	Workshop on Cancer Therapy: "Translating Computational Insights into Clinical Oncology and Future	Department of Biomedical Science, Alagappa University	13th October, 2019	Felicitation Address	N

	Therapeutics”				
36.	Three Days Skill Training Workshop on Structural Bioinformatics and Computer Aided Drug Design (WSBCADD-2025)	Department of Bioinformatics, Alagappa University	23rd -25th October , 2025	Welcome Address	N

J. Jeyakanthan