

Dr. J. JEYAKANTHAN Professor and Head

### **Contact**

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## **Academic Qualifications:**

<b>Year of Passing</b>	Degree	University / Institute
2020-21	D.Sc (Submitted)	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
1991	B.Ed.	University of Madras
1989	B.Sc (Physics)	M. K. University

## **Teaching Experience: 12 Years**

Position	institute/University	Perioa
Professor and Head	Department of Bioinformatics	March 2010 – till date

### Research Experience: 29 Years

Position	Institute/University	Period
Professor and Head	Department of Bioinformatics	March 2010 – till date
Research Scientist	SPring-8, Japan	May 2007 – March 2010
Researcher	RIKEN Harima Institute, SPring-8, Japan	June 2003 – May 2007
PDF	Indian Institute of Science, Bangalore	January 2000 – May 2003
CSIR SRF-JRF	University of Madras, Chennai	June 1995 – December 1999

### **Additional Responsibilities**

- 1. 2022 -\*: Member, Project Monitoring Unit Academic Core Committee of RUSA 2.0
- 2. 2022-\*: Coordinator, DBT-Bioinformatics and Computational Biology Centre,
  Department of Bioinformatics
- 3. 2021-\*: Member, Learning Outcome Based Curriculum Frame Work (LOCF)
- 4. 2021-\*: Member, Guru Dakshata UGC Quality Mandates
- 5. 2021-\*: Member, Paramarsh UGC Quality Mandates
- 6. 2021-\*: Member, CARE/STRIDE UGC Quality Mandates
- 7. 2019-\*: Director, Alagappa University Ranking Cell (AURC)
- 8. 2019-\* : Director, Center for Internal Quality Assurance Committee, Directorate of Online Programmes
- 9. 2018 -\* : Member, Internal Quality Assurance Committee, Directorate of Distance Education (DDE)
- 10. 2018 -\*: Member, Sports Advisory Board
- 11. 2018 -\*: Coordinator, Tamil Nadu State University Rating Framework (TANSURF)
- 12. 2017 \*: Coordinator, DST-PURSE Program (Phase-II) All Science Departments
- 13. 2017 \*: Coordinator, DST-FIST Program (Level-I)
- 14. 2016 \*: Member, Research Advisory Committee (RAC)
- 15. 2016 \*: Academic staff, Anti-Ragging Committee
- 16. 2015 \* : Chairperson, School of Biological Sciences
- 17. 2013 \* : Coordinator, UGC Innovative Program (PG diploma)
- 18. 2010 \*: Member, Senate of Alagappa University
- 19. 2010 \*: Member, Website Maintenance Committee
- 20. 2010 -\* : Member, Standing Committee on Academic Affairs, Alagappa University

- 21. 2010 \*: Chairman, Board of Studies of Bioinformatics
- 22. 2010 -\*: Head of the Department, Department of Bioinformatics

### **Completed:**

- 23. 2019-19: Head in-charge, Department of Botany
- 24. 2019-19: Chairman, Board of Studies of Botany
- 25. 2018-19: Member, Finance Committee
- 26. 2018-19: Member, Governing Council for DDE
- 27. 2018-19: Member, Board of Governors, RUSA 2.0 (Representing Syndicate)
- 28. 2017-19: Coordinator, National Institutional Ranking Framework Cell
- 29. 2016-19: Member, Purchase Committee
- 30. 2016-19: Member, Syndicate of Alagappa University (Nominated by Governor of Tamil Nadu)
- 31. 2015–17: Director, Directorate of Collaborative Programmes
- 32. 2012 16: Director, Centre for International Relations
- 33. 2012 15: Member, Research Advisory Committee
- 34. 2012 13: Coordinator, Career Guidance & Counselling Cell
- 35. 2010 16: Member, Internal Quality Assurance Cell (IQAC)

#### **Areas of Research**

**Broad subject** : Structural Biology and Bio-Computing

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

#### **Current Research focus**

## Structural and Functional studies on vital drug targets

- ❖ Proteins from *Thermus thermophilus* HB8, *Pyrococcus horikoshii* OT3, *Aquifex aelicous* VF5, *Mycobacterium tuberculosis, Brugia malayi, Nocardia sps.* and ESKAPE pathogens.
- Computational screening of proteins responsible for life-threatening diseases such as TB, Filariasis, Cancer, Diabetes, Chikungunya, Dengue, Malaria and nosocomial infection

### > Development of Tools and databases

❖ Web based search engines for analyzing macromolecular interactions

## **Research Supervision / Guidance**

Progra	m of Study	Completed	Ongoing
Research	PDF	04	03
	Ph.D.	08	10
	M.Phil.	08	-

Project	PG	22	03
	UG / Others	08	02

## **Publications**

Interna	itional	Nati	Others	
Journals	Conferences	Journals	Conferences	Books / Chapters / Monographs / Manuals
176	88	01	146	12

Cumulative Impact Factor (as per JCR): 639.739

h-index : 25 i10 index : 63 Total Citations : 2232

# **Funded Research Projects**

# **Completed Projects**

S.	Agency	Per	iod	Project Title	Budget (Rs. In
No		From	To		lakhs)
1	DBT	2012	2015	Structural and Functional Analysisfrom <i>Thermus</i> thermophilus HB8	50.25
2	UGC	2012	2015	Structural and Functional Protein from Pyrococus horikoshii OT3	12.90
3	DBT	2012	2015	Structure Determination of and Identification of Potential Inhibitors	32.16
4	DBT	2013	2016	Structural and Functional <i>Pyrococcus horikoshii</i> OT3	77.00
5	DST	2013	2016	Structural and Functional Studies from Pyrococcus horikoshii OT3	48.98
6	UGC	2016	2018	Structural and Functional Stat2 Protein From <i>Homo Sapiens</i>	37.80
7	DBT	2015	2018	Development of Web Based Fatty acids and Buffers	13.81
8	DST- SERB	2016	2019	Identification of Potential Anti-Filiarial drug targeted enzymes Wbm0441, Wbm0042 from Wolbachia endosymbiont <i>Brugia malayi</i>	69.38
9	ICMR	2017	2020	Structural insights of SIRT from <i>Homo</i> sapiensdiabetes	33.34
10	DAE- BRNS	2018	2021	Design, Synthesis and <i>in vitro</i> activated kinase	30.33
11	DBT- Twin	2014	2017	Identification of novel drug of the pathogen (TWIN Program)	73.69
12	DBT- Twin	2010	2013	The use of biodiversity as a molecular targets of Tuberculosis	83.49

# **Ongoing Projects**

S.			Period Project Title		Budget (Rs.
No	Agency	From	To	Project Title	In lakhs)
1	DST INDO- TAIWAN	2020	2023	Structural and functional insights of potential anti-malarial drug targets of G6PD and 6PGD from <i>Plasmodium falciparum</i> (3D7)	73.72
2	TANSCHE	2021	2023	Structural and functional characterization of phospeotransacetylase (PTA) and Acetate Kinase (ACKA) from Mycobacterium tuberculosis H3R7Rv using <i>in silico</i> and <i>in vitro</i> studies	29.81
3	ICMR	2022	2024	Computational and functional characterization of peptide inhibitors disrupting LIMK2-cofilin interaction as a novel therapeutic target towards Glaucoma	29.45

# **Others**

S.	S. Agency From To		iod	D	Budget (Rs.
No			To	Project Title	In lakhs)
1	ICMR - RA	2022	2024	Three-dimensional structure determination of Bacterial DNA Adenine Methyltransferase from Acinetobacter baumannii to be used as drug targets for designing antibiotics	13.2
2	ICMR - RA	2022	2024	Structural and Functional Insights of Vancomycin Resistant Protein VanR from Enterococcus faecium using In vitro and in silico Approach	13.2
3	ICMR - SRF	2022	2024	Structural studies on polyamine biosynthesis enzymes	08.80
4	UGC Kothari Fellow	2022	2024	Investigation of potential inhibitors for alpha linolenic acid (ALA) metabolism in the human malaria parasite	20.96
5	UGC (MANF)	2014	2019	Structural and functional studies on Transcriptional regulatory proteins from <i>Thermus thermophilus</i> HB8 and <i>Pyrococcus horikoshii</i> OT3 - <i>In silico</i> and <i>in vitro</i> studies	18.16
6	UGC (OBC)	2016	2021	Transcriptional Regulation by p21- Activating kinase-1 with an Agonist RUNX3 and Antagonist peptides	19.06

				modulating Pancreatic Cancer: A Structural and Computational approach	
7	ICMR (SRF)	2018	2020	Structural and functional elucidation and inhibitors identification for SMATase from <i>Serratia marcescens</i> to overcome antibiotic resistance	08.97
8	ICMR (SRF)	2019	2021	Structural insights mechanism of type II diabetes proteins from <i>home sapiens</i> to identify potential inhibitors computational and biochemical studies	08.80
9	ICMR (SRF)	2020	2022	Experimental and Computational studies on Proteins involved in Peptidoglycan biosynthesis pathway from <i>Wolbachia</i> Endosymbiont of <i>Brugia malayi</i>	09.472

# **Consultancy Projects**

S.	Agency	Per	iod	Project Title	Budget (Rs.
No	Agency	From	To	Froject ritie	In lakhs)
1	Schrödinger, USA	2011	Till date	Computer Aided Drug Design	Collaboration and skill training for Research Scholars and Students
2	University/ Institution	2012	2016	Computer Aided Drug Design	0.60
3	GE Health care	2012	Till date	Protein Purification and Downstream Bioprocessing	Collaboration and skill training for Research Scholars and Students

# Others

S.	Agency	Per	iod	Scheme/Research Support	Budget (Rs.
No	Agency	From	To	Scheme/Research Support	In lakhs)
1	DST	2017	2021	<b>FIST</b> (Fund for Improvement of S&T Infrastructure in Universities and Higher Educational Institutions) <b>Level – I</b>	62.00

2	UGC	2013	2018	Innovative Programme - PG Diploma in Structural Pharmacogenomics (Post M.Sc One year Course)	54.00 + 2AP*
3	DST	2017	*	DST-PURSE Programme (Phase 2) – All Science Departments	700
4	DBT	2022	2027	Bioinformatics and Computational Biology Center	183.8

<sup>\*</sup> Two Assistant Professors

### **Distinctive Achievements / Awards**

- Tamilnadu Scientist Award (TANSA) by Tamilnadu State Council for Science and Technology (2020)
- 2. UGC Research Award (2016)
- 3. Fellow of Academy of Sciences, Chennai (2015)
- 4. Research Scientist (2003-2010) –RIKEN Japan; NSRRC Taiwan; Spring-8 Japan
- 5. Post Doctoral Fellowship DST, DBT and IRPHA (2000-2003)
- 6. IUCr Young Scientist (1999)
- 7. Young Scientist Travel Award by DST and UNESCO (1999)
- 8. Research Fellow award by CSIR (1997)
- 9. Research award by Marquis (2007)
- 10. MHRD LEAP award by NIT-Trichy & NTU-Singapore (2019)

## **Events organized in leading roles**

Number of Seminars / Conferences / Workshops / Events organized: 21

- 1. E-Learning Program on "BIOINFORMATICS AS CARTOGRAPHIC TOOL IN DRUG DISCOVERY", May 19<sup>th</sup> -30<sup>th</sup>, 2020, Alagappa University, Karaikudi, Tamil Nadu, India
- International Conference on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (ICSBCADD'2019), Dec. 11<sup>th</sup> -13<sup>th</sup>, 2019, Alagappa University, Karaikudi, Tamil Nadu, India.
- 3. International Conference on Innovative and Emerging Trends in Botany (ICIETB-2019), Nov. 6<sup>th</sup> -7<sup>th</sup>, 2019, Alagappa University, Karaikudi, Tamil Nadu, India.
- 4. 11th National Symposium cum Workshop on Recent Trends in Structural Bioinformatics

- and Computer Aided Drug Design (SBCADD'2019), Feb. 12th-15th, 2019, Alagappa University, Karaikudi, Tamil Nadu, India.
- 10<sup>th</sup> National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (SBCADD'2018), Feb. 20<sup>th</sup>-23<sup>rd</sup>, 2018, Alagappa University, Karaikudi, Tamil Nadu, India.
- 6. 9th National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (SBCADD'2017), Feb. 14th-17th, 2017, Alagappa University, Karaikudi, Tamil Nadu, India.
- 7. Fire and Safety Awareness Camp for our University Students and Staff members, Oct. 19th, 2016.
- 8. Eye Camp for Faculty members, Administrative Staffs and Students of our University, Oct. 5<sup>th</sup>, 2016.
- 9. World Habitat Day, Oct. 03<sup>rd</sup>, 2016, Alagappa University, Karaikudi, Tamil Nadu, India.
- 10. International Conference on Recent Trends in Biosciences-2016 (ICRTB-2016), Apr. 07<sup>th</sup> 09<sup>th</sup>, 2016, Alagappa University, Karaikudi, Tamil Nadu, India.
- 11. 8<sup>th</sup> National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (SBCADD'2016), Feb. 16<sup>th</sup>-19<sup>th</sup>, 2016, Alagappa University, Karaikudi, Tamil Nadu, India.
- 12. World Habitat Day, Oct. 15th, 2015, Alagappa University, Karaikudi, Tamil Nadu, India.
- 13. 7<sup>th</sup> National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (SBCADD'2015), Feb. 24<sup>th</sup>-27<sup>th</sup>, 2015, Alagappa University, Karaikudi, Tamil Nadu, India.
- 14. World Creativity and Innovation Day, Apr. 21st, 2014, Alagappa University, Karaikudi, Tamil Nadu, India.
- 15. 6<sup>th</sup> National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (SBCADD'2014), Feb. 18<sup>th</sup>-21<sup>st</sup>, 2014, Alagappa University, Karaikudi, Tamil Nadu, India.

- 16. 5<sup>th</sup> National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (SBCADD'2013), Feb. 19<sup>th</sup>-22<sup>nd</sup>, 2013, Alagappa University, Karaikudi, Tamil Nadu, India.
- 17. Career Guidance and Soft Skill training, Oct. 29th, 2012, Alagappa University, Karaikudi, Tamil Nadu, India
- 18. 4<sup>th</sup> National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (SBCADD'2012), Feb. 20<sup>th</sup>-23<sup>rd</sup>, 2012, Alagappa University, Karaikudi, Tamil Nadu, India.
- 19. National Youth day, Jan. 12th, 2012, Alagappa University, Karaikudi, Tamil Nadu, India.
- 20. World water day celebration, Mar22<sup>nd</sup>, 2011
- 21. 3<sup>rd</sup> National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (SBCADD'2010), Dec. 20<sup>th</sup>-22<sup>nd</sup>, 2010, Alagappa University, Karaikudi, Tamil Nadu, India.

### **Events Participated**

Conferences / Seminars / Workshops: 234

## Overseas Exposure / Visits

- National Synchrotron Radiation Research Centre, Taiwan 05th -09th December, 2017
- Osaka University and RIKEN SPring-8, Japan 22<sup>nd</sup> -30<sup>th</sup> June, 2014
- Osaka University and RIKEN SPring-8, Japan 02<sup>nd</sup> -08<sup>th</sup> December, 2012
- Osaka University and RIKEN SPring-8, Japan 09<sup>th</sup> -16<sup>th</sup> December, 2011
- Osaka University and RIKEN SPring-8, Japan 22<sup>nd</sup> March- 30<sup>th</sup> May, 2010

### Membership in

#### **Professional Bodies**

- 1. Member in American Crystallographic Association
- 2. Vice-President & Life Member, Bioinformatics and Drug Discovery Society (BIDDS)
- 3. Member in British Crystallographic Association
- 4. Executive Committee Member in Indian Crystallographic Association

- 5. Life Member, Indian Science Congress Association
- 6. Life Member, Chemical Research Society of India
- 7. Life Member, Society of Biological Chemists, India
- 8. Life Member, Biotech Research Society, India
- 9. Member in the World Directory of Crystallographers

# **Advisory Board**

## Academic Bodies in Other Institutes/ Universities

1.	2022 - *	:	Member, Board of Studies in Department of Bioinformatics, University of Madras, Chennai
2.	2020 - *	:	Member, Board of Studies in Department of Bioinformatics, School of Chemical and Biotechnology, SASTRA Deemed University, Thanjavur
3.	2019 - *	:	Member, Research Advisory Committee, Karpagam Academy of Higher Education, Coimbatore.
4.	2019 - *	:	Member, Local Program Planning & Management Committee (LPPMC), Bharathiar University, Coimbatore
5.	2018 - *	:	Member, Board of Studies in Bioinformatics, Bharathiar University, Coimbatore
6.	2018 - *	:	Board of Studies in Environmental Biotechnology, Bharathidasan University, Trichy
7.	2018 - *	:	Member, Research Committee, Bharathidasan University, Trichy

# **Academic Bodies Completed**

1.	2012 - 15	:	Member, Board of Studies of Bioinformatics, Periyar University, Salem
2.	2012 - 15	:	Member, Board of Studies of Physics, V.H.N.S.N. College, Virudhunagar.
3.	2013 - 16	:	Bharathidasan University Representative, Board of Studies of
			Bioinformatics, Holy Cross College, Trichy.
4.	2015 - 18	:	Member, Standing Committee on Academic Affairs, Bharathidasan
			University, Trichy.
5.	2015 - 18	:	Chairman, Board of Studies in Bioinformatics (UG, PG & PG Diploma),
			Bharathidasan University, Trichy.
6.	2015 - 18	:	Member, Board of Studies in Bioinformatics and Information
			Technology, Thiruvalluvar University, Vellore.
7.	2015 - 17		Member, Board of Studies in Bioinformatics, Bharathiar University,
/.			Coimbatore.
8.	2014 - 17	:	Member, Board of Studies in Faculty of Bio and Chemical Engineering,
			Sathyabama University, Chennai.
9.	2017 -19		Member, Academic Council, Thassim Beevi Abdul Kader College for
			Women, Ramanathapuram
10.	2015 -20	į	UGC Nominee, SAP DSA-I program promotion in Biophysics Department,
10.			Punjab University.

### Resource persons in various capacities

Number of Invited / Special Lectures delivered: 234

### **Others**

- 1. No. of PhD Thesis evaluated: 39
- 2. No. of PhD Public Viva Voce Examination conducted: 17

### **Recent Publications**

- 1. 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. *Structural Chemistry*, 2022. **(IF:** 1.494)
- 2. Alexpandi, R., Gendrot, M., Abirami, G., Delandre, O., Fonta, I., Mosnier, J., & Veera Ravi, A. Repurposing of doxycycline to hinder the viral replication of SARS-CoV-2: From in silico to in vitro validation. *Frontiers in Microbiology*, 2022. **(IF:** 5.64)
- 3. 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. *Structural Chemistry*, 2022. (**IF:** 1.494)
- 4. 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*, 27(10):gaab059, 2021. **(IF:** 4.025)
- 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. (IF: 4.475)
- 6. Rahul Kanumuri, Aruna Kumar Chelluboyina, Jayashree Biswal, Ravichandran Vignesh, Akkanapally Venu, Vaishnavi B, Leena DJ, **Jeyakanthan Jeyaraman**, Ganesan Kumaresan, Gopala Krishna Aradhyam, and Ganesh Venkatraman, Suresh Rayala. 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. **(IF**: 9.867)

- 7. Richard Mariadasse, Raji Rajmichael, Abhisek Dwivedy, Mathimaran Amala, Mohammed Ahmad, Nachiappan Mutharasappan, Bichitra K. Biswal and **J Jeyakanthan**. Characterization of putative transcriptional regulator (PH0140) and its distal homologue. *Cell Signal.* 2021; 84:110031. (**IF**: 4.315)
- 8. Arul MN, Kumar S, **Jeyakanthan J** & Srivastav V. Searching for target-specific and multitargeting organics for Covid-19 in the Drugbank database with a double scoring approach. *Sci Rep.* 2020; 10(1):19125. (**IF**: 4.379)
- 9. Murugan, NA, 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, 7648, 2020 (**IF**: 5.923)
- 10. Chaudhary SK, Elayappan M, **Jeyakanthan J**, Sekar K. Structural and functional characterization of oligomeric states of proteins in RecFOR pathway. *Int J Biol. Macromol.*, 163,943-953, 2020 (**IF**:6.953)
- 11. Ahmed, 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 (**IF**: 3.512)
- 12. Arul Murugan N, Chitra JP & **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.*, Jun 16;1-12, 2020. (**IF**: 3.310)
- 13. Prabhu D, Amala M, Saritha P, Rajamanikandan S, Veerapandiyan M, **Jeyakanthan J**. Functional characterization of streptomycin adenylyltransferase from *Serratia marcescens*: An experimental approach to understand the Antibiotic Resistance mechanism. *BMC Infectious Diseases*, 20(Suppl 1):324, ISSHID P-31,20, 2020. (**IF**: 3.090)
- 14. Rajendran Santhosh, Namrata Bankoti, Padmashri Adgonda Malgonnavar, Daliah Michael, **Jeyaraman Jeyakanthan** and K. Sekar. MRPC: Missing Regions in Polypeptide Chains A Knowledgebase, *Journal of Applied Crystallography*, Vol 52, 1422-1426, 2019. **(IF:** 3.304)
- 15. Richard Mariadasse, Sanjay Kumar Choubey and **Jeyaraman Jeyakanthan**. 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). **(IF:** 4.956)

- 16. Jayashree Biswal, Jayaprakash Prajisha, Suresh K. Rayala, Ganesh Venkatraman, Poopandi Saritha, Raghu Rangaswamy & **J Jeyakanthan**. Identification of Pak1 inhibitors using water thermodynamic analysis. *J Biomol Struct Dyn.* 38(1), 13–31. (2020) (**IF:** 3.310)
- 17. Amala. M, Rajamanikandan. S, Prabhu. D, Surekha, K & **J Jeyakanthan.** 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) (**IF:** 3.310)
- 18. 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. *Int.J Bio Macromol*,120; 1379-1386, 2018. (**IF**: 6.953)
- 19. Sanjay K. Choubey & **J Jeyakanthan**. 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. (**IF**: 2.518).
- 20. S. Jagadeeshan, A. Subramanian, S. Tentu, S. Beesetti, M. Singhal, S. Raghavan, R. P. Surabhi, J. Mavuluri, H. Bhoopalan, J. Biswal, R. S. Pitani, S. Chidambaram, S. Sundaram, R. Malathi, J Jeyakanthan, A. S. Nair, G. Venkatraman& S. K. Rayala. p21 activated kinase 1 (Pak1) signaling influences therapeutic outcome in pancreatic cancer. *Annals of Oncology Advance Access*, 27(8):1546-56, 2016. (IF: 32.976)
- 21. 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: 102-111. 2016. (**IF**: 3.688)
- 22. Richard M, Biswal J, Prajisha J, Raj Rao G, Choubey SK, Santhosh R & **Jeyakanthan J**. Mechanical insights of Oxythiamine compound as potent inhibitor for Human Transketolase like protein 1. *J Recept Signal Transduct*, 36(3). pp: 233-42. 2016. (**IF**: 1.78)
- 23. Gowri M, Beaula WS, Biswal J, Prabhu D, Saiharish R, Rohanprasad S, Pitani R, Kandaswamy D, Raghunathan R, **J Jeyakanthan**, Rayala SK& Ganesh V. 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). pp: 636-647. 2016. (**IF**: 5.08)

- 24. Ravi M, Tentu S, Baskar G, Rohan Prasad S, Raghavan S, Jayaprakash P, **J Jeyakanthan**, Rayala SK& Venkatraman G. Molecular mechanism of anti-cancer activity of phycocyanin in triple-negative breast cancer cells. *BMC Cancer*, 15(1) PP: 768. 2015. (**IF**: 4.430)
- 25. Anita R.Chacko, Mohammed Arifullah, Narayan P. Sastri, **J Jeyakanthan**, Go Ueno, Kanagaraj Sekar, Randy J. Read, Eleanor J. Dodson, Durga C. Rao & Kaza Suguna. A Novel Pentameric Structure of the Diarrhea-inducing Region of the Rotavirus Enterotoxigenic Protein NSP4. *J Virol.*, 85(23), pp. 12721-12732, 2011. (**IF**: 5.103)
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