



**Dr. J. JEYAKANTHAN**  
**Professor and Head**

### Contact

Address : Department of Bioinformatics  
Alagappa University  
Karaikudi – 630 003  
Tamil Nadu, INDIA

Employee Number : 34101

Contact Phone (Office) : +91 4565 223725/340/341

Contact Phone (Mobile) : +91 9789809245

Contact e-mail(s) : jjkanthan@gmail.com

Skype id : jeyakanthan.jeyaraman

Website : www.jjeyakanthan.bioinfoau.org

### Academic Qualifications:

Year of Passing	Degree	University / Institute
2000	Ph.D. Crystallography and Biophysics	University of Madras
1995	M. Phil. Physics	M. K. University
1993	M.Sc. Physics	M. K. University
1991	B.Ed.	University of Madras
1999	P.G.D.C.A	MIT, Anna University

### Teaching (8 Years)/Research Experience: 23 Years

Position	Institute/University	Period
Professor and Head	Department of Bioinformatics	March 2010 – *
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

### Additional Responsibilities

1. 2017 - \* : Coordinator, DST-PURSE (Phase-II)
2. 2017 - \* : Coordinator, DST-FIST (Level-I).
3. 2016 - \* : Member of Syndicate (Governor-Chancellor Nominee).
4. 2016 - \* : Member, Research Advisory Committee (RAC).
5. 2015 - \* : Chairperson, School of Biological Sciences.
6. 2013 - \* : Coordinator, UGC Innovative Program (PG diploma).
7. 2010 - \* : Member of Senate.
8. 2010 - \* : Member, Website Maintenance Committee.
9. 2010 - \* : Chairman, Board of Studies of Bioinformatics.

### Completed:

1. 2015 - 17: Director, Directorate of Collaborative Programmes.
2. 2012 - 16: Director, Centre for International Relations.
3. 2012 - 15: Member, Research Advisory Committee.
4. 2012 - 13: Coordinator, Career Guidance and Counselling Cell.
5. 2010 - 15: 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**

1. Proteins from *Thermus thermophilus* HB8, *Pyrococcus horikoshii* OT3, *Aquifex aelicous* VF5, *Mycobacterium tuberculosis* and *Brugia malayi*.
2. Proteins responsible for *Dengue*, *Chikungunya*, Cancer, Diabetes, etc.,

➤ **Development of Tools and databases**

3. Web based search engines for analyzing macromolecular interactions

### Research Supervision / Guidance

	Program of Study	Completed	Ongoing
Research	Ph.D.	-	11
	M.Phil.	06	-

Project	PG	16	-
	UG / Others	02	-

## Publications

International		National		Others
Journals	Conferences	Journals	Conferences	Books / Chapters / Monographs / Manuals
104	82	01	92	01

Cumulative Impact Factor (as per JCR) :	274.67
h-index	: 13
i10 index	: 21
Total Citations	: 760

## Funded Research Projects

### Completed Projects

S. No	Agency	Period		Project Title	Budget (Rs. In lakhs)
		From	To		
1	DBT	2012	2015	Structural and Functional Analysis ....from <i>Thermus thermophilus</i> HB8	50.25
2	UGC	2012	2015	Structural and Functional ..... Protein from <i>Pyrococcus horikoshii</i> 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 <i>Pyrococcus horikoshii</i> OT3	48.98

### Ongoing Projects

S. No	Agency	Period		Project Title	Budget (Rs. In lakhs)
		From	To		
1	DST	2016	2019	Identification of potential antifilarial drug ..... <i>Brugia malayi</i>	69.38
2	UGC	2016	2018	Structural and Functional ..... Stat2 Protein From <i>Homo Sapiens</i>	37.80
3	DBT	2015	2018	Development of Web Based ..... Fatty acids and Buffers	13.81

### Consultancy Projects

S. No	Agency	Period		Project Title	Budget (Rs. In lakhs)
		From	To		
1	University/Institution	2012	2016	Computer Aided Drug Design	0.60

### Others

S. No	Agency	Period		Scheme/Research Support	Budget (Rs. In lakhs)
		From	To		
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*

\* Two Assistant Professors

### Distinctive Achievements / Awards

1. UGC Research Award (2016)
2. Fellow of Academy of Sciences, Chennai (FASCh) (2015)
3. Marquis Who's Who Scientific Directory (2007)
4. Post Doctoral Fellowship - DST, DBT and IRPHA (2000-2003)
5. IUCr Young Scientist (1999)
6. Young Scientist Travel Award by DST and UNESCO (1999)
7. Research Fellow Award by CSIR (1997)

### Events organized in leading roles

Number of Seminars / Conferences / Workshops / Events organized: 12

1. 9<sup>th</sup> National Symposium cum Workshop on Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (SBCADD'2017), Feb. 14<sup>th</sup>-17<sup>th</sup>, 2017, Alagappa University, Karaikudi, Tamil Nadu, India.
2. 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.
3. 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.

4. 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.
5. 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.
6. 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.
7. 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.
8. 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: 77**

## Overseas Exposure / Visits

- 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. Life Member, Bioinformatics and Drug Discovery Society
2. Member in American Crystallographic Association
3. Member in British Crystallographic Association
4. Life member in Indian Crystallographic Association
5. Member in the World Directory of Crystallographers
6. Life Member, Indian Science Congress Association

### Advisory Board

#### National Committee

2016 - *	:	UGC Women PDF Selection Committee.
2015 - *	:	UGC Nominee, SAP DSA-I program promotion in Biophysics Department, Punjab University.

#### International Committee

2017 - *	:	Netherlands Organisation for Scientific Research (NWO, the Dutch Research Council) to review the Research Grant Proposal.
----------	---	---

#### Academic Bodies in Other Institutes/ Universities

1. 2015 - \* : Member, Standing Committee on Academic Affairs, Bharathidasan University, Trichy.
2. 2015 - \* : Chairman, Board of Studies in Bioinformatics (UG, PG & PG Diploma), Bharathidasan University, Trichy.
3. 2015 - \* : Member, Board of Studies in Bioinformatics and Information Technology, Thiruvalluvar University, Vellore.
4. 2015 - \* : Member, Board of Studies in Bioinformatics, Bharathiar University, Coimbatore.
5. 2014 - \* : Member, Board of Studies in Faculty of Bio and Chemical Engineering, Sathyabama University, Chennai.

### Academic Bodies Completed

1.	2013 - 16	:	Bharathidasan University Representative, Board of Studies of Bioinformatics, Holy Cross College, Trichy.
2.	2012 - 15	:	Member, Board of Studies of Bioinformatics, Periyar University, Salem
3.	2012 - 15	:	Member, Board of Studies of Physics, V.H.N.S.N. College, Virudhunagar.

### Resource persons in various capacities

Number of Invited / Special Lectures delivered: 43

### Others

1. No. of PhD Thesis evaluated : 23
2. No. of PhD Public Viva Voce Examination conducted : 16

### Recent Publications

1. M. Maniyazagan, R. Mariadasse, M. Nachiappan, **J. Jeyakanthan**, N.K. Lokanath, S. Naveen, G. Sivaraman, P. Muthuraja, P. Manisankar, T. Stalin Synthesis of rhodamine based organic nanorods for efficient chemosensor probe for Al (III) ions and its biological applications. *Sensors and Actuators B*, S0925 - 4005 (17) 31314 - X; **2017**. DOI: 10.1016/j.snb.2017.07.106.
2. Singal, B., Balakrishna, A. M., Nartey, W., Manimekalai, M. S. S., **Jeyakanthan, J.** and Grüber, G. Crystallographic and solution structure of the N-terminal domain of the Rel protein from *Mycobacterium tuberculosis*. *FEBS Lett.*, **2017**. DOI:10.1002/1873-3468.12739.
3. Ansuman Biswas, Arpit Shukla, Santosh Kumar Chaudhary, Santhosh Rajendran, **Jeyaraman Jeyakanthan**, Kanagaraj Sekar. Structural studies of a hyperthermophilic Thymidylate Kinase enzyme reveal conformational sub-states along the reaction coordinate. *FEBS Journal*, **2017**.
4. Ansuman Biswas, Arpit Shukla, R. S. K. Vijayan, **Jeyaraman Jeyakanthan** and K. Sekar. 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**.
5. Rajamanikandan S, **Jeyaraman J**, Pappu S. 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**.
6. M. Maniyazagana, C. Rameshwaran, R. Mariadasse, **J. Jeyaraman**, K. Premkumar, T. Stalin. Fluorescence Sensor for Hg<sup>2+</sup> and Fe<sup>3+</sup> 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. Jayashree Biswal, Mutharasappan Nachiappan, Dhamodharan Prabhu, **Jeyaraman Jeyakanthan**. Unraveling the importance of Multidrug Efflux Transporter protein from *Thermus thermophilus* HB8 - an in silico approach. **Research Journal of Medical and Allied Sciences**. Vol 1; Issue 1, **2017**.
8. Prabhu D, Vidhyavathi R, **Jeyakanthan J**. Computational identification of potent inhibitors for Streptomycin 3''-adenylyltransferase of *Serratia marcescens*. **Microb Pathog**.103, 94-106, **2017**.
9. 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**.
10. Sundaraj Rajamanikandan, **Jeyaraman Jeyakanthan** & Pappu Srinivasan. 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, 192-218, **2017**.
11. M. Maniyazagan, R. Mariadasse, **J. Jeyakanthan**, N.K. Lokanath, S. Naveen, K. Premkumar, P. Muthuraja, P. Manisankar, T. Stalin. 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**.
12. Kanagarajan Surekha, Mutharasappan Nachiappan, Dhamodharan Prabhu, Sanjay Kumar Choubey, Jayashree Biswal and **Jeyakanthan Jeyaraman**. Identification of potential inhibitors for oncogenic target of Dihydroorotate dehydrogenase using In silico approaches. **J Mol Struct.**, 1127, 675-688, **2017**.
13. Dakshinamurthy Sasikala, **Jeyaraman Jeyakanthan**, Pappu Srinivasan. 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**.
14. Choubey SK, 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**. Nov 18:1-14, **2016**.
15. Sanjay K. Choubey, **Jeyaraman 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**.



16. Sanjay K. Choubey, Richard Mariadasse, Santhosh Rajendran, **Jeyaraman Jeyakanthan**. 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**.
17. 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, 1754-1767, **2016**.
18. Ansuman Biswas, Subbarao Jasti, **J. Jeyakathan** and K. Sekar. Role of sequence evolution and conformational dynamics in the substrate specificity and oligomerization mode of thymidylate kinases. *J Biomol Struct Dyn* .Jul 27:1-19, **2016**.
19. Guru Raj Rao R, Biswal J, Prabhu D, Sureka K, **Jeyakanthan 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), 2199-213, **2016**.
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. Jayaraman**, A. S. Nair, G. Venkatraman, and 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**.
21. R. Santhosh, S.N. Satheesh, M. Gurusaran, Daliah Michael, K. Sekar and **J. Jeyakanthan**. NIMS: A database on Nucleobase compounds and their Interactions in Macromolecular Structures. *Journal of Applied Crystallography.* 49, PP:1093-1098, **2016**.
22. D Sasikala, **J Jeyakanthan**, P Srinivasan. Structural insights on identification of potential lead compounds targeting WbpP in *Vibrio vulnificus* through structure-based approaches. *Journal of Receptors and Signal Transduction.* 36(5), PP 515-30, **2016**.
23. Kanagarajan Surekha, Damodharan Prabhu, Mariadasse Richard, Mutharasappan Nachiappan, Jayashree Biswal, **Jeyaraman Jeyakanthan**. Investigation of vital pathogenic target orotate phosphoribosyltransferases (OPRTase) from *Thermus thermophilus* HB8: Phylogenetic and molecular modeling approach. *Gene.* 583(2). PP:102-111. **2016**.
24. Mariadasse Richard, Jayashree Biswal, Jayaprakash Prajisha, Guru Raj Rao, Sanjay Kumar Choubey, Rajendran Santhosh and **Jeyaraman Jeyakanthan**. Mechanical insights of Oxythiamine compound as potent inhibitor for Human Transketolase like protein 1 (TKTL1 protein). *Journal of Receptors and Signal Transduction*, 36(3). pp:233-42. **2016**.
25. Gowri M, Beaula WS, Biswal J, Prabhu D, Saiharish R, Rohanprasad S, Pitani R, Kandaswamy D, Raghunathan R, **Jeyakanthan J**, Rayala SK, Ganesh V.  $\beta$ -lactam substituted polycyclic fused pyrrolidine/pyrrolizidine derivatives eradicate *C. albicans* in an ex vivo human dentinal tubule model by inhibiting sterol 14- $\alpha$  demethylase and cAMP pathway. *Biochim Biophys Acta.* 1860(4). pp:636-647. **2016**.