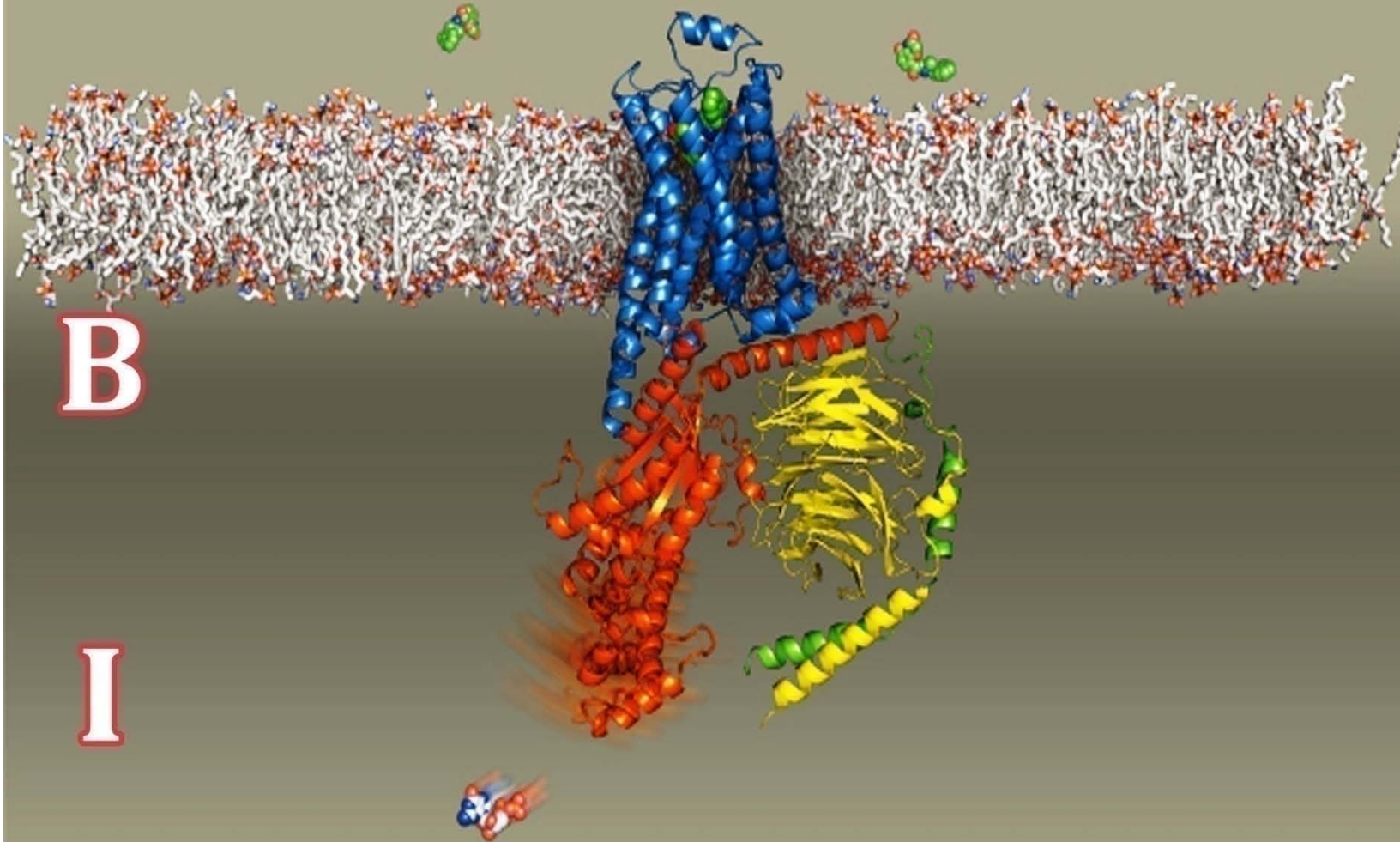




# e-BIOINFORMATICS MAGAZINE



**B**

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**ISSUE: 3  
2013 - 2014**

## **About the DBI - BIM**

The *e*-magazine delivers simple, concise, and relevant information of the happenings at Department of Bioinformatics. This periodical is published annually as per the academic calendar.

The magazine is sent free of charge to all alumni of DBI, as well as to faculty, staff, and students.

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DBI-BIM

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## Message from the Chief Editor



Dear all,

I am very happy to note that Department of Bioinformatics is bringing out the “e- Magazine” e-Bioinformatics Magazine (BIM) for the academic year 2013-14. Each year, the magazine outlines the progress that the department has made during the previous academic year and recapitulates all events, showcasing the various activities of the department. This year has passed swiftly in a blur of achievements and accomplishments, and I would like to congratulate and extend my best wishes to all those who have worked hard to ensure that the magazine is published with a treasure trove of memories. To me, the magazine will always be an event-filled journal, chronicling another exciting year that will be cherished by our department students, research scholars and staffs in the years to come. Through this magazine, I would like to greet the entire Bioinfo family.

I hope this magazine will be a treasure for those associated with Bioinformatics area and will help in providing a platform for sharing experiences and learning in this area. I once again congratulate the Department of Bioinformatics and the entire team on this endeavour and wish the “e-Magazine” all success.

Heartly congratulations to the editorial team and I am thankful to all the authors who have send their articles who made this magazine so informative. I heartly congratulate and convey my best wishes to all faculty, students, Research scholars for a successful future. Wish you all the best!!!!

A handwritten signature in blue ink, which appears to read "Sunil". The signature is written in a cursive style and is followed by a period.

**Sunil Kumar Tripathi**  
**Chief Editor**

## **Department Events**

### **6<sup>th</sup> National Symposium cum Workshop on “Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (SBCADD-2014)**

SBCADD'2014 is a Symposium cum Workshop which focuses on enriching the growing scientific community consisting of budding young minds acting as a driving force in their research and also amalgamates researchers from all over india and outside to strengthen the connections in all fields of Bioinformatics. This symposium cum workshop is being organized from 18<sup>th</sup> to 21<sup>st</sup> Feb 2014. This four day event will feature primary lectures, Poster presentation and workshop to a number of scientists and academicians dealing with basic science and allied parallel research. The main aim is to share the ideas and knowledge about the molecule, its interaction with the drug and awareness on new drug development. The occasion was glorified by Dr. S. Kaliyamoorthy the Convener, Vice-Chancellor Officiating Committee of Alagappa University, Dr. T. P. Singh Distinguished Biotechnology Research Professor AIIMS New Delhi, Dr. B. Jayaram Coordinator, IIT Delhi, Dr. Manju Bansal, Indian Institute of Science, Bangalore, Dr. D. Velmurugan, Professor & Head, CAS in Crystallography & Biophysics.

Eighteen Eminent Scientists and experts from various premier institutes such as IISc Bangalore, AIIMS New delhi, IIT Delhi, IIT Madras, NIPER, MKU Madurai, University of Madras, VIT Vellore, Pondicherry University, Anna University and Schrodinger U.S.A delivered talks that are thought-provoking and were of much use to young budding scientists. Furthermore, more than 152 participants were gained in hands-on training sessions provided by Application Scientists from Schrödinger, USA in many areas of Structural Bioinformatics, Computer Aided Drug Design Problem solving sessions along with demonstrations incorporated as a part of the Symposium cum Workshop will familiarize the participants with molecular modeling and drug discovery tools. SBCADD'2014 would provide an excellent opportunity to keep up with the cutting-edge research and also serve as a platform for delivering new lead molecules more quickly at lower cost through *in silico* methods facilitate target identification, structure prediction and lead/drug discovery.









**Glimpses of SBCADD 2014 moments**

## World Creativity Day 21.04.2014

World Creativity Day was celebrated by the Department of Bioinformatics, Alagappa University on 21<sup>st</sup> April 2014. Dr. Karuthiah Pandian I.A.S (Retd), Director, Bharathidasan Institute of Management, Tiruchirappalli was the Chief Guest. In Plenary address, he requested the students to reveal their individuality for enhancing the quality of research to meet the global standards. Dr. Subas Chandra Bose, Member-Vice Chancellor officiating Committee, Alagappa University described the importance of the existing rules for the Human resource and Management are for the welfare of the society. Prof. A. Narayanamoorthy, Dean-Faculty of Arts delivered the Key-note address and Prof. Gurumallesh Prabhu, Special Officer (Planning) provided the felicitation address. Earlier Prof. J. Jeyakanthan welcomed the gathering and explained the importance of celebrating World Creativity Day. Dr. Sanjeev Kumar Singh, Associate Professor proposed the vote of thanks.





World creativity day was celebrated on 21<sup>st</sup> April

## **Conference Attended**

### **UGC-ASC**

Dr. J. Jeyakanthan delivered a lecture on High Throughput X-ray Crystallography organized by the Academic Staff College, Bharathiar University, Coimbatore during 5<sup>th</sup> July 2013.

### **Workshop on Molecular Modeling & Drug Design**

Dr. Sanjeev Kumar Singh attended the workshop and delivered a talk on Current trends in Pharmacoinformatics at PSG College Coimbatore during 14<sup>th</sup> -20<sup>th</sup> July 2013.

### **State level seminar on Advanced Bio Chem Development (ABCD-2013)**

Dr. J. Jeyakanthan delivered a lecture on Structural biology and Bioinformatics at Sri Sarada Niketan College for Women, Karaikudi, during 21 August 2013.

### **Conference on Recent Advances in Computational Drug Design.**

Mr. K. Gopinath, Mr. C. Sathish Kumar, Ms. D. Sasikala, Mr. D. Prabhu and Ms. J. Prajisha attended and presented poster at Conference on Recent Advances in Computational Drug Design IISC, Bangalore during 16<sup>th</sup> -17<sup>th</sup> September 2013.

### **2<sup>nd</sup> IITM- Tokyo Tech Joint Symposium on Techniques and Application of Bioinformatics**

Mr.Guru Raj Rao, Mr.Richard Maridasse and Mr.Sanjay Kumar Choubey under the guidance of Dr. J. Jeyakanthan attended and presented poster at 2<sup>nd</sup> IITM- Tokyo Tech Joint Symposium on Techniques and Application of Bioinformatics IIT Madras during 27<sup>th</sup> -28<sup>th</sup> September 2013.

### **American Society for Borne and Mineral Research (ASBMR) Annual meeting**

Dr. M. Karthikeyan attended and presented paper at American Society for Borne and Mineral Research (ASBMR) Annual meeting Baltimore, Maryland, USA during 4<sup>th</sup>-7<sup>th</sup> October 2013.

### **International Seminar on Recent Trends in Aquatic Animal Biotechnology (RTAAB 2013)**

Dr. P. Srinivasan and his student A.Sudha attended the International Seminar on Recent Trends in Aquatic Animal Biotechnology at Dept of animal Health & Management, Alagappa University during 21<sup>st</sup>-22<sup>nd</sup> October 2013.

### **42<sup>nd</sup> National Seminar on Crystallography**

Dr. J. Jeyakanthan attended and delivered a lecture on Structural and Functional studies of Leucine Responsive Regulatory protein at 42<sup>nd</sup> National Seminar on Crystallography AIIMS New Delhi during 8<sup>th</sup> -10<sup>th</sup> November 2013.

### **54<sup>th</sup> Annual Conference of Association of Microbiologists of India (AMI-2013)**

Ms. D. Sasikala under the guidance of Dr. P. Srinivasan attended and presented poster at 54<sup>th</sup> Annual Conference of Association of Microbiologists of India (AMI-2013) during 17<sup>th</sup>-20<sup>th</sup> November 2013.

### **International Conference on Biomolecular Simulations & Dynamics: Recent Advances & Future Perspectives**

Dr. P. Kirubikaran attended the International Conference on Biomolecular Simulations & Dynamics: Recent Advances & Future Perspectives at IIT Madras 28<sup>th</sup> -30<sup>th</sup> November 2013.

### **International Science Congress-2013**

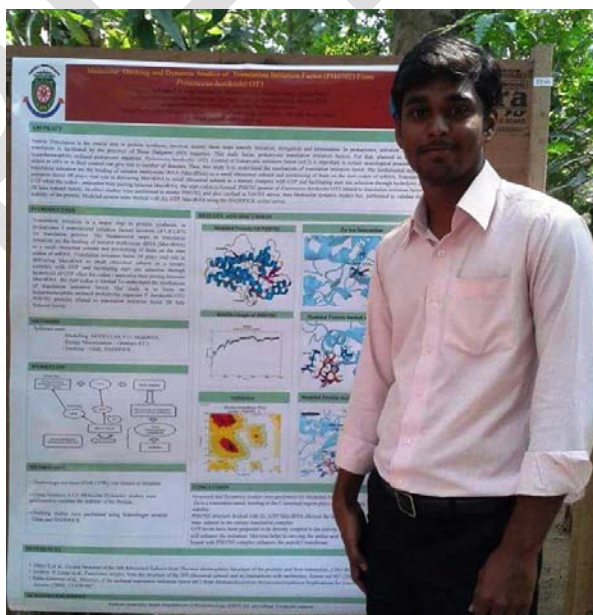
Mrs. A. Sudha, Ms. Vanajothi attended the International Science Congress-2013 Karunya University during 8<sup>th</sup> -9<sup>th</sup> December 2013.

### **Phoenix- Macromolecular Structure Solution Workshop 2014**

Dr. J. Jeyakanthan had attended Phoenix- Macromolecular Structure Solution Workshop at University of Madras 21<sup>st</sup> January 2014.

### **Recent Trends in Macromolecular Structure and Function (ISRTMSF-2014)**

Dr. J. Jeyakanthan along with his two Ph.D Students Mr. D. Prabhu and Ms. J. Prajisha had attended and presented a poster at “Recent Trends in Macromolecular Structure and Function” at University of Madras, Chennai, India during 22<sup>nd</sup>-24<sup>th</sup> January, 2014.



### **National Workshop on Molecular Modelling**

Mr. D. Prabhu has attended the National Workshop on Molecular Modelling organized by University of Madras on 25<sup>th</sup> January 2014.

### **Recent trends in Macromolecular Crystallography**

Dr. J. Jeyakanthan along with his two Ph.D Students, Ms. Prajisha. J and Ms. Jayashree Biswal had attended and presented oral presentation at “Recent Trends in Macromolecular Crystallography” at Pondicherry University Puducherry, India during 12<sup>th</sup>-13<sup>th</sup> March, 2014.

### **National Conference on Innovations, Implementations and Controversies of Animal Biotechnology**

Dr. P. Srinivasan attended the National Conference on Innovations, Implementations and Controversies of Animal Biotechnology at Bharathidasan University during 20<sup>th</sup> & 21<sup>st</sup> March, 2014.

### **Insightful Preaching's and Enrichment Program**



**Invited talk by Dr. C.J. Chen, Professor and Division Head, Life Science Group, Scientific Research Division, National Synchrotron Radiation Research Centre, Taiwan on 28<sup>th</sup> March, 2013**



**Visiting Faculties Prof. D. Velmurugan, University of Madras, Chennai (21<sup>st</sup> – 23<sup>rd</sup> December, 2013); Dr. V. Subramanian, CLRI, Chennai (24<sup>th</sup> – 25<sup>th</sup> December, 2013) and Dr. K. Gunasekaran, University of Madras, Chennai (21<sup>st</sup> – 22<sup>nd</sup> October, 2013) to deliver lectures for the PGDSP programme.**



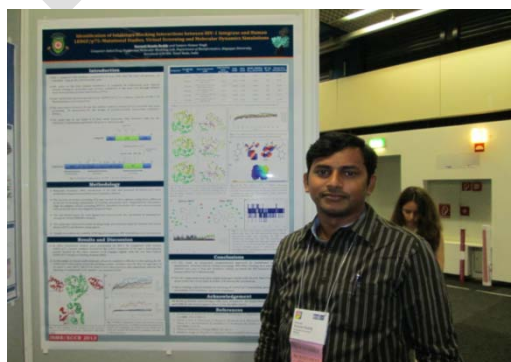
**Eminent Scientists Prof. T.P Singh, AIIMS and Prof. Manju Bansal, IISc Bangalore visited and delivered plenary lectures at SBCADD'2014 on 18<sup>th</sup> February, 2014.**

**DBI as a Springboard  
Consultancy for Research Training and Technical Exposure**

The abundance of enriched computational and experimental facilities at Department of Bioinformatics a collective sum of revenue has been generated from the consultancy services provided to many students hailing from different institutions to complete their M.Sc Dissertation thesis and carry out their part of Doctoral Research based on their objectives and requirement

1.	Ms. M. Gowri	Sri Ramachandra University	17 <sup>th</sup> – 30 <sup>th</sup> July, 2013
2.	Mr. U. Dinesh Babu	SASTRA University	14 <sup>th</sup> – 30 <sup>th</sup> August, 2013
3.	Dr. N. Ramesh Kannan	Srimad Andavan Arts and Science College	21 <sup>st</sup> – 31 <sup>st</sup> January, 2014

**Students Achievements**



**Dr. Karnati Konda Reddy's poster presentation at ISMB/ECCB Conference, Berlin, Germany from July, 21<sup>st</sup> – 23<sup>rd</sup>, 2013**

## Research Projects

S. No.	Principal Investigator	Project Title	Period		Funding Agency	Amount ₹ (in lakhs)
			From	To		
1.	Dr. J. Jeyakanthan	Structure and functional studies on PH0140 protein from <i>Pyrococcus horikoshii</i> OT3	07/2012	06/2015	UGC	12.90
		Structural and Functional analysis of Orotate Phosphoribosyl transferase (TTHA1742) and Dihydroorotate Dehydrogenase (TTHA0779) from <i>Thermus thermophilus</i> HB8	07/2012	06/2015	DBT	50.25
		Structure determination of CPS and ATCase of <i>Thermus thermophilus</i> HB8 and identification of potential inhibitors	09/2012	08/2015	DBT	32.16
		Structural and Functional Studies of Translation Initiation factors from <i>Pyrococcus horikoshii</i> OT3	01/2013	05/2016	DBT - Twin	77.00
		Structural and Functional Studies of Purine Biosynthesis complex from <i>Pyrococcus horikoshii</i> OT3	07/2013	08/2016	DST	48.98
		Shape and chemical feature based 3D-Pharmacophore Model generation, Virtual Screening and MESP studies to identify Potential	02/2011	01/2014	UGC	7.48



		Leads for Antifungal Azoles.				
		Computational Screening of CDK2 Inhibitors by Combined approach of Pharmacophoric study, QPLD and Molecular Dynamics Simulation analysis	05/2011	04/2014	DST	18.95
		QM/MM partial charges, binding pocket contours analysis and FEP calculation for designing potent inhibitors of HTLV-Protease: A de novo drug design approach	03/2012	03/2015	CSIR	16.02
		Molecular characterization, molecular docking and biocontrol effect of Vibrio bacteriophages from shrimp aquaculture environment	07/2011	07/2014	UGC	7.64
		Diversity of Salmonella specific bacteriophages in Tamilnadu and screening potent phages to treat salmonellosis	08/2012	08/2015	ICMR	16.33
		Development of Microarray for the detection of Bacteria / Bacteriophages and controlling measures against pathogenic bacteria from shrimp aquaculture environment	08/2012	08/2015	DST-FAST TRACK	23.44
		Investigation of binding of HA Protein with sialic acid ligand	02/2011	01/2014	CSIR	15.98

		base identification of neuraminidase inhibitor of H1N1 2009 influenza virus	lead of				
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## Publications

1. L. Karthik, M. Nachiappan, D. Velmurugan, **J. Jeyakanthan**, K. Gunasekaran. (2013), "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) PP: 59-70.
2. Santosh Kumar Chaudhary, **J. Jeyakanthan**, K. Sekar. (2013), "Cloning, expression, purification, crystallization and preliminary X-ray crystallographic study of thymidylate kinase(TTHA1607) from *Thermus thermophilus* HB8". *Acta Cryst.* F69, PP: 118-121. **(IF: 0.56)**.
3. T. Balakrishnan, K. Ramamurthi, **J. Jeyakanthan** and S. Thamotharan. (2013) "*catena*-Poly[[[aqua(glycine- $\kappa$ O)lithium]- $\mu$ -glycine- $\kappa_2$ O:O'] bromide]". *Acta Cryst.* E69, m60–m61.
4. Kavyashree Manjunath, Shankar Prasad Kanaujia, K. Surekha, **J. Jeyakanthan**, K. Sekar. (2013), "Structure of SAICAR synthetase from *Pyrococcus horikoshii* OT3: Insights into thermal stability". *Int J Biol Macromol.* 53, pp: 7-19. **(IF: 3.096)**.
5. Suryanarayanan V, **Singh SK**, Tripathi SK, Selvaraj C, Reddy KK, Karthiga A., (2013), "A three-dimensional chemical phase pharmacophore mapping, QSAR modelling and electronic feature analysis of benzofuran salicylic acid derivatives as LYP inhibitors", *SAR QSAR Environ Res.*, 24(12):1025-40 **(IF:1.59)**.
6. Tripathi SK, Muttineni R, **Singh SK.**, (2013), "Extra precision docking, free energy calculation and molecular dynamics simulation studies of CDK2 inhibitors", *J Theor Biol.*, 334: 87-100 **(IF:2.11)**.
7. Reddy KK, **Singh SK**, Tripathi SK, Selvaraj C, Suryanarayanan V., (2013), "Shape and pharmacophore-based virtual screening to identify potential cytochrome P450 sterol 14 $\alpha$ -demethylase inhibitors", *J Recept Signal Transduct Res.*, Aug; 33(4): 234-43 **(IF:2.27)**.
8. Reddy KK, **Singh SK**, Tripathi SK, Selvaraj C., (2013), "Identification of potential HIV-1 integrase strand transfer inhibitors: in silico virtual screening and QM/MM docking studies", *SAR QSAR Environ Res.*, 24(7):581-95 **(IF:1.59)**.
9. Shafreen RM, Selvaraj C, **Singh SK**, Pandian SK., (2013), "Exploration of fluoroquinolone resistance in *Streptococcus pyogenes*: comparative structure analysis of wild-type and mutant DNA gyrase", *J Mol Recognit.*, 26(6): 276-85 **(IF:2.15)**.

10. Vijayalakshmi P, Selvaraj C, **Singh SK**, Nisha J, Saipriya K, Daisy P., (2013), "Exploration of the binding of DNA binding ligands to *Staphylococcal* DNA through QM/MM docking and molecular dynamics simulation", *J Biomol Struct Dyn.*, 31(6):561-71 (IF: 2.91).
11. Singh P, **Singh SK**, Selvaraj C, Singh RK., (2013), "195 In silico study on HIV-PRIs substructures to terminate proteolytic activity in HTLV", *J Biomol Struct Dyn.*, 31 (Sup1):127-127 (IF:2.91).
12. **Singh SK**, Selvaraj C., (2013), "Molecular dynamics and ligand based studies for the validation of potential inhibitors for SrtA against *Bacillus anthracis*", *J Biomol Struct Dyn.*, 31 (Sup1):119-120 (IF:2.919).
13. Durai Prabhu, Chinnasamy Arulvasu, Gajendran Babu, Ramar Manikandan & **Pappu Srinivasan**, (2013), "Biologically synthesized green silver nanoparticles from leaf extract of *Vitex negundo*. L. induces growth-inhibitory effect of human colon cancer cell line HCT15", *Process Biochemistry*, 48, 317-324. (IF: 2.51).
14. Nallathambi Sengottuvelan, **Pappu Srinivasan**, Kandasamy, M. & Hoong Kun Fun, (2013), "DNA Cleavage Electrochemical and Magnetic studies of Scorpion and copperII complex", *International Journal of ChemTech Research*, 5, 367-375. (IF: 0.23).
15. Venkatesan Suryanarayanan, Arumugam Sudha, Sundaraj Rajamanikandan, Ramar Vanajothi & **Pappu Srinivasan**, (2013), "Atom-based 3D QSAR studies on novel N- $\beta$ -D-Xylosylindole derivatives as SGLT2 inhibitors", *Medicinal Chemistry Research*, 22, 615-624. (IF: 1.61).
16. Arumugam Sudha, Sumathi, K., Manikandaselvi, N. S., Narayanan Marimuthu Prabhu & **Pappu Srinivasan**, (2013), "Anti-hepatotoxic Activity of Crude Flavonoid Fraction of *Lippia nodiflora* L. on Ethanol Induced Liver Injury in Rats", *Asian Journal of Animal Sciences*, 7, 1-3.
17. Arumugam Sudha, & **Pappu Srinivasan**, (2013), Physicochemical and Phytochemical profiles of aerial parts of *Lippia nodiflora* L. *International Journal of Pharmaceutical Sciences and Research*, 4, 4263-4271.
18. **Karthikeyan M**, Shridevi V, Rajiv Rose, Anandan B, Singh KhD, Shanmugasundaram S, Mohan D, Ramesh, Jayaraman G, (2013), "Angiotensin Gene Polymorphisms (T174M and M235T) are Significantly Associated with the Hypertensive Patients of Tamil Nadu, South India", *International Journal of Human Genetics*, 13(4): 201-207. (IF: 0.382)
19. Singh KhD, **Karthikeyan M**, (2013), "Molecular Modeling, Quantum Polarized Ligand Docking and Structure Based 3D-QSAR study of imidazole series as Dual Endothelin and Angiotensin II Receptor Antagonists", *Acta Pharmacologica Sinica (NPG)*, 34, 1592-1606. PMID: 24304920, DOI: 10.1038/aps.2013.129 (IF: 2.496)

20. Kirubakaran P, **Karthikeyan M**, (2013), “Pharmacophore modeling, 3D-QSAR and DFT studies of IWR small-molecule inhibitors of Wnt response”, *Journal of Receptors and Signal Transduction*, 33 (5) 276-285. PMID: 23914783, DOI: 10.3109/10799893.2013.822888 (IF: 1.63)
21. Kirubakaran P, **Karthikeyan M**, Singh KhD, Nagamani S, (2013), “Pharmacophore modeling, 3D-QSAR and molecular docking study on naphthyridine derivatives as inhibitors of 3-phosphoinositide-dependent protein kinase-1”, *Medicinal Chemistry Research*, 22 (8): 3812-3822. DOI: 10.1007/s00044-012-0383-5 (IF: 1.61)
22. **Karthikeyan M**, Singh KhD, Sathishkumar C, Nagamani S, Gopinath K, Thiyagarajan C, Premkumar P, Anusuyadevi M, (2013), “High Throughput Screening and E-pharmacophore filtering in the discovery of new BACE-1 inhibitors”, *Interdisciplinary Sciences: Computational Life Sciences*, 5(2): 119-126. PMID: 23740393, DOI: 10.1007/s12539-013-0157-x (IF: 0.662)
23. Devi Kasinathan, , Nisha RG, Prabhu NM, Manikandan R, **Karthikeyan M**, (2013), “Awareness on Type II Diabetes and Its Complication among Sivaganga District Population in Tamilnadu: A Cross Section Survey”, *Journal of Advanced Scientific Research*, 4(1): 38-42. ISSN 0976-9595
24. Kirubakaran P, **Karthikeyan M**, Singh KhD, Nagamani S, Premkumar K, (2013), “*In silico* structural and functional characterization of the human TOPK by protein structure modeling and molecular dynamics studies”, *Journal of Molecular Modeling*, 19(1):407-19. DOI: 10.1007/s00894-012-1566-1 (IF: 1.98)

### Student’s/Scholar’s Corner

#### Scientific BrainBank

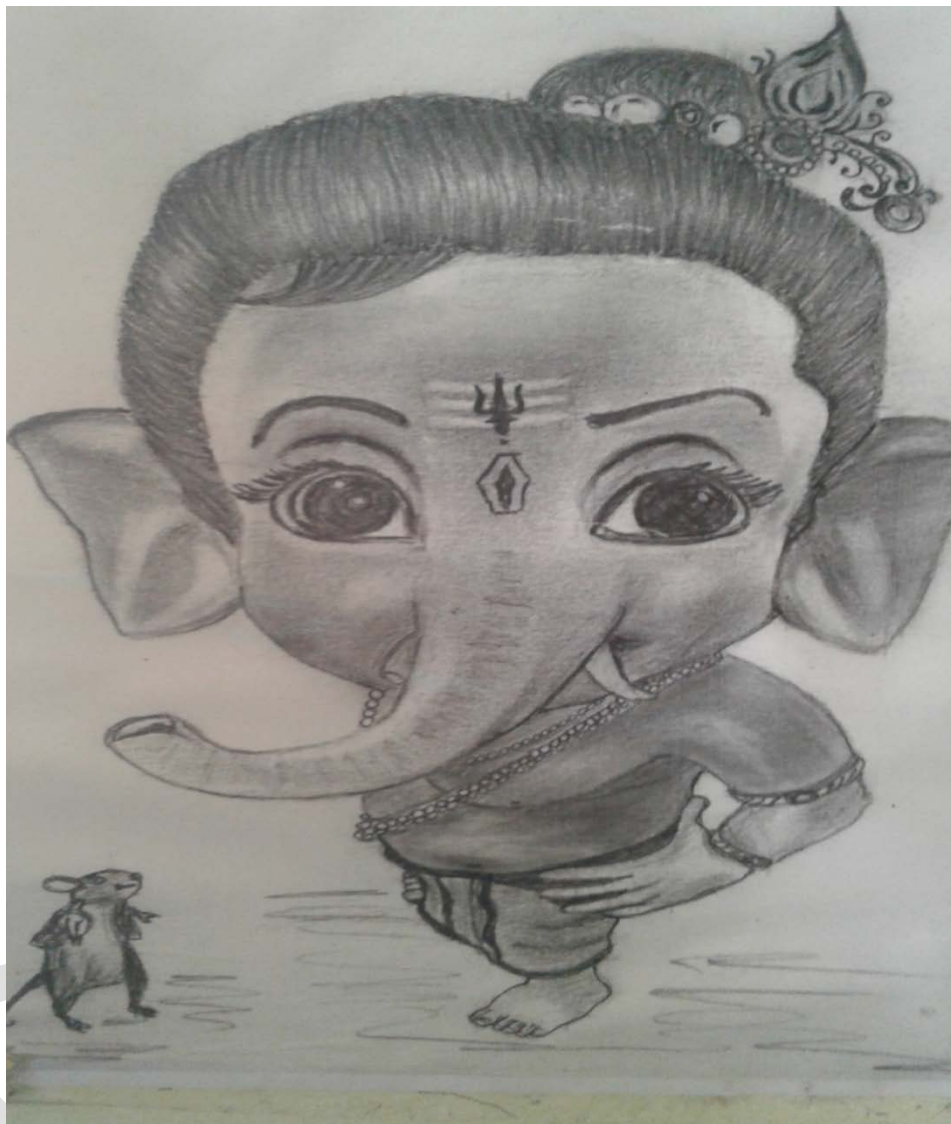
Journal Club has been initiated and followed as a regular practice where the research scholars are made to present on recent research topic of their interest for about 45 – 60 minutes and thereafter deliberations on the much hyped subject leads to the stimulation of thought provoking process and formation of novel ideas for their research doings.

#### Journal club Schedule

Name	Title of the Paper	Date
Mr. D. Prabhu	Structure based functional inference of hypothetical proteins from mycoplasma hyopneumoniae	05-07-2013
A. Sudha	Anti-inflammatory and Anticancer activities of extracts and compounds from the mushroom <i>Inonotus obliquus</i>	12-07-2013
Kh. Dhanachandra Singh	RYR3 gene polymorphisms and cardiovascular disease outcomes in the context of antihypertensive treatment	19-07-2013
R. Vanajothi	Green tea epigallocatechin-3-gallate protects against oxidative stress-induced nuclear translocation of P53	26-07-2013

	and apoptosis in retinal pigment epithelial cells, ARPE-19	
Sunil Kumar Tripathi	Molecular modeling studies on cell cycle regulatory protein and its inhibitors towards therapeutic target for cancer	02-08-2013
P. Kirubakaran	Mechanism of Taq DNA Polymerase inhibition by fulberene derivatives: Insight from computer simulation	16-08-2013
Karnati Konda Reddy	Insights into the Glycyl radical enzyme active site of benzyl succinate synthase A computational study	23-08-2013
Selvaraj. C	Molecular Dynamics simulation study and hybrid pharmacophore model development in human LTA4H inhibitor design	30-08-2013
Gopinath. K	Mispred: a resource for identification of erroneous protein sequence in public databases.	6-09-2013
Nachiappan. M	Molecular dynamics approach to probe the allosteric inhibition of PTP1B by chlorogenic and cichoric acid	13-09-2013
Rajamanikandan. S	An inhibitory compound produced by pseudomonas with effectiveness of V.harveyi	20-09-2013
Sathish Kumar. C	Green synthesis of biopolymer-silver nanoparticle nanocomposite: An optical sensor for AMMONIA detection.	27-09-2013
Sindhu. T	Scutellarin from Scutellaria baicalensis suppresses adipogenesis by upregulating PPAR $\alpha$ in 3T3-L1 cells	04-10-2013
Sureka. K	Structure of PIN-domain protein from Pyrococcus horikoshii OT3	11-10-2013
Sasikala. D	Characterization of induced staphylococcus aureus bacteriophage SAP-26 & its anti-biofilm activity with rifampicin	18-10-2013
Suryanarayanan. V	An innovative strategy for dual inhibitor design and its application in dual inhibition of human thymidylate synthase and dihydrofolate reductase enzymes	25-10-2013
Karthiga. A	Investigating citrullinated proteins in tumor cell lines	08-11-2013
Stalin. N	Isolation and characterization of five lytic bacteriophages infecting a vibrio strain closely related to vibrio owensii	22-11-2013
Prabhu. D	Hypoxia increases antibiotic resistance in pseudomonas aeruginosa through altering the composition of multi drug efflux pumps	29-11-2013
Sureka. K	Crystal structure of cryptosporidium parvum pyruvate kinase	29-11-2013
Renganayaki. M	Complex genetic origin of Indian populations and its implications	06-12-2013
Prajisha. J	Mycobacterium tuberculosis shikimate kinase inhibitors: Design and simulation studies of the catalytic turn over	13-12-2013

**Student's Corner**



**k. Sureka  
Research Scholar**



**k. Sureka**  
**Research Scholar**



**k. Sureka**  
**Research Scholar**



MADURAI  
THE HINDU • THURSDAY, FEBRUARY 20, 2014

## Emphasis on extensive research

Special Correspondent

**KARAIKUDI:** S. Kaliyamoorthy, Convener, Vice-Chancellor, Officiating Committee, Alagappa University, has called upon students to carry out extensive research on structural biology and bioinformatics by developing drugs for killer-diseases.

Inaugurating the four-day sixth national symposium cum workshop on 'Recent trends in

structural bioinformatics and computer-aided drug design' here on Wednesday, he said scientists and research scholars should work in a dedicated manner to tap the potential of bioinformatics in solving the problems faced by the medicinal chemist.

Prof. T.P. Singh of the Department of Biophysics at All India Institute of Medical Sciences (AIMS) in New Delhi

stressed the need for human resource development in the areas of bioinformatics and computer-aided drug design.

Prof. B. Jayaram, Coordinator, School of Biological Sciences, IIT-Delhi, explained the crucial role bioinformatics tools played in designing toxic-free drug molecule. Prof. Manju Bansal of Indian Institute of Science, Bangalore, said human genome sequence and biologi-

cal databases were great resources in specialised biology.

Prof. D. Velmurugan of Crystallography and Biophysics department in University of Madras focused on structural bioinformatics and X-ray crystallography and its contribution in the field of drug designing.

All bioinformatics software could be used as a filtration tool for the identification of new drugs, he said.

# உடல் நலம் குறித்த ஆராய்ச்சிக்கு போதிய நிதி ஒதுக்குவது இல்லை

## தேசிய கருத்தரங்கில் தகவல்

காரைக்குடி, பிப்.21: உடல் நலம் குறித்த ஆராய்ச்சிக்கு போதிய நிதி ஒதுக்குவது இல்லை என தேசிய கருத்தரங்கில் தெரிவிக்கப்பட்டது.

காரைக்குடி அழகப்பா பல்கலைக்கழக உயிர் தகவலியல் துறை சார்பில் கட்டமைப்பு உயிரி தகவலியல் மற்றும் கணினி சார்ந்த மருந்து கண்டு பிடிப்புகள் குறித்த தேசிய அளவிலான கருத்தரங்கு துவக்க விழா நடந்தது. உயிரி தகவலியல் துறை தலைவர் ஜெயகாந்தன் வரவேற்றார்.

பல்கலைக் கழக துணை வேந்தர் பொறுப்புக்குழு தலைவர்களிய மூர்த்தி துவக்கி வைத்து பேசுகையில், மூலக் கூறுகளின் செயல்பாடுகள் பற்றி அறிந்து கொள்வதற்கும், மனித வள மேம்

பாட்டிற்கும் கம்ப்யூட்டர் சார்ந்த மருந்து கண்டுபிடிப்பு துறை பல புதிய வழிமுறைகளை உருவாக்கி தருகிறது. அறிவியல் வல்லுநர்கள் இத்துறையில் மிகவும் ஈடுபாட்டுடன் செயல்பட வேண்டும் என்றார்.

ஸ்டீராடிங்கர் அமைப்பின் துணை தலைவர் ரகு பேசுகையில், உயிரி தகவல் தொழில் நுட்பத்தில் புதிய

ஆராய்ச்சி மேற்கொள்ள வேண்டும். ஆராய்ச்சி தொழில் கூடங்கள் உருவாக்க வேண்டும். சீனாவில் உயிர் தொழில் நுட்ப வளர்ச்சிக்கு அதிக அளவில் நிதி ஒதுக்கப்பட்டு தொழில் நுட்ப கூடங்கள் அதிக அளவில் உருவாக்கப்பட்டுள்ளன. ஐ.டி துறை மற்றும் வினவெளி ஆராய்ச்சிக்கு அதிக

அளவில் நிதி ஒதுக்கப்பட்டு புதிய கண்டுபிடிப்புகள் உருவாக்கப்படுகின்றன. ஆனால் உடல் நலம் ஆராய்ச்சிக்கு இது போன்று அதிக அளவில் நிதி ஒதுக்கப்படுவது இல்லை என்றார்.

இதில் அகில இந்திய மருத்துவ அறிவியல் நிறுவனத்தின் உயிரி இயற்பியல் துறை பேராசிரியர் டிபிசிங், உயிர் அறிவியல் துறை இந்திய தொழில் நுட்ப நிறுவன ஒருங்கிணைப்பாளர் ஜெயராமன், பெங்களூரு இந்திய அறிவியல் கழகத்தின் மூலக்கூறு உயிரி இயற்பியல் துறை பேராசிரியர் மஞ்சபன்சால், சென்னை பல்கலைக்கழக படிக்கவியல் மற்றும் உயிர் இயற்பியல் துறை தலைவர் வேல்முருகன் உள்பட பலர் கலந்து கொண்டனர். இணைப் பேராசிரியர் சஞ்சீவ் குமார் நன்றி கூறினார்.

/சிவகங்கை நகராட்சியில்  
கலப்பு உரக்கிடங்கின்  
ளவு.

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சிவகங்கை நகராட்சியில் கழிப்பறை  
வசதி உள்ள வீடுகளின் எண்ணிக்கை.

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## 'அவுட்சோர்சிங்' மூலம் பெருகி வரும் உயிரி தகவல் தொழில் நுட்ப பணிகள்

காரைக்குடி, பிப்.21-

இந்தியாவில், உயிரி தகவல் தொழில் நுட்ப பணிகள், 'அவுட்சோர்சிங்' முறையில், மேற்கொள்ளும் முறை பெருகி வருவதாக 'ஸ்கோர்டிங்கர்' துணை தலைவராக ரகு பேசினார்.

காரைக்குடி அழகப்பா பல்கலை கழக உயிரி தகவல் துறை சார்பில், 'கட்டமைப்பு உயிரி தகவலியல், மற்றும் கணினி மருந்து கண்டுபிடிப்புகளின் நவீன வளர்ச்சி' குறித்த தேசிய கருத்தரங்கு துணைவேந்தர் பொறுப்பு குழு தலைவர் கலியமூர்த்தி தலைமையில் நடந்தது.

இதில் ரகு பேசியதாவது: மனித உடலில் 23 ஆயிரம் புரதங்கள் உள்ளன. ஒவ்வொரு புரதமும் ஒவ்வொரு பணியை செய்கிறது. 23 ஆயிரம் புரதங்களின் முப்பரிமாண மூலக்கூறு வடிவமைப்பை கண்டுபிடித்தால் தான், இவற்றால் ஏற்படும் நோய் தாக்கத்துக்கு, உரிய மருந்து

களை கண்டுபிடிக்க முடியும்.

ஆனால், 4 சதவீதம் புரதங்களுக்குரிய முப்பரிமாண மூலக்கூறு அமைப்பை கண்டுபிடிக்கப்பட்டு உள்ளது. ஒரு புரதத்துக்குரிய முப்பரிமாண வடிவமைப்பு கண்டுபிடிக்க, 15 ஆண்டு வரை ஆகிறது. 8 ஆயிரம் முதல் 10 ஆயிரம் கோடி வரை இதற்கு செலவாகிறது.

இவற்றை விரைவாக கண்டுபிடிக்க வேண்டுமானால், பல்கலை அளவில் உள்ள பழைய பாடத்திட்டங்கள் களையப்பட வேண்டும்.

இந்தியாவில், அவுட்சோர்சிங் முறையில், உயிரி சம்பந்தமான, ஆராய்ச்சிக்கு தேவையான பணிகள் செய்யப்படுகிறது. இந்திய இளைஞர்களின் திறமை இதற்கு செலவழிக்கப்படுகிறது.

ஆனால், கண்டுபிடிக்கப்படும், மருந்துகள் பன்னாட்டு கம்பெனிகள், பெயரில் வெளி வருகிறது. 12க்கும் மேற்பட்ட கம்பெனிகள்,

வெளிநாட்டு உயிரி தகவல் துறைக்கு பணி செய்து கொண்டிருக்கிறது. இது பெருகி கொண்டே வருகிறது. இதை மாற்ற, இந்திய அளவில் பல்கலைக்கழகங்களின் ஆராய்ச்சி திறனை மேம்படுத்த வேண்டும். பல்கலை கழக ஆராய்ச்சி நூலகம் அமைக்க வேண்டும்.

மத்திய, மாநில அரசும், அறிவியல் துறைக்கு தேவையான கட்டமைப்பை மேற்கொள்ள முன் வர வேண்டும். ஆராய்ச்சி தொழிற்சூடங்கள் உருவாக வேண்டும், என்றார்.

துறை தலைவர் ஜெயகாந்தன் வரவேற்றார். எய்ம்ஸ் பேராசிரியர் சிங், உயிரி அறிவியல் துறை இந்திய தொழில் நுட்ப நிறுவன ஒருங்கிணைப்பாளர் ஜெயராம், பேராசிரியர் வேல்முருகன், சஞ்சீவகுமார், பாலமுருகன் பங்கேற்றனர். 50க்கும் மேற்பட்ட மாணவர்கள் ஆராய்ச்சி கட்டுரை சமர்ப்பித்தனர்.



## Contact Us

**The Chief Editor  
DBI-BIM**

Department of Bioinformatics

Alagappa University

Karaikudi-630 004

Tamil Nadu, India

E-Mail: [bioinfoau@gmail.com](mailto:bioinfoau@gmail.com)

Ph no: +91-4565-230725

Fax: +91-04565-225202

