



# e-BIOINFORMATICS MAGAZINE



**B**



**I**

**M**

**ISSUE: 4  
2014 - 2015**

## **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.

The contents of the magazine ©2014-2015 by the DBI, Alagappa University.

DBI-BIM

## **EDITOR IN CHIEF**

Mr. Gopinath. K

## **EDITORS**

Ms. T. Sindhu

Ms. D. Sasikala

Mr. V. Suryanarayanan

## **EDITORIAL BOARD**

Mr. R. Guru Raj Rao

Mr. L. Lakshmanan

Mr. M. Richard

Mr. N. Stalin

Ms. Jayashree Biswal

Mr. S. Vijaya Prabhu

## **TECHNICAL SUPPORT (M.SC II<sup>nd</sup> yr)**

Mr. V. Jagasiripian

Mr. S. Saravanakumar

Mr. M. Veerapandiyam

## **ADVISORY COMMITTEE**

**Dr. J. Jeyakanthan**

Professor & Head

**Dr. Sanjeev Kumar Singh**

Associate Professor

**Dr. M. Karthikeyan**

Assistant Professor

**Dr. RM. Vidhayavathi**

Assistant Professor

**Dr. J. Joseph Sahayarayan**

Assistant Professor

**Dr. P. Boomi**

Assistant Professor

<b>Contents</b>	<b>Pg no</b>
<b>Message from the Chief Editor</b>	<b>5</b>
<b>Department Events</b>	<b>6-9</b>
<b>Conference</b>	<b>10-11</b>
<b>Collaboration/Invited lectures</b>	<b>12-13</b>
<b>Consultancy Services</b>	<b>14</b>
<b>Projects</b>	<b>14</b>
<b>Student's Achievements</b>	<b>15</b>
<b>Journal Club</b>	<b>17</b>
<b>Publications</b>	<b>18-20</b>
<b>Student's Corner</b>	<b>21-24</b>
<b>Press Releases</b>	<b>25-26</b>

## Message from the Chief Editor



**Dear all,**

The Department of Bioinformatics, Alagappa University feels excited and proud for releasing the fifth issues of “The e- Bioinformatics Magazine” (BIM). Our department always aims to provide best platform for students growth through symposiums, workshop, and research collaboration. Department has been recognized in national and International level through the national level symposium cum workshop. This department also funded by various funding agencies to support the research in Small and Macro Molecule X-ray Crystallography, Structural Biology, Molecular Modelling, Computer Aided Drug Design, Pharmacoinformatics, Chemoinformatics, Molecular Cell Biology, Genetic Engineering, Genomics, Proteomics, Bio-computing, Quantum Chemistry, Database and Software development.

e-BIM aims to provide research activities of Department of Bioinformatics. This issue focused to provide department activities, e-BIM summaries extension activities, research collaboration, and invited talks by eminent scientist, research achievements, research outcome and publication. Future, e-BIM is expected to provide the recent development in the field of bioinformatics.

The world is on the hand, the technological advancement always helps to connect the research community to collect and share the information easier and faster. Thus, it is expected that e-BIM can serve among students as an effective tool for exploring the advances in Bioinformatics. I thank all the editors and reports for the marvellous support for compiling this issue.

A handwritten signature in blue ink, appearing to read 'Gopinath'.

**Mr. K.Gopinath**  
**Chief Editor**

**Innings during June 2k14-December 2k15**

**7<sup>th</sup> National Symposium cum Workshop on “Recent Trends in Structural Bioinformatics and Computer Aided Drug Design (SBCADD-2015)”**

SBCADD’2015 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 24<sup>th</sup> to 27<sup>th</sup> Feb 2015. 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 Prof. S. Kaliyamoorthy the Convener, Vice-Chancellor Officiating Committee of Alagappa University, Prof. P. Gunasekaran, Vice-Chancellor, Thiruvalluvar University, Vellore, Prof. K. Muniyappa, Indian Institute of Science, Bangalore, Dr. D. Velmurugan, Professor & Head, CAS in Crystallography & Biophysics, Dr. S. Karutha Pandian Member Vice-Chancellor Officiating Committee, Professor & Head, Department of Biotechnology, Alagappa University.

Seventeen Eminent Scientists and experts from various premier institutes such as IISc Bangalore, Thiruvalluvar University Vellore, IIT Madras, IIT Guwahati, CLRI Chennai, Bharathiar University Coimbatore, Chhatrapati Shahu Ji Maharaj University Kanpur, Sri Ramachandra University, Madras University, Anna University Chennai, Pondicherry University and Schrodinger U.S.A delivered talks that are thought-provoking and were of much use to young budding scientists. Furthermore, more than 120 participants were gained in hands-on training sessions provided by Application Scientists from Schrodinger, 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’2015 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.



**Dr. J. Jeyakanthan H.O.D of the Bioinformatics is honouring the Vice-Chancellor Officiating Committee Prof. S. Kaliyamoorthy with shawl.**





## **Conference Attended**

### **State Level Conference on Advanced Bio-Chem Development (ABCD-2014)**

On 11<sup>th</sup> August 2014, Dr. J. Jeyakanthan delivered an invited talk on “Structural Bioinformatics and Drug Discovery” at Sri Sarada Niketan College for Women, Karaikudi.

### **National Workshop on Essentials of Bioinformatics**

Dr. J. Jeyakanthan delivered an invited talk on “Bioinformatics and Drug Discovery” at Dr. Umayal Ramanathan College for Women”, Karaikudi 14<sup>th</sup> August 2014.

### **Recent Strategies in Drug Discovery-III**

Dr. Sanjeev Kumar Singh attended Recent Strategies in Drug Discovery-III at PSG college of Arts & Science Coimbatore 25<sup>th</sup>-27<sup>th</sup> September 2014.

### **Physics Association**

On 26<sup>th</sup> September 2014, Dr. J. Jeyakanthan delivered an invited talk on “High Throughput X-ray Crystallography” at Kandaswami Kandar’s College, Velur.

### **International Conference on Physiology and Medicine**

Mr. T. Stalin under the guidance of Dr. P. Srinivasan had attended and presented a poster at “International Conference on Physiology and Medicine” organized by the Department of Zoology, Periyar University, Salem India during 15<sup>th</sup>-17<sup>th</sup> October, 2014.

### **National Conference on Bioengineering and Biotechnology an Industrial Perspective**

Dr. Sanjeev Kumar Singh attended and delivered a lecture on “Computer aided drug design & its importance in current drug discovery at the “National Conference on Bioengineering and Biotechnology an Industrial Perspective” AMITY, Lucknow, India 16<sup>th</sup> -17<sup>th</sup> October 2014.

### **Indo-US Conference Molecular modeling & informatics in drug design**

Umesh Panwar under the guidance of Dr. Sanjeev Kumar Singh attended and presented a poster on PPRID-Phage Protein resource information data at National Institute of Pharmaceutical education & research (NIPER) Punjab, 3<sup>rd</sup> -6<sup>th</sup> November 2014

### **43<sup>rd</sup> C National Seminar on Crystallography**

Mr. M. Nachiappan and Mr. D. Prabhu under the guidance of Dr. J. Jeyakanthan had attended and presented a poster at “43<sup>rd</sup> C National Seminar on Crystallography” at CSIR-CDRI, Lucknow, India during 12<sup>th</sup>-14<sup>th</sup> November, 2014.

### **55<sup>th</sup> Annual Conference of Association of Microbiologists of India**

Ms. D. Sasikala under the guidance of Dr. P. Srinivasan had attended and presented a poster at “55<sup>th</sup> Annual Conference of Association of Microbiologists of India” organized by the

Association of Microbiologists of India, Coimbatore Unit, TNAU, and Coimbatore during 12<sup>th</sup>-14<sup>th</sup> November, 2014.

#### **Theoretical Chemistry Symposium**

Dr. Sanjeev Kumar Singh along with his Research scholar V. Suryanarayanan attended and presented poster on Structural & Mechanistic insights into the pyridine 1-oxide derivatives as PCAF BRD inhibitors at the “Theoretical Chemistry Symposium” CSIR-NCL, Pune, India 18<sup>th</sup>-21<sup>st</sup> December 2014.

#### **International Conference on Computational Intelligence: Health and Disease and DNA 2014: Next Generation DNA Led Technologies**

Dr. J. Jeyakanthan delivered an invited talk on “Structural Biology and its importance in drug discovery” at Institute of Bioinformatics and Computational Biology (IBCB) Viskhapatnam, 27<sup>th</sup>-28<sup>th</sup> December 2014.

#### **UGC Sponsored State level Seminar on Progress in Condensed Matter physics**

Dr. J. Jeyakanthan delivers a lecture on Structural Biology and its importance in drug discovery at The Madura College, Madurai, 7<sup>th</sup> January 2015.

#### **National Seminar on Frontier Areas in Chemical Technologies (FACTs-2015)**

Dr. J. Jeyakanthan attended the conference “National Seminar on Frontier Areas in Chemical Technologies” at Alagappa University 2015.

#### **Workshop on Metrohm Autolab electrochemical Instruments for Biosensors, Energy and Corrosion Applications**

Dr. M. Karthikeyan participated in Workshop on Metrohm Autolab electrochemical Instruments for Biosensors, Energy and Corrosion Applications at Department of Biosensors and Bioelectronics, Alagappa University, Karaikudi during 16<sup>th</sup> February 2015.

#### **National Seminar on Genomics & Proteomics: A Computation approach**

Dr. Sanjeev Kumar Singh attended and delivered a talk on Current topics in CADD at Lady Dock College, Madurai, 6<sup>th</sup> March 2015.

#### **Workshop on Structural biology an Introduction to protein Crystallography**

Mr. D. Prabhu and Mr. Guru Raj Rao under the guidance of Dr. J. Jeyakanthan had attended the “Workshop on Structural biology an Introduction to protein Crystallography” organized by Department of Biophysics NIMHANS, Bangalore on April 15<sup>th</sup>-18<sup>th</sup> 2015.

#### **Faculty Development Program**

Dr. Sanjeev Kumar Singh attended the Faculty Development Program on Comprehensive approach of biotechnological applications at BIT Anna University 16<sup>th</sup> -29<sup>th</sup> April 2015.

## Collaboration



**R. Santhosh (Research Scholar) visit at IISC Bangalore during 2014 for research discussion.**

### Invited Lectures

**Dr. Shandar Ahmad**, Eminent Scientist, National Institute of Biomedical Innovation, Osaka, Japan delivered an invited talk on Predicting Biomolecular Interactions and miRNA Regulatory modules and shared his expertise and experience with the students during 5<sup>th</sup>-9<sup>th</sup> March, 2014.

Also, the Department invited **Dr. Shandar Ahmad**, to discuss matters on the enrichment of existing curriculum of Bioinformatics programs. The Departmental curriculum Development Committee met in the presence of Dr. Shandar Ahmad, as a Subject Expert on 7<sup>th</sup> March in the Department of Bioinformatics.



**Invited talk by Dr. Shandar Ahmad, National Institute of Biomedical Innovation, Japan on 7<sup>th</sup> March, 2014.**



**Visiting Faculties Dr. R. Sankaranarayanan, SASTRA University, Thanjavur (6<sup>th</sup> December, 2014) Dr. Mohane S. Coumar, Pondicherry University, Puducherry (21<sup>st</sup> – 22<sup>nd</sup> November, 2014) and Dr. Ganesh Venkatraman, Sri Ramachandra University, Chennai (27<sup>th</sup> - 29<sup>th</sup> November, 2014) to deliver lectures for the PGDSP programme.**

### DBI as a Spring board

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

Mr. S. Ramkumar	Bharathiar University	21 <sup>st</sup> –30 <sup>th</sup> August, 2014
Ms. Mathangi Ravi	Sri Ramachandra University	21 <sup>st</sup> –27 <sup>th</sup> August, 2014
Ms. Ritu Khare	SRM University	17 <sup>th</sup> –23 <sup>rd</sup> March, 2015

### Research Project

S. No	Principal Investigator	Project Title with Period	Funding Agency	Amount (In Lakhs)
1.	Dr. J. Jeyakanthan	Development of Web Based Search Engines for the Analyses of Protein interactions with Nucleotide, Fatty Acids and Buffers (05/2015 - 04/2018)	DBT	13.81
		Structural and Functional Insights of Potential therapeutic dengue fever target STAT2 protein from <i>Homo Sapiens</i> (04/2016– 05/2018)	UGC-Research Award	37.8
		Identification of Potential Anti-Filarial drug targeted enzymes Wbm0441, Wbm0042 from <i>Wolbachia</i> endosymbiont <i>Brugia malayi</i> (09/2016-08/2019)	DST	69.38
2.	Dr. Sanjeev Kumar Singh	Identification of novel drug targets of <i>Leishmania donovani</i> : Studies on CAAX prenyl protease I and II of the pathogen. (08/2014-07/2017)	DBT	73.69
		<i>In silico</i> screening, theoretical calculation and <i>in vitro</i> studies for development of potential HIV1-PR inhibitors. (04/2016-03/2019)	DBT	19.51
3.	Dr. M. Karthikeyan	Pharmacogenomics Study of Anti Hypertensive Treatment in South Indian Population (05/2014-04/2017)	ICMR	21.25
		Computational Identification and <i>In vitro</i> validation of small molecule inhibitors for tankyrase protein to inhibit the over expression of Wnt/ $\beta$ catenin signaling mechanism using HCA-7, HCT116 and MDST8/HCA-46 colon cancer cell lines: A new drug target for Colorectal Cancer (03/2016-02/2019)	DBT	30.48
4.	Dr. RM. Vidhyavathi	Classification of hierarchical clustering with FP-Growth algorithm to analyzing and creating the solution for Chromosomal disorder (01/2016-05/2018)	AURF	0.80

## Ph.D Awardees

Sl.No	Name	Faculty	Year of Passing
1.	Dr. Sunil.K.Tripathi	Dr. Sanjeev Kumar Singh	2014
2.	Dr. C. Selvaraj	Dr. Sanjeev Kumar Singh	2014
3.	Dr. Kh. Dhana Chandra Singh	Dr. M. Karthikeyan	2014
4.	Dr. Karnati Konda Reddy	Dr. Sanjeev Kumar Singh	2014
5.	Dr. P. Kirubakaran	Dr. M. Karthikeyan	2014

## Student's Achievement



**Mr. P. Kirubakaran receiving the IJPS Best paper award in Medicinal & Synthetic Chemistry by The Indian Pharmaceutical Association's Prof. M. L. Khorana Memorial, Indian Journal of Pharmaceutical Sciences on August, 7<sup>th</sup> 2014.**

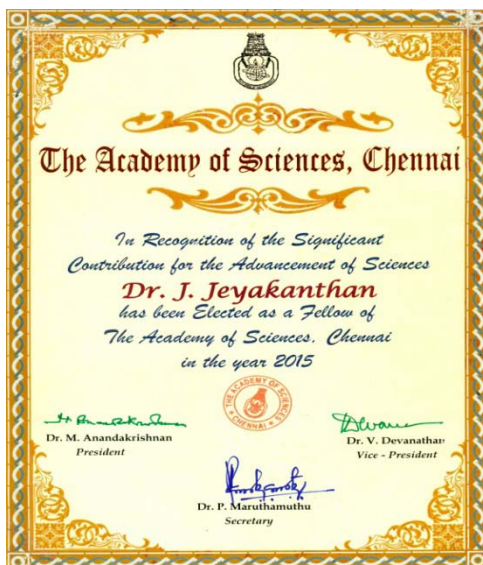


**Mr. M. Nachiappan has received the Best Poster Award at 43<sup>rd</sup> C National Seminar on Crystallography, held on 12<sup>th</sup>-14<sup>th</sup> November, 2014.**

Mr. Nagamani. S, Research scholar under the guidance of Dr. M. Karthikeyan has been selected for the ICMR-SRF, 2014.

Mr. M. Richard, Research scholar under the guidance of Dr. J. Jeyakanthan has been selected for the Moulana Azad National Fellowship (MANF) - UGC, 2015.

## Faculty's Achievement



**Dr. J. Jeyakanthan has been elected as a fellow of “The Academy of sciences” in recognition of the significant contribution for the Advancement of Sciences in the year 2015.**

## Pooja Celebrations

On the auspicious day of Ayudha and Saraswati Pooja, the students, faculty and non-teaching staff come together to witness the Dusherra Celebrations on October 1, 2014 at Department of Bioinformatics. The occasion was graced in the presence of Dr. J. Jeyakanthan, Professor and Head, Dr. Sanjeev Kumar Singh, Associate Professor, Dr. P. Srinivasan Assistant Professor and Dr. M. Karthikeyan, Assistant Professor all the teaching faculties. Saraswati Pooja is just another attempt by the students and staff to preserve the Indian culture and to impart a sense of respect towards long-established traditions. This celebration ensures that students find a home away from home. Both the faculty and students joined hands together, with great deal to make the event a memorable one also evoking the blessing of the goddess of knowledge to have a successful academic and carrier growth.

## 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 mins 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
Mrs. A. Sudha	Synthesis and evaluation of resveratrol derivatives as new chemical entities for cancer.	04.07.2014
Ms. R. Vanajothi	Condurango glycoside rich components stimulate DNA damage-induced cell cycle arrest & ROS mediated caspase 3 dependent apoptosis through inhibition of cell-proliferation in lung cancer <i>in vitro</i> & <i>in vivo</i>	18.07.2014
Ms. K. Sureka	Structure & Function of RNase as a Polyadenylate Specific exoribonuclease affecting mycobacterial virulence <i>in vivo</i>	01.08.2014
Mr. S. Nagamani	Sequence derived 3D Pharmacophore models for G Protein Coupled receptor & their application in virtual screening	22.08.2014
Mr.M. Nachiappan	An append domain results in an unusual architecture for malaria parasite trypanophenyl tRNA synthetase	19.09.2014
Mr. K. Gopinath	Fixpred: a resource for correction of erroneous protein sequences	19.09.2014
Mr.C.Sathish Kumar	Triketramides A-D, Indole alkaloids from the Australian sponge Triketron fiabeliforme	24.10.2014
Mr.S.Rajamanikandan	Computational prediction of a putative binding site on Drpl: Implications for antiparkinsonian therapy	07.11.2014
Ms. T. Sindhu	Multiple e-pharmacophore modeling combined with high throughput virtual screening & docking to identify potential inhibitors of $\beta$ -secretase (BACE1)	18.12.2014
Ms. D. Sasikala	Evaluating efficacy of bacteriophage therapy against Staphylococcus aureus infections using a silkworm larval infection model	9.01.2015
Mr.V. Suryanarayanan	Protein like dynamics of polycarbonate polymers in water	23.01.2015
Mr.R. Guru Raj Rao	Structural features of interfacial tyrosine residue in ROBO1 fibronectin domain antibody complex crystallographic thermodynamic & molecular dynamic analysis	06.02.2015
Mr. Sanjay Kumar Choubey	Pharmacophore generation atom based 3D QSAR docking & virtual screening studies of P38- $\alpha$ mitogen activated protein kinase inhibitors pyridopyridazine	20.02.2015
Mr. M. Richard	Molecular evolution of the neuropeptide S-Receptor	06.03.2015
Mr. N. Stalin	Efficiency of phage cocktail in the inactivation of vibrio in aquaculture	20.03.2015

## Research Articles

1. Surekha K, Nachiappan M, Prabhu D, Muthukumar J, Krishna R, **Jeyakanthan J.** (2014), "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), PP: 591-601. (IF: 2.91).
2. Selvaraj C, Singh P, **Singh SK.**, (2014), "Molecular insights on analogs of HIV PR inhibitors toward HTLV-1 PR through QM/MM interactions and molecular dynamics studies: comparative structure analysis of wild and mutant HTLV-1 PR", *J Mol Recognit.*, 27(12), 696-706 (IF: 2.15).
3. Sivakamavalli J, Selvaraj C, **Singh SK**, Vaseeharan. B, (2014), "Exploration of protein-protein interaction effects on alpha-2-macroglobulin in an inhibition of serine protease through gene expression and molecular simulations studies", *J Biomol Struct Dyn.*, 32(11), 1841-54 (IF: 2.91).
4. Selvaraj C, Bharathi PR, **Singh SK.**, (2014), "Communication of  $\gamma$  phage lysine plyG enzymes binding toward SrtA for inhibition of *Bacillus anthracis*: protein-protein interaction and molecular dynamics study", *Cell Commun Adhes.*, 21(5), 257-65 (IF: 2.41).
5. Selvaraj C, Singh P, **Singh SK.**, (2014), "Molecular modeling studies and Comparative analysis on structurally similar HTLV and HIV protease using HIV-PR inhibitors", *J Recept Signal Transduct Res.*, 34(5), 361-71 (IF: 2.27).
6. Yadav S, Gupta S, Selvaraj C, Doharey PK, Verma A, Singh SK, Saxena JK. , (2014), "In silico and in vitro studies on the protein-protein interactions between *Brugia malayi* immunomodulatory protein calreticulin and human C1q", *PLoS One.*, 9(9):e106413 (IF: 3.23).
7. Selvaraj C, **Singh SK.**, (2014), "Validation of potential inhibitors for SrtA against *Bacillus anthracis* by combined approach of ligand-based and molecular dynamics simulation", *J Biomol Struct Dyn.*, 32(8): 1333-49 (IF:2.91).
8. Selvaraj C, Sivakamavalli J, Vaseeharan B, Singh P, **Singh SK.**, (2014), "Examine the characterization of biofilm formation and inhibition by targeting SrtA mechanism in *Bacillus subtilis*: a combined experimental and theoretical study", *J Mol Model.*, 20(8): 2364. (IF: 1.73).
9. Reddy KK, **Singh SK.**, (2014), "Combined ligand and structure-based approaches on HIV-1 integrase strand transfer inhibitors", *Chem Biol Interact.*, 218: 71-81 (IF: 2.57).
10. Vijayalakshmi P, Selvaraj C, Shafreen RMB, **Singh SK**, Pandian, SK, Daisy P., (2014), "Ligand based pharmacophore modelling and screening of DNA minor groove binders targeting *Staphylococcus aureus*. *J Mol Recognit.*, 27(7):429-37 (IF: 2.15).
11. Selvaraj C, Sivakamavalli J, Vaseeharan B, **Singh SK.**, (2014), "Virtual Screening of LPXTG competitive SrtA inhibitors targeting signal transduction mechanism in *Bacillus anthracis*: A combined experimental and theoretical study", *J Recept Signal Transduct Res.*,34(3):221-32 (IF: 2.27).
12. Muralidharan A, Selvaraj C, **Singh SK**, Nelson Jesudasan CA, Geraldine P, Thomas P., (2014), "Virtual screening based on pharmacophoric features of known calpain inhibitors to identify potent inhibitors of calpain", *Med Chem Res.*, 23(5):2445-55 (IF: 1.40).

13. Sivakamavalli J, Selvaraj C, **Singh SK**, Vaseeharan B., (2014), "Interaction investigations of crustacean  $\beta$ -GBP recognition towards pathogenic microbial cell membrane and stimulate upon Prophenoloxidase activation", *J Mol Recognit.*, 27(4):173-183. (IF:2.15)
14. Shafreen RM, Selvaraj C, **Singh SK**, Pandian SK., (2014), "In silico and in vitro studies of cinnamaldehyde and their derivatives against LuxS in *Streptococcus pyogenes*: effects on biofilm and virulence genes", *J Mol Recognit.*, 27(2):106-116 (IF:2.15).
15. Selvaraj C, Singh P, **Singh SK.**, (2014), "Investigations on the Interactions of lambda Phage-Derived Peptides against the SrtA Mechanism in *Bacillus anthracis*", *Appl Biochem Biotechnol.*, 172(4): 1790-806 (IF:1.73).
16. Tripathi SK, **Singh SK.**, (2014), "Insights into the structural basis of 3,5-diaminoindazoles as CDK2 inhibitors: prediction of binding modes and potency by QM-MM interaction, MESP and MD simulation", *Mol Biosyst.*, 10(8): 2189-201 (IF:3.21).
17. Selvaraj C, Sivakamavalli J, Vaseeharan B, Singh P, **Singh SK.**, (2014), "Structural Elucidation of SrtA enzyme in *Enterococcus faecalis*: An Emphasis on Screening of Potential Inhibitors against the Biofilm Formation", *Mol BioSyst.*, 10(7): 1775-89 (IF:3.21).
18. Reddy KK, Singh P, **Singh SK.**, (2014), "Blocking the interaction between HIV-1 integrase and human LEDGF/p75: mutational studies, virtual screening and molecular dynamics simulations", *Mol BioSyst.*, 10(3):526-36. (IF:3.21)
19. **Pappu Srinivasan**, Palanisamy Chella Perumal, & Arumugam Sudha, (2014), "Discovery of novel inhibitors for Nek6 protein through homology model assisted structure based virtual screening and molecular docking approaches", *The Scientific World Journal*, 967873 (IF: 1.73).
20. Arumugam Sudha, **Pappu Srinivasan** & Palanivel Rameshthangam, (2014), "Exploration of potential EGFR inhibitors: a combination of Pharmacophore-based virtual screening, atom-based 3D-QSAR and molecular docking analysis", *Journal of Receptors and Signal Transduction*, 29, 1-12. (IF: 2.27).
21. Thangaraj Sindhu, Sundaraj Rajamanikandan and **Pappu Srinivasan**, (2014), "In vitro anti-oxidant and anti-bacterial activities of *Kyllinga nemoralis*", *Indian Journal of Pharmaceutical Sciences*, 76, 170-174. (IF: 0.76).
22. Arumugam Sudha & **Pappu Srinivasan**, (2014), "Bioassay-guided isolation and antioxidant evaluation of flavonoid compound from aerial parts of *Lippia nodiflora* L", *BioMed Research International*, 549836, (IF: 2.13).
23. Durai Prabhu, Chinnasamy Arulvasu, Gajendran Babu, Ramar Manikandan, **Pappu Srinivasan**, Govindaraju Kasivelu, Ashokkumar Thirunavukkarasu, (2014), "Synthesis and characterization of silver nanoparticles using crystal compound of sodium para-hydroxybenzoate tetrahydrate isolated from *Vitex negundo*. L leaves and its apoptotic effect on human colon cancer cell lines", *European Journal of Medicinal Chemistry*, 84, 90-99. (IF: 3.44).
24. Thangaraj Sindhu and **Pappu Srinivasan**, (2014), "Pharmacophore modeling, 3D QSAR and molecular docking studies of benzimidazole derivatives as potential FXR agonists", *Journal of Receptors and Signal Transduction*, 34, 241-253. (IF: 2.27).

25. Arumugam Sudha & **Pappu Srinivasan**, (2014), “Bioassay-guided isolation, identification and molecular ligand-target insight of lipoxygenase inhibitors from leaves of *Anisomeles malabarica* R.Br”, *Pharmacognosy Magazine*, 10, 596-605. (IF: 1.25).
26. P. Arthi, Haleel Azees, **Pappu Srinivasan**, Chinnasamy Arulvasu, Durai Prabhu & A. Kalilur Rahiman, (2014), “Antibacterial, DNA interaction and cytotoxic activities of pendant-armed polyamine macrocyclic dinuclear nickel(II) and copper(II) complexes”, *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy*, 129, 400–414. (IF: 2.65).
27. P. Arthi, S. Shobana, **Pappu Srinivasan**, A. Kalilur Rahiman, (2014), “Synthesis, antibacterial, docking and anticancer evaluation of N-substituted benzoyl derivatives”, *Journal of Chosun Natural Science*, 7, 241–252. (IF: 0.44).
28. Singh KhD, Ajay J, Kaur H, Kukreti R, **Karthikeyan M\***, (2014), “Renin Angiotensin System gene polymorphisms in response to antihypertensive drugs and visit-to-visit blood pressure variability in essential hypertensive patients” *Current Pharmacogenomics and Personalized Medicine*, , 227-235 (Bentham Science Publishers). DOI: 10.2174/1875692113666150420225829.
29. Singh KhD, **Karthikeyan M\***, (2014), “Combined sequence and sequence-structure-based methods for analyzing RAAS gene SNPs: a computational approach”, *Journal of Receptors and Signal Transduction Research*, 34(6): 513-526. PMID: 24878201, DOI: 10.3109/10799893.2014.922575 (IF:1.611)
30. Kirubakaran P, Arunkumar P, Premkumar K, **Karthikeyan M\***, (2014), “Sighting of Tankyrase inhibitors by structure and ligand based screening and in vitro approach”, *Molecular BioSystems (RSC)*, 10, 2699-2712. PMID: 25091558, DOI: 10.1039/c4mb00309h (IF: 3.35)
31. **Karthikeyan M\***, Kirubakaran P, Singh KhD, Bhuvaneshwari S, Gopinath K, (2014), “Understanding the evolutionary relationship of HA protein from influenza viruses using phylogenetic approach and molecular modeling studies”, *Journal of Biomolecular Structure & Dynamics*, 32 (5), 816-830. PMID: 23782165, DOI: 10.1080/07391102.2013.793211, (IF: 2.983)
32. Singh KhD, Naveena Q, **Karthikeyan M\***, (2014), “Jak2 inhibitor – a jackpot for pharmaceutical industries: a comprehensive computational method in the discovery of new potent Jak2 inhibitors”, *Molecular BioSystems (RSC)*, 10, 2146-2159. PMID: 24874539, DOI: 10.1039/c4mb00071d (IF: 3.35)
33. Singh KhD, Ajay J, Harpreet K, Ritushree K, **Karthikeyan M\***, (2014), “Gender specific association of RAS gene polymorphism with essential hypertension – a case control study”, *BioMed Research International*, PMID: 24860821, (DOI: 10.1155/2014/538053), (IF: 2.706)
34. Kirubakaran P, Kothandan G, Cho SJ, **Karthikeyan M\***, (2014), “Molecular insights on TNKS1/TNKS2 and inhibitor-IWR1 interactions”, *Molecular BioSystems (RSC)*, 10, 281-293. PMID: 24291818, DOI: 10.1039/c3mb70305c, (IF: 3.3)
35. Kirubakaran P, Kothandan G, Cho SJ, **Karthikeyan M\***, (2014), “Molecular insights on TNKS1/TNKS2 and inhibitor-IWR1 interactions”, *Molecular BioSystems (RSC)*, 10, 281-293. PMID: 24291818, DOI: 10.1039/c3mb70305c (IF: 3.35)

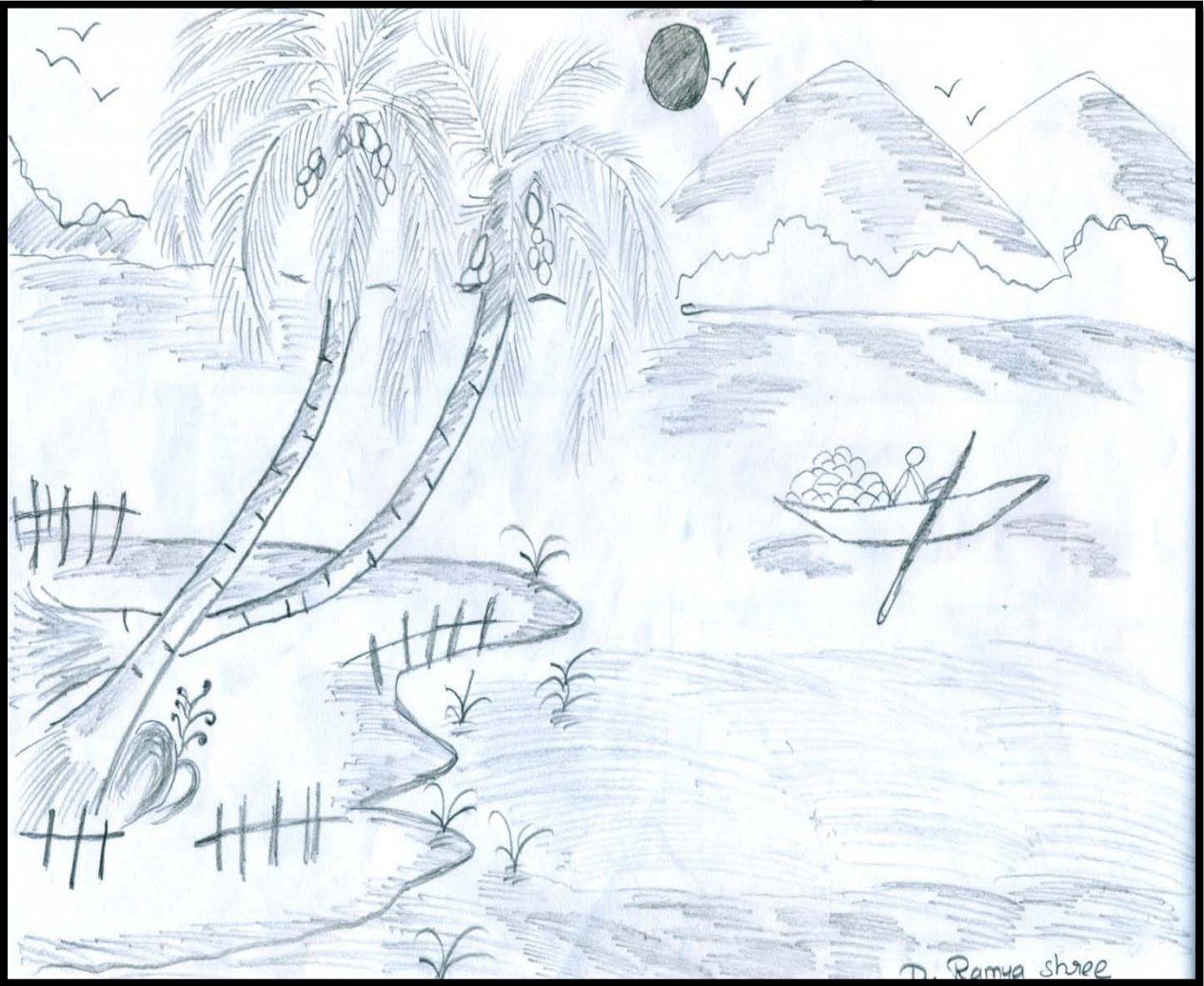
**Student's Corner**



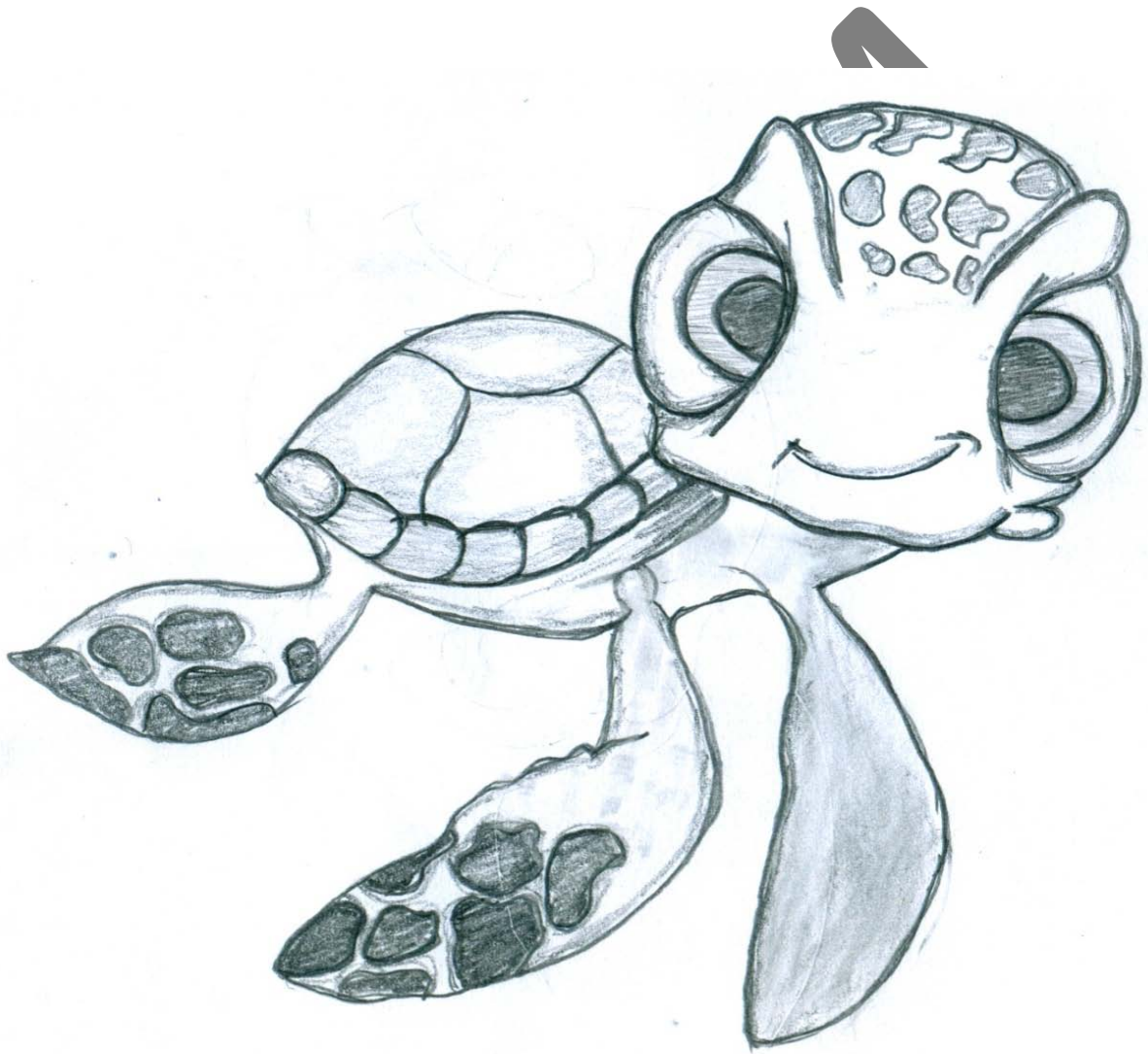
**Ms. S. Deepika**  
**M.SC II yr**



**Ms. R. Kanimozhi**  
**M.SC II yr**



**Ms. T. Nithya**  
**M.SC II yr**



**Ms. P. Pappathi**  
**M.SC II yr**



▶ காரைக்குடி அழகப்பா பல்கலைக்கழகத்தில் நடந்த கருத்தரங்கில் மேலாண்மை நிறுவன இயக்குனர் கருத்தையாண்டியன் பேசினார்.

## புதிய கண்டுபிடிப்புகளில் மாணவர்கள் ஈடுபடுவது குறைவாக உள்ளது

### மேலாண்மை நிறுவன இயக்குநர் வருத்தம்

காரைக்குடி, ஏப். 23: மாணவர்கள் சமுதாயத்துக்கு தேவையான புதிய கண்டுபிடிப்புகளில் ஈடுபடுவது குறைந்து வருகிறது என திருச்சி பாராதிதாசன் மேலாண்மை நிறுவன இயக்குநர் கருத்தையாண்டியன் ஐ.ஏ.எஸ் தெரிவித்தார்.

காரைக்குடி அழகப்பா பல்கலைக்கழக உயிரிதகவலியல் துறைசார்பில் உலக படைப்பாற்றல் தினம் கொண்டாடப்பட்டது. உயிரிதகவலியல் துறை தலைவர் ஜெயகாந்தன் வரவேற்றார். திருச்சி பாரதிதாசன் மேலாண்மை நிறுவனத்தின் இயக்குநர் கருத்தையாண்டியன் தனது தலைவரின் தலைவரின் முன்னோடி என அழைக்கப்படும் வியானார்டோ டாவின்கி பிறந்தநாள் உலக படைப்பாற்றல் தினமாக கொண்டாடப்பட்டு வருகிறது.

இந்தியா மட்டுமல்லாமல் உலகில் 46 நாடுகளில் இந்நாள் கொண்டாடப்படுகிறது. படைப்பாற்றல் என்பது புதிய திட்டங்களை திறம்பட யோசித்து செயல்படிவம் கொடுப்பதே யாகும். ஆனால் தற்போது உள்ள நிலையில் புதிய கண்டுபிடிப்புகளில் மாணவர்கள் ஈடுபடுவது என்பது மிகவும் குறைவாக உள்ளது. பணம் சம்பாதிக்க வேண்டும் என்பதில் மட்டும்தான் தங்களது கவனத்தை செலுத்துகின்றனர். தங்களது அறிவு, திறமைகளை சமுதாய முன்னேற்றத்துக்கு பயன்படுத்த தயங்குகின்றனர். புதிய கண்டுபிடிப்புகளில் மாணவர்கள் ஈடுபட வேண்டும்.

மாணவர்கள் தங்களின் தனித்திறமையை வெளிக்கொண்டுவந்து கண்டுபிடிப்புகளில் புதுமையை புகுத்த வேண்டும். இதன் மூலம் நமது சமூகம், சமுதாயம் முன்னேற்றம் அடைவதோடு, பொருளாதார வளர்ச்சிக்கும் உதவும். இனம் ஆராய்ச்சியாளர்களை உருவாக்க இந்திய அறிவியல் தொழில்நுட்ப கழகம் மற்றும் யூஜிஜி ஊக்கத்தொகை வழங்குகிறது. பின்னர் 2 முதல் பல்கலைக்கழக உயர்கல்வி

மற்றும் பி.எச்.டி வரை ரூ.5000 முதல் 80 ஆயிரம் வரை ஊக்கத்தொகை வழங்கிறது. இதில் மாணவர்களுக்கு என தனியாக சிறப்பு திட்டங்களும் செயல்படுத்தப்பட்டு வருகின்றன என பேசினார்.

பல்கலைக்கழக துணைவேந்தர் பொறுப்புக்குழு உறுப்பினர் கபால்சந்திரபோஸ் பேசுகையில், 'சமுதாயத்திற்கும், தனிமனித வளர்ச்சிக்கும் படைப்பாற்றல் அளப்பரிய பங்காற்றுகின்றன. சட்டங்கள் மனிதவள மேம்பாட்டிற்கு மட்டுமே பயன்பட வேண்டும். வளர்ச்சி மேம்பாட்டிற்கு உதவும் வகையில் சட்டங்கள் மாற்றப்பட வேண்டும். புதிய சிந்தனை கொண்ட மனிதர்களே புதிய உலகை உருவாக்குவார்கள். சிந்தனை பகிர்மானம், குழு முயற்சி போன்றவை இன்றைய சமுதாயத்திற்கு தேவையாக உள்ளது என பேசினார்.

அழகப்பா பல்கலைக்கழக கலைத்துறை உண்நாராயணமூர்த்தி, திட்டம் மற்றும் வளர்ச்சி பிரிவு அதிகாரி குருமல்லேஷ் பிரபு உள்பட பலர் கலந்து கொண்டனர். இணைப்பேராசிரியர் சஞ்சீவகுமார்சிங் நன்றி கூறினார்.

## மனித வள மேம்பாட்டுக்கு மட்டுமே சட்டங்கள்

காரைக்குடி, ஏப்.25-

காலை அழகப்பா பல்கலைக் கழக உயிரி தகவலியல் துறை சார்பில், உலக படைப்பாற்றல் தினம், அறிவியல் வளாக கருத்தரங்கு கூடத்தில் நடந்தது. திருச்சி பாரதிதாசன் மேலான்மை நிறுவன இயக்குனர், கருத்தையா பாண்டியன் தலைமை வகித்தார். அழகப்பா பல்கலை துணைவேந்தர் பொறுப்புக்குழு உறுப்பினர் சுபாஷ் சந்திரபோஸ் பேசியதாவது: மனித சமுதாயத்திற்கும், தனி மனித வளர்ச்சிக்கும் படைப்பாற்றல் மற்றும் புதுமுறை

### பொறுப்புக்குழு உறுப்பினர் பேச்சு

காணல், அளப்பரிய பங்காற்றுகின்றன. சட்டங்கள் மனித வள மேம்பாட்டிற்கு மட்டுமே, சட்டங்களைக் காக மனிதர்கள் இல்லை. வளர்ச்சி மேம்பாட்டிற்கு உதவும் வகையில், சட்டங்கள் மாற்றப்பட வேண்டும். புதிய சிந்தனைகளை மனித குலம் ஏற்று கொள்ள வேண்டும். இத்தகைய சமுதாயமே, சமூக

பொருளாதாரத்தில் முன்னேற்றம் அடையும். புதிய சிந்தனை கொண்ட மனிதர்களே, புதிய உலகை உருவாக்குவார்கள். சிந்தனை பகிர்மானம், குழு முயற்சி போன்றவை, இன்றைய சமுதாயத்திற்கு தேவையாக இருக்கிறது, என்றார்.

கலைத்துறை முதன்மையர் நாராயணமூர்த்தி, திட்டம் மற்றும் வளர்ச்சி பிரிவு சிறப்பு அதிகாரி குருமல்லேஷ்பிரபு பங்கேற்றனர். துறை தலைவர் ஜெயகாந்தன் வரவேற்றார். பேராசிரியர் சஞ்சீவகுமார் சிங் நன்றி கூறினார்.

தினமலர்

திங்கள் ■ ஆகஸ்ட் 11, 2014

## கருத்தரங்கு

காரைக்குடி, ஆக.11-

காரைக்குடி உமையாள் ராமனாதன் மகளிர் கல்லூரியில், உயிர் தொழில் நுட்பவியல் துறை சார்பில், தேசிய செயல் விளக்க கருத்தரங்கு நடந்தது. கல்லூரி தலைவர் ராமனாதன் வைரவன் முன்னிலை வகித்தார். முதல்வர் ஹேமாமாலினி, துணை முதல்வர் லட்சுமி வரவேற்றனர். அழகப்பா பல்கலை உயிர் தகவலியல் பேராசிரியர் ஜெயகாந்தன், கொச்சி லியாட்ரிஸ் பயோசயின்ஸ் முதன்மை தொழில் நுட்ப அலுவலர் சிடியன், நிர்வாக அலுவலர் ரஞ்சித் பாலோஸ் பேசினார். துறை தலைவர் சித்ரா, மாரீஸ்வரி, செல்வி ஒருங்கிணைப்பாளர்களாக செயல்பட்டனர். பேராசிரியை வினோதினி நன்றி கூறினார்.



## 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

