# DEPARTMENT OF BIOINFORMATICS

# ALAGAPPA UNIVERSITY

*(A State University Reaccredited with 'A' Grade by NAAC)*

**KARAIKUDI-630 004, TAMIL NADU, INDIA**

## 8th National Symposium cum Workshop on "RECENT TRENDS IN STRUCTURAL BIOINFORMATICS AND COMPUTER AIDED DRUG DESIGN" (SBCADD'2016)

**16th – 19th February, 2016**

**ABSTRACTS RECEIVED FOR POSTER PRESENTATION**

| S.No | Title of Abstract | Status |
|---|---|---|
| 1. | **Crystal structure and docking studies of 3-phenyl-3a,4-dihydro-3H-chromeno[4,3-c]isoxazole-3a-carbonitrile**<br>**M.Sivakumar**, S.Aravindhan*<br>Department of Physics, Presidency College, Chennai-5, Tamil Nadu, India. | **Accepted** |
| 2. | **Toxicity of Au and Au-Pt metal nanoparticles against cancer cell lines (HepG2): Recent insights from *in vitro* study**<br>**P.Boomi[1]** and H.Gurumallesh Prabu[2*]<br>[1]Department of Bioinformatics, Alagappa University, Karaikudi-4.<br>[2]Department of Industrial Chemistry, School of Chemistry, Alagappa University, Karaikudi-3. | **Accepted** |
| 3. | **Biochemical and Structural analysis of ID3 protein by X-Ray Crystallography: An important therapeutic target for various cancers**<br>**Guneswar Sethi[1]**, **Krishna Kant Gupta[1]**, Sharad Awasthi[2], Arunkumar Dhayalan[2], Ramadas Krishna[1*]<br>[1]Centre for Bioinformatics, Pondicherry University, Pondicherry, 605014, India<br>[2]Department of Biotechnology, Pondicherry University, Pondicherry, 605014, India | **Accepted** |
| 4. | **Atom-based 3D-QSAR studies on 5-(Substituted Benzylidene)Thiazolidine-2,4-dione Derivatives as PTP1B inhibitors**<br>**Gopinath Krishnasamy** and Karthikeyan Muthusamy*<br>Department of Bioinformatics, Science Block, Alagappa University, Karaikudi – 630 004, Tamil Nadu, India. | **Accepted** |
| 5. | **E-Pharmacophore based virtual screening to identify potent inhibitors against snake venom Phospholipase A2 (PLA2)**<br>**Sathishkumar Chinnasamy** and Karthikeyan Muthusamy*<br>Department of Bioinformatics, Science Block, Alagappa University, Karaikudi – 630 004, Tamil Nadu, India. | **Accepted** |
| 6. | **Pharmacophore, 3D-QSAR, MDs studies on 4-hydroxy-2-isopropylhexanamides and piperidine-3-carboxamides as Direct Renin Inhibitors**<br>**Loganathan Lakshmanan**, John Marshal Jayaraj, Karthikeyan Muthusamy*<br>Department of Bioinformatics, Alagappa University, Karaikudi – 630 004 | **Accepted** |

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| 7. | **Identification of potent active compounds against SUB3 protein of Dermatophytes. A Virtual Screening, MM-GBSA and Molecular Dynamics studies**<br>**Umamaheswari. S[1], Rajasekaran Kanimozhi[2]**, Loganathan Lakshmanan[2], D. Arvind Prasanth[1] and Karthikeyan Muthusamy[2]*<br>[1]Department of Microbiology, Periyar University, Salem – 636 011, Tamil Nadu, India<br>[2]Department of Bioinformatics, Alagappa University, Karaikudi – 630 004, Tamil Nadu, India | **Accepted** |
| 8. | **Assessment on Superior Protein Structure of Transgenic Cucumber (*Cucumis sativus* L.) using Computational Tools and Software's**<br>**J. Joseph Sahayarayan[1]**, A. Ganapathi[2]*<br>[1]Department of Bioinformatics, Science Block, Alagappa University, Karaikudi – 630 004.<br>[2]Department of biotechnology and Genetic Engineering, Bharathidasan University, Thiruchirapalli – 620 024. | **Accepted** |
| 9. | **Calcium Phosphate Metabolic Inhibitors Regulate the Chronic Kidney Disease (CKD) Disease Pathogenesis – Theoretical Insights**<br>**Selvaraman Nagamani[1]**, Chandrasekhar Kesavan[2], Karthikeyan Muthusamy[1*]<br>[1] Department of Bioinformatics, Science Block, Alagappa University, Karaikudi – 630004, Tamilnadu, India.<br>[2] Loma Linda Veterans Medical Center and Loma Linda University, 11201 Benton Street, Loma Linda, CA 92357, United States of America. | **Accepted** |
| 10. | **Selective agonists for VDR through E-Pharmacophore screening, Molecular Docking, Molecular Dynamics study.**<br>**John Marshal Jayaraj**, Karthikeyan Muthusamy*<br>Department of Bioinformatics, Alagappa University, Karaikudi – 630 004. | **Accepted** |
| 11. | **Protein-Protein Docking and Molecular dynamics of CAD protein from hyperthermophilic *Thermus thermophilus* HB8**<br>**Sureka Kanagarajan**, Nachiappan Muthurasappan, Dhamodharan Prabhu and Jeyaraman Jeyakanthan*<br>Structural Biology and Bio - Computing Lab, Department of Bioinformatics, Science Block, Alagappa University, Karaikudi - 630 004, Tamil Nadu, India. | **Accepted** |
| 12. | **The Functional characterization of *Streptococcus agalactiae* surface protein, PavA**<br>**Shobana Ponnuvel** and Karthe Ponnuraj*<br>Centre of Advanced Study in Crystallography & Biophysics, University of Madras, Guindy Campus, Chennai – 600 025 | **Accepted** |
| 13. | **Understanding the mechanism of specific t-RNA synthetase from *Thermus thermophilus* HB8 - An *in silico* approach**<br>**Nachiappan Muthurasappan** and Jeyaraman Jeyakanthan*<br>Structural Biology and Bio-Computing Laboratory, Department of Bioinformatics, Science Block, Alagappa University, Karaikudi - 630 004, Tamil Nadu, India. | **Accepted** |
| 14. | **Identification of Potent Lead molecules for Streptomycin 3'' - adenylyltransferase from *Serratia marcescens* using computational approach**<br>**Dhamodharan Prabhu** and Jeyaraman Jeyakanthan*<br>Structural Biology and Bio - Computing Lab, Department of Bioinformatics, Tamil Nadu, India, Science Block, Alagappa University, Karaikudi - 630 004. | **Accepted** |

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| 15. | **Cloning, Expression and Purification of Glycinamide Ribonucelotide Synthetase (GARS) from *Pyrococcous horikoshii* OT3**<br>**R. Guru Raj Rao[1]**, Nachiappan Muthurasappan[1], Sureka Kanagarajan[1], Jayashree Biswal[1], K. Sekar[2] and Jeyaraman Jeyakanthan[1]*<br>[1]Structural Biology and Bio - Computing Lab, Department of Bioinformatics, Science Block, Alagappa University, Karaikudi - 630 004, Tamil Nadu, India<br>[2]Supercomputer Education and Research Center, Indian Institute of Science, Bangalore – 560 012. | **Accepted** |
| 16. | **Exploring the binding specificity of exogenous amino acids in response to transcriptional interactions of TRP protein – DNA complex using computational studies**<br>**Mariadasse Richard** and Jeyaraman Jeyakanthan*<br>Structural Biology and Bio - Computing Lab, Department of Bioinformatics, Science Block, Alagappa University, Karaikudi - 630 004, Tamil Nadu, India. | **Accepted** |
| 17. | **Database of Medicinal Plants for the Treatment of Jaundice**<br>**M.L. Abillasha**, N. Vithya, C. Lakshmi Priya, Santhosh Solomon, N. Bharathi*<br>Department of Plant Molecular Biology &Bioinformatics, Tamil Nadu Agricultural University, Coimbatore-641003. | **Accepted** |
| 18. | **Structural and Mechanistic insights on novel target Calcium/Calmodulin dependent protein Kinase Kinase 1 (CAMKK1) using *In silico* approaches**<br>**Prajisha. J** and Jeyaraman Jeyakanthan*<br>Structural Biology and Bio - Computing Lab, Department of Bioinformatics, Science Block, Alagappa University, Karaikudi - 630 004, Tamil Nadu, India. | **Accepted** |
| 19. | **Transcriptional Regulation by p21-Activating Kinase-1 with an Agonist RUNX3 and Antagonist Peptides modulating Pancreatic Cancer: A Structural and Computational Approach.**<br>**Jayashree Biswal[1]**, Suresh Kumar Rayala[2], Ganesh Venkatraman[3] and Jeyaraman Jeyakanthan[1*]<br>[1]Structural Biology and Bio – Computing Lab, Department of Bioinformatics, Science Block, Alagappa University, Karaikudi - 630 004, Tamil Nadu, India.<br>[2]Department of Biotechnology, Indian Institute of Technology Madras, Room No. BT 306, Chennai-600 036, Tamil Nadu, India.<br>[3]Department of Human Genetics, College of Biomedical Sciences, Sri Ramachandra University, Porur, Chennai-600 116, Tamil Nadu, India. | **Accepted** |
| 20. | **Pharmacogenomics study of UDP-glucuronosyl transferase enzyme**<br>**Ida Malarselvi R[1]**, Niraimathi S[2*], Ramachandra Raja C[1] and Priscilla J[3]<br>[1]Centre for Advanced Material Research, Government Arts College(Autonomous), Kumbakonam-612001,TamilNadu,India.<br>[2]Sri Issac Newton College of Arts & Science, Pappakovil, Nagapattinam -611001.Tamil Nadu, India.<br>[3]PG and Research Department of Physics, A.D.M.College for Women(Autonomous), Nagapattinam- 611001.Tamil Nadu, India | **Accepted** |
| 21. | **Pharmacophore modeling and structure based virtual screening to identify potent inhibitors targeting LuxP of *Vibrio harveyi***<br>**Sundaraj Rajamanikandan[1]** and Pappu Srinivasan[2*]<br>[1]Department of Bioinformatics, [2]Department of Animal Health and Management, Science Block, Alagappa University, Karaikudi, Tamilnadu, India | **Accepted** |
| 22. | **Molecular modeling, Molecular dynamics and Structure-Based Virtual screening of LuxS protein from *V. alginolyticus***<br>**Dakshinamurthy Sasikala[1]** and Pappu Srinivasan[2*]<br>[1]Department of Bioinformatics, [2]Department of Animal Health and Management, Science Block, Alagappa University, Karaikudi, Tamilnadu, India | **Accepted** |

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| 23. | ***In Silico* evaluation of LuxR Inhibition by Cinnamaldehyde analogues and phage particles**<br>**Nattan Stalin**[a] and Pappu Srinivasan[b]*<br>[a]Molecular Biology Laboratory, Department of Bioinformatics,<br>[b]Department of Animal Health and Management, Alagappa University, Karaikudi - 630 004, Tamilnadu, India | **Accepted** |
| 24. | **An insight into understanding activity of potential inhibitors for Juvenile Idiopathic Arthritis**<br>**N. Bharathi*, M. Jayakanthan***, L.T. Saravanakumar , N. K. Kavinkumar, U. Sathvika<br>Department of Plant Molecular Biology &Bioinformatics, Tamil Nadu Agricultural University, Coimbatore-641003. | **Accepted** |
| 25. | **Investigation of nsSNPs with uncertain significance in extracellular domains 1&2 of Cadherin 23 – a structural bioinformatics approach**<br>**Paridhy Vanniya S** and C R Srikumari Srisailapathy*<br>Department of Genetics, Dr. ALM PG IBMS, University of Madras, Taramani, Chennai – 600113 | **Accepted** |
| 26. | **Molecular Modeling studies on Grp94 inhibitors: Assessment of various partial atomic charges on Statistical Quality of 3D-QSAR CoMSIA models.**<br>**Saikiran Reddy Peddi**, **Sree Kanth Sivan**, Vijjulatha Manga*<br>MMMC, Department of Chemistry, University College of Science, Osmania University, Hyderabad – 500007 | **Accepted** |
| 27. | **FABP-db: A database on the Fatty Acid-Binding Proteins**<br>**R. Santhosh**[1], Daliah Michael[2], K. Sekar[2] and J. Jeyakanthan[1]*<br>[1]Structural Biology and Bio Computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi - 630 004, Tamil Nadu, India<br>[2]Department of Computational and Data Sciences, Indian Institute of Science, Bangalore - 560 012, Karnataka India | **Accepted** |
| 28. | **Microseed matrix-screening (rMMS): introduction, theory, practice and a new technique for membrane protein crystallization in LCP**<br>Stefan A. Kolek[1], Patrick D. Shaw Stewart[1] and Bastian Bräuning[2].<br>[1]Douglas Instruments Ltd, UK, [2]Technische Universität München, Germany | **Accepted** |
| 29. | **Fourier analysis of orientation of protein structure**<br>**Ashok Palaniappan**<br>Department of Computational Biology, Faculty of Allied Health Sciences, Chettinad Academy of Research and Education, Kelambakkam – 603103 | **Accepted** |
| 30. | **Molecular Docking and Structural analysis of Calcium dependent CatSper ion channels.**<br>**J.M.Jeffrey**, S.Gopinath and C.R.Srikumari Srisailapathy*<br>Department of Genetics, Dr.ALM PG IBMS, University of Madras, Taramani, Chennai-113. | **Accepted** |
| 31. | **Identification of Allosteric Inhibitor for Protein Kinase B (AKT) Using Pharmacophore Based Virtual Screening and its Biological Evaluation**<br>**Pragna Lakshmi[1, 2]**, Veena Vijaykumar[3], Sakthivel Natarajan[3], Krishna Ramadas[1*]<br>[1]Centre for Bioinformatics, Pondicherry University, Pondicherry.<br>[2]Interdisciplinary Program in Life Sciences, Pondicherry University, Pondicherry.<br>[3]Department of Biotechnology, Pondicherry University, Pondicherry. | **Accepted** |
| 32. | **Target Identification in *Fusobacterium nucleatum* by Subtractive Genomics Approach and Enrichment Analysis of Host-Pathogen Protein-Protein Interactions**<br>**Amit Kumar[1]**, Pragna Lakshmi[1], Basant Kumar Tiwary[2], Ramadas Krishna[1*]<br>[1] Centre for Bioinformatics, Pondicherry University, Puducherry-605014, India.<br>[2] Centre Head, Centre for Bioinformatics, Pondicherry University, Puducherry-605014, India. | **Accepted** |
| 33. | **Pharmacophore Modeling and Molecular Docking Studies on 4-Aminoquinolone Piperidine Amide Derivatives as DprE1 Inhibitors**<br>**Tanmoy Mukherjee[1*]**, Sudipta Mondal[2] , Debanjan Sen[1]<br>[1]Bengal Institute of Pharmaceutical Sciences, Kalyani, Nadia-741235, W.B<br>[2]Department of Bioinformatics, Alagappa University, Karaikudi-630003, T.N | **Accepted** |

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| 34. | **Hoxc8 inhibition design in disease relation to Osteopontin gene - A therapeutic approach using molecular docking**<br>**Kalaimathi.M[1]*** and Sujatha Roy Saha[2]<br>[1]Department of Genetics, Dr.ALM Post Graduate Institute of Basic Medical Sciences, University of Madras, Chennai-600113.<br>[2]Bionteq Biosciences, Vadapalani, Chennai-600026. | **Accepted** |
| 35. | ***in silico* Screening of Derivatives of Active Compounds As B-Raf (V600e) Receptor Inhibitors For Anticancer Activity**<br>**Aiswarya Pradeep** and Dr. Puniethaa Prabhu*<br>Department of Biotechnology, K.S.Rangasamy College Of Technology, Tiruchengode, Namakkal- 637215. | **Accepted** |
| 36. | **Conformational flexibility and Electrostatic properties of Dilantin molecule in the active site of estrogen receptor-α : A Quantum chemical and charge density Study**<br>**C. Kalaiarasi** and P. Kumaradhas*<br>Laboratory of Biocrystallography and Computational Molecular Biology, Department of Physics, Periyar University, Salem-636 011, India | **Accepted** |
| 37. | **Understanding the structure and Electronic properties of Galangin in the active site of AChE via Molecular docking and Charge density analysis**<br>**K. Saravanan** and P. Kumaradhas*<br>Laboratory of Biocrystallography and Computational Molecular Biology, Department of Physics, Periyar University, Salem–636 011 | **Accepted** |
| 38. | **Structure, charge density distribution and electrostatic potential of catechin derivatives in the active site of p300 enzyme: A Molecular docking and Charge density analysis**<br>**M. Sivanandam**, D. Aruna and P. Kumaradhas*<br>Laboratory of Biocrystallography and Computational Molecular Biology, Department of Physics, Periyar University, Salem- 636 011, India | **Accepted** |
| 39. | **Exploration on the stability and interactions of the HPV virus through combined Structure and Ligand based methods**<br>**Murali Aarthy**, Ravi Ponnazhagu and Sanjeev Kumar Singh*<br>Computer Aided Drug Design and Molecular Modelling Lab, Department of Bioinformatics, Alagappa University, Karaikudi-630004, Tamil Nadu, India | **Accepted** |
| 40. | **Atomic charge, Electrostatic potential, solvation energy and MMGBSA binding free energy calculation on PCAF BRD inhibitors**<br>**Venkatesan Suryanarayanan**, Aasaithambi Kasthuri and Sanjeev Kumar Singh*<br>Computer Aided Drug Design and Molecular Modelling Lab, Department of Bioinformatics, Alagappa University, Karaikudi-630004, Tamil Nadu, India | **Accepted** |
| 41. | **Water-mediated interactions in the structural discrimination between purines and between pyrimidines by proteins**<br>**S. Usha[1]**, S. Selvaraj[2], Sanjeev Kumar Singh[1]*<br>[1]Department of Bioinformatics, Alagappa University, Science Block, Karaikudi – 630004<br>[2]Department of Bioinformatics, Bharathidasan University, Tiruchirappalli – 620024 | **Accepted** |
| 42. | **Shape-based virtual screening, docking and dynamics to identify the novel negative allosteric modulators for mGluR5**<br>**Vijaya Prabhu. S** , Sanjeev Kumar Singh*<br>Department of Bioinformatics, Alagappa University, Science Block, Karaikudi – 630004 | **Accepted** |
| 43. | **Structure analysis of single nucleotide polymorphism G241R occurring in Human Apex1- a molecular dynamics study**<br>**K Keerthi**, K Anbarasu and S Jayanthi*<br>School of Bio Sciences and Technology, VIT University, Vellore-632014 | **Accepted** |

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| 44. | **Molecular Modeling and Designing of Inhibitors against HLA-DQB1 gene of Type 1 Diabetes**<br>**Radha Mahendran*,** Lakshmi Narayanan, Annie Absala Trace, Suganya Jeyabaskar, Agnal Vincent Paul, Hubert.J<br>Department of Bioinformatics, School of Life Science, Vels University, Chennai-600 043. | **Accepted** |
| 45. | ***In silico* Identification of PTP1B Inhibitors isolated from *Sterculia foetida* against Diabetes mellitus Type II**<br>**Suganya Jeyabaskar**, Hubert. J, Radha Mahendran*, Annie absala trace, Marimuthu Nishandhini, Lakshmi Narayanan.S, Agnal Vincent paul,<br>Department of Bioinformatics, Vels University, Chennai- 600 117, India. | **Accepted** |
| 46. | **Inhibition of Claudin-10 expression using promising naturalplant compounds: An in silico approach**<br>**Majji Rambabu**, Sivaraman Jayanthi*<br>School of Bio Sciences and Technology, VIT University, Vellore-632014 | **Accepted** |
| 47. | **Crystal Structure and Docking Studies of N-((4 methoxyphenyl) carbamothioyl) cyclohexanecarboxamide**<br>**P. Periyannan, K. Ravichandran*** and M. Beemaro<br>Department of Physics, Kandaswami Kandar's College, Velur (PO), Namakkal-638 182. | **Accepted** |
| 48. | **Computational Investigation of POMC gene through SNP analysis, modeling, and simulations**<br>**Sai Somesh V**, Ingle Surabhi S, Karthik N and Sajitha Lulu.S*<br>Department of Biotechnology, School of Bio Sciences and Technology, VIT University, Vellore – 632014, Tamil Nadu, India | **Accepted** |
| 49. | **Epitope-based vaccine design for Mycoplasma pneumoniae – An immunoinformatics approach**<br>**Ambili Unni, Madhusmita Rout**, Tabitha A and Sajitha Lulu S*<br>Department of Biotechnology, School of Biosciences and Technology, VIT University, Vellore - 632014, Tamil Nadu | **Accepted** |
| 50. | **Pharmacophore mapping, 3D QSAR, Molecular Docking and Binding Free Energy Calculations on quinoli(on)ne congeners as inhibitors of CD38**<br>**Sudipta Mondal**, Venkatesan Suryanarayanan and Sanjeev Kumar Singh*<br>Computer Aided Drug Design and Molecular Modelling Lab, Department of Bioinformatics, Alagappa University, Karaikudi-630004, Tamil Nadu, India | **Accepted** |
| 51. | **Structural insight on estrogen receptor β and their interaction towards estrogen and tamoxifen in breast cancer**<br>**Divya G** and Venkat Kumar S*<br>Department of Biotechnology, SBST, VIT University, Vellore - 632014 | **Accepted** |