



DEPARTMENT OF BIOINFORMATICS

ALAGAPPA UNIVERSITY

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KARAIKUDI-630 004, TAMIL NADU, INDIA



7th National Symposium cum Workshop on "RECENT TRENDS IN STRUCTURAL BIOINFORMATICS AND COMPUTER AIDED DRUG DESIGN" (SBCADD-2015) February 24th – 27th, 2015

LIST OF PARTICIPANTS

S.No	Title of Abstract	Status
1.	An <i>insilico</i> approach to predict directional evolution of Oxacillinase substrate-specificity Arijit Pal and AnusriTripathi* Department of Biochemistry and Medical Biotechnology; Calcutta School of Tropical Medicine; 108, C.R. Avenue; Kolkata – 700 073; India.	Accepted
2.	Crystallographic and DFT studies on pyrrolo [1, 2-c] imidazole scaffolds Manikandan Jayaraman, Rajarathinam Balakrishnan, Kannan Muthu, Manivel Panneerselvam, Vasuki Gnanasambandam and Krishna Ramadas* Centre for Bioinformatics, Pondicherry University, Puducherry-605014	Accepted
3.	Leveraging ICT for setting up of Drug Discovery Repositories P.Muthukumar ¹ , Thirumalai Parthiban ¹ , G.Radhakrishnan ¹ , P.Suresh ² , J.Nafeesa Begum ³ 1Computer and Networking Unit, CSIR-CECRI, Karaikudi, Tamilnadu, India 2IT Division, CSIR Madras Complex Taramani, Chennai Tamilnadu, India 3Department of CSE, Govt. College of Engg., Bargur Krishnagiri Distt.,	Accepted
4.	Insilco Design of Novel Antimalarial Agents Applying Receptor Based 3D-QSAR Technique G.S. Nandini, S. Sree Kanth and M. Vijjulatha*, MMMC, Department of Chemistry, University College of Science, Osmania University, Hyderabad – 500007	Accepted
5.	Developing novel inhibitors of HIV-1 entry using Insilico studies V.Radhika, N.V.S.S. Kanthi and M. Vijjulatha* MMMC group, Department of Chemistry, University College of Science, Osmania University, Hyderabad – 500007	Accepted
6.	Insights into protein interaction networks reveal non-receptor kinases as significant druggable targets for psoriasis Sudharsana Sundarrajan*, Sajitha Lulu and Mohanapriya Arumugam Bioinformatics division, School of Biosciences and Technology, VIT University, Vellore-632014	Accepted
7.	Molecular dynamics studies on β-lactamases and Penicillin binding proteins Sudha Ramaiah*, K.M.Kumar, Anand Anbarasu Bioinformatics Division, School of Biosciences and Technology.VIT University, Vellore – 632014	Accepted
8.	Protein aggregation due to nsSNP resulting in P56S VABP protein is associated with amyotrophic lateral sclerosis Rayapadi G Swetha, Kullappan Malathi, Sudha Ramaiah, Anand Anbarasu* Medical & Biological Computing Laboratory, Bioinformatics Division, VIT University, Vellore – 632 014	Accepted

9.	A Functional network-based polymorphic study of fabp4 gene Susmita Bag, Anitha. P, Sudha Ramaiah, Anand Anbarasu* Medical and Biological Computing Laboratory, School of Biosciences and Technology.VIT University, Vellore – 632014, Tamil Nadu, India	Accepted
10.	Computational gene network study on antibiotic resistance genes of <i>Acinetobacter baumannii</i> P. Anitha, Anand Anbarasu, Sudha Ramaiah* Medical and Biological Computing Laboratory, School of Biosciences and Technology.VIT University, Vellore – 632014, Tamil Nadu, India.	Accepted
11.	Preliminary crystallization studies of extracellular alkalophilic lipase from <i>Acinetobacter radioresistens</i> PR8. Krishna Kant Gupta* ¹ , Priya R. ² , Sharmili Jagtap ² , Ramadas Krishna ¹ . ¹ Center for Bioinformatics, Pondicherry University, Pondicherry 605014, India. ² Department of Microbiology, Pondicherry University, Pondicherry 605014, India	Accepted
12.	Crystal Structure of Pyrazole Derivative M.Sivakumar*, S.Aravindhan Department of Physics, Presidency College, Chennai-5, Tamil Nadu, India.	Accepted
13.	2D-QSAR and Pharmacophore Modelling of Non-Sulfonyl Selective COX-2 Inhibitors E. Manivannan*, and S. C. Chaturvedi School of Pharmacy, Devi Ahilya University, Ring Road, Indore-452001 (M.P.)	Accepted
14.	Structure Determination of Great Cormorant (<i>Phalacrocorax Carbo</i>) Haemoglobin through X-Ray Crystallography G. Jagadeesan and S. Aravindhan* Department of Physics, Presidency College, Chennai 600 005, India	Accepted
15.	Molecular Modeling, Docking and Dynamics Studies of Wolbachia Endosymbiont of <i>Brugia Malayi</i> Carbonic Anhydrase G. Jagadeesan and S. Aravindhan* Department of Physics, Presidency College, Chennai 600 005, India	Accepted
16.	Pyrrrolidine inhibitors for Tuberculosis G. Jagadeesan and S. Aravindhan* Department of Physics, Presidency College, Chennai 600 005, India	Accepted
17.	Wnt canonical and non-canonical pathways: Sequence and Structural difference favors a distinct preference of Wnt3a binding with co-receptor LRP6 Itishri Sahu ¹ , Seema Mishra ¹ , Rambabu Undi ¹ , Ravinder Kandi ¹ , Usha Gutti ² and Ravi Kumar Gutti ^{1*} ¹ Stem Cells and Haematological Disorders Laboratory, Department of Biochemistry, School of Life Sciences , University of Hyderabad , (PO) Gachibowli, Hyderabad 500046 , AP , India. ² Department of Biotechnology, GITAM Institute of Science, GITAM University, Visakhapatnam-530 045 (AP), INDIA	Accepted
18.	Docking Analysis of Human Androgen Receptor to Decipher Curcumin as Anticancer Agents Chitra Jeyaraj Pandian, Vinodhini Jayaraj, Soffiya James, MareeswariNagarajan, <u>Meena Kottaisamy</u> , Chandralekha Kasi Department of Biotechnology, Dr.UmayalRamanathan College for Women, Karaikudi	Accepted

19.	Discovery of potent inhibitors of human Mirk/Dyrk1B receptor by molecular modeling, virtual screening and dynamics studies Ramar Vanajothi and Pappu Srinivasan* Department of Bioinformatics, Alagappa University, Karaikudi – 630 004, Tamilnadu, India	Accepted
20.	In silico evaluation of 5-hydroxy- 3', 4', 7- trimethoxyflavone as new natural entity for cancer A. Sudha and P. Srinivasan* Department of Bioinformatics, Alagappa University, Karaikudi - 630 004, India	Accepted
21.	Novel drug identified for bladder cancer – Insilico Approach P. Saravana Prabha*, D. Malarvizhi, V. K. Gopalakrishnan Department of Bioinformatics and Biochemistry, Karpagam University, Coimbatore - 641021	Accepted
22.	Constructing the interactome to identify human miRNA – lung cancer association. Thabitha Amalraj ¹ , Madhusmita Rout ¹ , Vino Sundararajan ² , Mohana Priya Arumugam ¹ , Sajitha Lulu Sudhakaran* Bioinformatics Division ¹ , Medical biotechnology ² , School of Bioscience and Technology, VIT University, Vellore - 632014	Accepted
23.	E-pharmacophore filtering and molecular docking studies of potential lead compounds against LuxPQ in <i>Vibrio harveyi</i> Nattan Stalin and Pappu Srinivasan* Department of Bioinformatics, Alagappa University, Karaikudi – 630 004, Tamilnadu, India	Accepted
24.	Big Data Analysis in mRNA Prediction Joshua Jebaraj, Sherly Mariem, Arul Mugilan. Department of Bioinformatics, Karunya University, Coimbatore	Accepted
25.	Pancreatic Lipase Plant Inhibitor database (PLPIndb) A. Joseph and P. Srinivasan* Department of Bioinformatics, Alagappa University, Karaikudi – 630 004, Tamilnadu, India	Accepted
26.	Heavy metal toxicity removal utilizing biocompatible peptides Praveen Bhai Patel, Antara Banerjee and Arpita Yadav UIET, Chhatrapati Shahu Ji Maharaj University, Kanpur 208024	Accepted
27.	Crystal structure and docking analysis of (2E, 4E)-ethyl 5-(phenyl sulfonyl)penta-2,4-dienoate, (2E,4E)-ethyl 5-(3-bromophenylsulfonyl)penta-2,4-dienoate and (2E,4E)-ethyl 5-(2,4-dichlorophenylsulfonyl)penta-2,4-dienoate V. Sabari ¹ , S. Aravindhan ² ¹ PG Department of Physics, Women's Christian College, Chennai-6, Tamil Nadu, India ² Department of Physics, Presidency College, Chennai-5, Tamil Nadu, India	Accepted
28.	Microbial siderophore exerts anti-cancer action displaying HDAC inhibitor activity M.Karthikeyan, S.Sivasankari, K.Prakash Shyam, RM.Murugappan Department of Zoology & Microbiology, Thiagarajar College, Madurai.	Accepted
29.	MATQC: A tool for next generation sequence quality check using MATLAB Varna.P and Vidya Niranjana Department of Biotechnology, RV college of engineering, Bangalore –560059	Accepted

30.	Virtual screening and molecular dynamics simulation studies on GP2 glycoprotein subunit of ebola virus Ruban Durairaj.D, Kanagaraj.M, Shanmughavel Piramanayagam. Computational Biology Lab, Department of Bioinformatics, Bharathiar University, Coimbatore.	Accepted
31.	E-Pharmacophore mapping and molecular docking studies on snake venom metalloproteinase (SVMPs) Sathishkumar Chinnasamy and Karthikeyan Muthusamy Department of Bioinformatics, Alagappa University, Science Block, Karaikudi – 630004	Accepted
32.	Molecular Docking and Molecular Dynamics Studies on Ellagic acid Derivatives compounds against Phospholipase A2 (PLA2) Jagasirpian Vinayagam, Sathishkumar Chinnasamy and Karthikeyan Muthusamy Department of Bioinformatics, Alagappa University, Science Block, Karaikudi – 630004	Accepted
33.	Pharmacophore Modelling and 3D-QSAR generation on series of phenylalanine based GPR142 agonists Gopinath Krishnasamy, Lakshmanan Loganathan, Karthikeyan Muthusamy* Department of Bioinformatics, Science Block, Alagappa University, Karaikudi – 630 004, Tamil Nadu.	Accepted
34.	Identification of natural inhibitors against <i>Grb14</i> protein: an <i>in silico</i> study Lakshmanan Loganathan, Gopinath Krishnasamy, Karthikeyan Muthusamy* Department of Bioinformatics, Science Block, Alagappa University, Karaikudi – 630 004, Tamil Nadu.	Accepted
35.	Effects of Cloiquinol on the copper binding domain of Amyloid Precursor Protein APP: A Molecular Dynamics study Selvaraman Nagamani, Karthikeyan Muthusamy* Department of Bioinformatics, Science Block, Alagappa University, Karaikudi – 630 004, Tamil Nadu.	Accepted
36.	Predicting the binding modes of non-secosteroidal ligands in the active site of Vitamin D Receptor by quantum mechanical calculations S. Saravanakumar ¹ , Selvaraman Nagamani ¹ , Chandrasekhar Kesavan ^{2,3} and Karthikeyan Muthusamy ¹ ¹ Department of Bioinformatics, Science Block, Alagappa University, Karaikudi – 630 004, Tamil Nadu ² Musculoskeletal Disease Center, JLP VA Medical Center, Loma Linda, CA 92357, USA. ³ Dept of Medicine, Loma Linda University, Loma Linda, CA 92354, USA.	Accepted
37.	Cloning, Expression and Purification of Alanyl related - tRNA synthetase from <i>Thermus thermophilus</i> HB8 Nachiappan. M, Veerapandiyan. M and Jeyakanthan. J Department of Bioinformatics, Alagappa University, Karaikudi - 630 004, Tamil Nadu.	Accepted
38.	Identification of Novel Inhibitors for Aminoimidazole Ribonucleotide (AIR) synthetase from <i>Pyrococcus horikoshii</i> OT3 through Homology modeling, Structure based screening and Molecular Dynamics approaches Jayashree Biswal ¹ , R.Guru Raj Rao ¹ , J.Prajisha ¹ , K.Sekar ² and J. Jeyakanthan ¹ ¹ Department of Bioinformatics, Science Block, Alagappa University, Karaikudi - 630 004, Tamil Nadu. ² Supercomputer Education and Research Center, Indian Institute of Science, Bangalore - 560 012.	Accepted
39.	Investigation of vital pathogenic target Orotate Phosphoribosyltransferases (OPRTase) from <i>Thermus thermophilus</i> HB8: Phylogenetic and Molecular modelling approach. Surekha K, Prabhu D, Richard M, Nachiappan M, Jayashree Biswal & Jeyakanthan J Department of Bioinformatics, Alagappa University, Alagappa University, Karaikudi-630004.	Accepted

40.	Pharmacophore, 3D-QSAR and Molecular Docking Studies of 6-Aminonicotinamide Derivatives to explore novel Histone Deacetylase 1 Inhibitors Sanjay K. Choubey, J. Jeyakanthan Department of Bioinformatics, Alagappa University, Karaikudi - 630 004, Tamil Nadu.	Accepted
41.	Identification of novel inhibitor for Translational Initiation Factor through Homology Modeling, Molecular Dynamics and Docking approaches J. Prajisha ¹ , Jayashree Biswal, J. Shankar Prasad Kanaujia ² and J. Jeyakanthan ¹ ¹ Department of Bioinformatics, Science Block, Alagappa University, Karaikudi - 630 004, Tamil Nadu. ² Department of Biotechnology, Indian Institute of Technology, Guwahati - 781 039, Assam.	Accepted
42.	Molecular Modeling and E-Pharmacophore generation of 4-Carboxy-5-aminoimidazole Ribonucleotide (CAIR) from <i>Pyrococcus horikoshii</i> OT3 R. Guru Raj Rao ¹ , Jayashree Biswal ¹ , J.Prajisha ¹ , K.Sekar ² and J. Jeyakanthan ¹ ¹ Department of Bioinformatics, Alagappa University, Karaikudi - 630 004, Tamil Nadu. ² Supercomputer Education and Research Center, Indian Institute of Science, Bangalore - 560 012.	Accepted
43.	An insight on Transcription Regulation of Tryptophan Responsive Regulatory Protein (PH0140) from <i>Pyrococcus horikoshii</i> OT3 Richard. M, Nachiappan. M, Sureka. K and Jeyakanthan. J Department of Bioinformatics, Science Block, Alagappa University, Karaikudi- 630 004, Tamil Nadu.	Accepted
44.	Identification of novel inhibitors of Dihydroorotate Dehydrogenase (DHODH) using Homology modeling, Virtual Screening, Free Energy Calculation and Molecular Dynamics Simulation Studies Sureka. K, Prabhu. D, Nachiappan. M, Jayashree Biswal. S, Prajisha. J and Jeyakanthan. J Department of Bioinformatics, Alagappa University, Karaikudi - 630 004, Tamil Nadu.	Accepted
45.	Docking and Molecular dynamics studies on Class C G protein coupled receptor Human mGluR5 Transmembrane Domain Sittrarasu Vijaya Prabhu and Sanjeev Kumar Singh Department of Bioinformatics, Alagappa University, Karaikudi-630004, Tamil Nadu.	Accepted
46.	Structural and mechanistic insights in to the pyridine 1-oxide derivatives as PCAF BRD inhibitors Venkatesan Suryanarayanan and Sanjeev Kumar Singh Department of Bioinformatics, Alagappa University, Karaikudi-630004, Tamil Nadu.	Accepted
47.	PPRID-Phage Protein Resource information database: A manually annotated Sequence and Structural information of phage proteins Umesh Panwar, Chandrabose Selvaraj and Sanjeev Kumar Singh Department of Bioinformatics, Alagappa University, Karaikudi-630003, Tamilnadu.	Accepted
48.	Cancerapp: A novel bioapp for cancer research Udit Setia ¹ , Thabitha Amalraj ¹ , Vino Sundararajan ² , Sajitha Lulu Sudhakaran Bioinformatics Division ¹ , Medical biotechnology ² , School of Bioscience and Technology, VIT University, Vellore - 632014.	Accepted
49.	A Data Mining Study on the Binding Sites Residues of Purine Bound Proteins to Enhance Protein Crystallizability Santhosh Rajendran ¹ , Gurusaran Manickam ² , Sekar Kanagaraj ² and Jeyakanthan Jeyaraman ^{1*} ¹ Department of Bioinformatics, Science Block, Alagappa University, Karaikudi - 630 004. ² Supercomputer Education and Research Centre, Indian Institute of Science Bangalore - 560 012	Accepted

50.	Investigation on the interaction of PCAF BRD with Histone H3 Murali Aarthi, Venkatesan Suryanarayanan and Sanjeev Kumar Singh Department of Bioinformatics, Alagappa University, Karaikudi-630004, Tamil Nadu.	Accepted
51.	Combined approach of Pharmacophore modelling, Atom based 3D-QSAR, Molecular docking and Molecular dynamics studies to identify and validate the Akt1 kinase inhibitors. Sankar Venkatesh and Jeyaraman Jeyakanthan Department of Bioinformatics, Alagappa University, Karaikudi - 630 004, Tamil Nadu.	Accepted