DEPARTMENT OF BIOINFORMATICS
ALAGAPPA UNIVERSITY
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ABSTRACTS RECEIVED FOR POSTER PRESENTATION

S. No	Title of Abstract	Status
1.	**Identification of Potent Angiotensin Converting Enzyme 2 Inhibitors through Virtual Screening and Structure-Based Pharmacophore Design** **C. Zozimus Divya Lobo**[1], A. Syed Mohamed[2]*, C.Vedhi[3] [1]Department of Chemistry, St.Mary's College,Tuticorin, Tamil Nadu, India [2]Department of Chemistry, Sadakathullah Appa College, Tirunelveli, Tamil Nadu, India [3]Department of Chemistry, VOC College,Tuticorin, Tamil Nadu. *(Email: asm2032@gmail.com)*	Accepted
2.	**Specific Binding of RVV-V with Cleavage Site of FV Explored** **Pradeep Kumar Yadav**, A. Christian Bharathi and B. Syed Ibrahim Department of Bioinformatics, Pondicherry University, Pondicherry, India *(Email: yadavpradeep755@gmail.com)*	Accepted
3.	**Study of Intermolecular Recognition Mechanism Involved in C4 Activation through Serine Protease – an *In Silico* Approach** **Vikrant Kumar Sinha,** and Muthuvel Suresh Kumar* Centre for Bioinformatics, School of Life Sciences, Pondicherry University, Pondicherry, India. *(E-mail: vik.nid13@gmail.com)*	Accepted
4.	**Alleviating Autism Spectrum Disorder through a Traditional Approach** **Vishnu Ranjit A[1]*** and R. Sathishkumar [2] [1] Department of Physiology, PSG College of Arts and Science, Coimbatore, Tamil Nadu, India [2] Assistant Professor, Department of Botany, PSG College of Arts and Science, Coimbatore, Tamil Nadu, India	Accepted
5.	**E-Pharmacophore Based Design of Novel Protease Inhibitors for HIV-1** **Ishwar Chandra,** Chirasmita Nayak and Sanjeev Kumar Singh* Computer Aided Drug Design and Molecular Modeling lab, Department of Bioinformatics, Alagappa University, Karaikudi – 630 004, Tamil Nadu, India. *(Email:skysanjeev@gmail.com)*	Accepted
6.	**3D-QSAR Pharmacophore Based Studies of Ache Complexes, with Resveratrol similar Compounds: a new Insight for *Alzheimer's Diseases* Treatment** **Mohd Babu Khan**[1], Bhagath Kumar P[1], Tuleshwori Devi S[1], Naidu Subbarao[2], Dinakara Rao A[1]* [1]Centre for Bioinformatics, School of Life Sciences, Pondicherry University, Pondicherry, India [2]School of Computational and Integrative Sciences, Jawaharlal Nehru University, New Delhi, India *(Email: mmbk.bioinfo@gmail.com,ampasaladr@gmail.com)*	Accepted
7.	**Alpha Amyrin and Beta Amyrin- Anti Cancer Compounds from Methanolic Bark Extract of Shorea Robusta** **V. Dhivya Jensi** and P. Ananda Gopu* Department for Advanced Computing and Bioinformatics, PRIST University, Thanjavur	Accepted

	(*Email : panandagopu.crd@prist.ac.in)	
8.	**Screening of Potent Inhibitor against TNKS 2 Using *In Silico* Approaches** **Josephine Julia Balthasar,** John Marshal Jayaraj and Karthikeyan Muthusamy* [1]Department of Bioinformatics, Alagappa University, Karaikudi – 630004, Tamil Nadu, India. (*Email: mkbioinformatics@gmail.com)	**Accepted**
9.	**Genome-Wide Analysis of Secretory Proteins in *Trypanosoma Brucei*: Insights into Functional Characteristics of the Secretome** **Gowdham M,** Murugesh Easwaran, Shanmughavel Piramanayagam* Department of Bioinformatics, Bharathiar University, Coimbatore-641046, India (Email:gowdhamgct@gmail.com.)	**Accepted**
10.	**Protein-Protein Interaction between *Vibrio Harveyi* Luxr and Phage Lysozyme using Molecular Docking and Molecular Dynamics Study** **Nattan Stalin[a],** Pappu Srinivasan[b]* *[a]Molecular Biology Laboratory, Department of Bioinformatics,* *[b]Department of Animal Health and Management, Alagappa University, Karaikudi - 630 003, Tamil Nadu, India.*	**Accepted**
11.	**Identification of Pathogenesis associated Leptospiral Outer Membrane Proteins (OMPs) as Vaccine Candidates for Leptospirosis** **Muthu Prasad[1]**, Paulsamy Chellapandi[2] and Kalimuthusamy Natarajaseenivasan[1]* [1]Department of Microbiology, [2]Department of Bioinformatics, School of Life Sciences, Bharathidasan University, Tiruchirappalli, Tamil Nadu – 620024. (*E-mail: natarajaseenivasan@gmail.com)	**Accepted**
12.	**Synthesis and Characterization of *Capsicum Annuum* Fruitextract (Capsaicin) Coated Silver Nanoparticle (Ca-Agnps) and Their Toxicity Assessment on *Ceriodaphniacornuta* through *In Vivo* and *In Silico* Approaches** **Sekar Vijayakumar[a]**, Venkatesan Suryanarayanan[b], BalasubramanianMalaikozhundan[a], Sanjeev Kumar Singh [b],Baskaralingam Vaseeharan[a]* [a]Nanobiosciences and Nanopharmacology Division, Biomaterials and Biotechnology in Animal Health Lab, Department of Animal Health and Management, Alagappa University, Karaikudi – 630 004,Tamil Nadu, India. [b]Computer Aided Drug Design and Molecular Modelling Lab, Department of Bioinformatics,Alagappa University, Karaikudi-630004, Tamil Nadu, India *(Email: vaseeharanb@gmail.com)*	**Accepted**
13.	**Anti-inflammatory and *in silico* studies of Loganic acid against COX-2** **Arumugam Sudha[1],** Jeyaraman Jeyakanthan[1] and Pappu Srinivasan[2]* [1]Department of Bioinformatics, [2]Department of Animal Health and Management, Alagappa University, Karaikudi -630 004, Tamil Nadu, India	**Accepted**
14.	**Distant Phe345 Mutation Compromises the Stability and Activity of *Mycobacterium Tuberculosis* Isocitrate Lyase (Mtbicl) By Modulating Its Structural Flexibility** **Rohit Shukla,** Harish Shukla, Timir Tripathi* Molecular and Structural Biophysics Laboratory, Department of Biochemistry, North-Eastern Hill University, Shillong 793022, India *(Email:shuklarohit815@gmail.com)*	**Accepted**
15.	**In silico Screening of Marine Bioactive Compounds against Kaposi's Sarcoma-associated Herpes virus** **Nirmaladevi Ponnusamy[a],** Rajasree Odumpatta[a], Sajitha Lulu[a], Mohanapriya Arumugam[a]* Department of Biotechnology, School of Biosciences and Technology, Vellore Institute of Technology University Vellore– 632014, Tamil Nadu, India (*Email: mohanapriyaa@vit.ac.in)	**Accepted**

16.	**Computational Study on Tankyrase-Ankyrin Complex for the Identification of Potent Inhibitors for Colon Cancer** **Sheela Rani Rajendran,** Lakshmanan Loganathan and Karthikeyan Muthusamy Department of Bioinformatics, Alagappa University, Karaikudi – 630 004, Tamil Nadu, India (*E-mail: mkbioinformatics@gmail.com)	**Accepted**
17.	**Computational Screening and Investigation of Algal Bioactive Compounds against E6 Oncoprotein of Human Papilloma Virus-HPV16** **Pavithra Damodharan[a]** , Sajitha Lulu[a] and Mohanapriya Arumugam[a]* [a]Department of Biotechnology, School of Biosciences and Technology, Vellore Institute of Technology University (Email: pavithradamodharan94@gmail.com)	**Accepted**
18.	**Identification of potent inhibitors for LuxS through Structure-Based Virtual screening, DFT and Molecular Dynamics Simulation study** **Dakshinamurthy Sasikala[a],** Jeyaraman Jeyakanthan[a] and Pappu Srinivasan[b]* [a]Molecular Biology Laboratory, Department of Bioinformatics, [b]Department of Animal Health and Management, Alagappa University, Karaikudi - 630 003, Tamil Nadu, India.	**Accepted**
19.	***In Silico* Redesigning of Hgstm1 towards Suppression of Oxidative Stress in Rheumatoid Synovium** **R Kowshik Aravilli**, Dr. V. Kohila* Department of Biotechnology, National Institue of Technology, Warangal-506001 (E.mail: arkowshik228@gmail.com, kohilav@gmail.com)	**Accepted**
20.	**Binding Mode Analysis of Viral Protein E7 and Retinoblastoma through *In Silico* Approaches** **Aarthy Murali** and Sanjeev Kumar Singh* Computer Aided Drug Design and Molecular Modelling Lab, Department of Bioinformatics, Alagappa University, Karaikudi-630004, Tamil Nadu, India (*E-mail: skysanjeev@gmail.com)	**Accepted**
21.	**Repurposing FDA Approved Drugs against Zika Virus Protease, a Computational Study** **Ankur Kumar[1]**, Aarthy Murali[2], Sanjeev Kumar Singh[2],Rajanish Giri[1] [1]School of Basic Science, Indian Institute of Technology Mandi, Kamand campus, Mandi – 175005 [2]Department of Bioinformatics, Alagappa University, Karaikudi- 630004 (Email : ankuranand89@gmail.com)	**Accepted**
22.	**Molecular Modeling and Screening Studies for Finding new N^5-CAIR Mutase Inhibitors from *Pyrococcus Horikoshii* OT3 – an *In Silico* Approach** **Guru Raj Rao R**., Jayashree Biswal, Surekha Kanagarajan, Jeyaraman Jeyakanthan* Structural Biology and Bio-Computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi, 630 004, Tamil Nadu, India. (*Email:jjkanthan@gmail.com)	**Accepted**
23.	**Kinase-Substrate Interplay and Proteome-Wide Phosphorylation Dynamics** **R. Shyama Prasad Rao**[1,*], and Nagib Ahsan[2] [1]Biostatistics and Bioinformatics Division, Yenepoya Research Center, Yenepoya University, Mangalore –575018, India [2]Division of Biology and Medicine, Alpert Medical School, Brown University; and Center for Cancer Research and Development, Proteomics Core Facility, Rhode Island Hospital, Providence, RI 02903, USA (*Email:drsprao@gmail.com)	**Accepted**
24.	***In Silico* and *In Vivo* Studies on Predicted Kanamycin Resistance Protein from *Thermus Thermophilus* HB8** **Arindam Ghosh,** Dhamodharan Prabhu, Mutharasappan Nachiappan, Jeyaraman Jeyakanthan*	**Accepted**

	Structural Biology and Bio-Computing Lab, Dept. of Bioinformatics, Alagappa University, Karaikudi- 630 004, Tamil Nadu, India. *(*Email: jjkanthan@gmail.com)*	
25.	**Structural and Functional Prediction of Hypothetical Protein TTHA0983 from Thermus thermophilus HB8: a Combined Experimental and Computational Approach** **Poopandi Saritha[1],** Mutharasappan Nachiappan[2], Guru Raj Rao[2], Dhamodharan Prabhu[2] and Jeyaraman Jeyakanthan[2]* [1]Department of Biotechnology, Rajalakshmi Engineering College, Thandalam, Chennai -602105. Structural Biology and Biocomputing Lab, Department of Bioinformatics, Alagappa University, Karaikudi - 630 004, Tamil Nadu, India. *(*Email:jjkanthan@gmail.com)*	**Accepted**
26.	**Crystal Structure of Asparaginyl tRNA Synthetase from *Thermus Thermophilus* HB8 and its Complexes** **Nachiappan Mutharasappan[1]**, Vitul Jain[2], Yogavel Manickam[2], Amit Sharma[2], and Jeyakanthan Jeyaraman[1*] [1]Structural Biology and Bio-Computing Laboratory, Department of Bioinformatics, Alagappa University, Karaikudi, Tamil Nadu, India - 630 004. [2]Structural Parasitology Lab, International Centre for Genetic Engineering and Biotechnology, Aruna Asaf Ali Marg, New Delhi - 110 067. *(*E-mail: jjkanthan@gmail.com)*	**Accepted**
27.	**Cloning, Expression and Preliminary Purification of Hypothetical Protein E3 Binding Protein (E3BP) from *Thermus Thermophilus* HB8.** **Malaisamy Veerapandiyan**, Mutharasappan Nachiappan, Dhamodharan Prabhu and Jeyaraman Jeyakanthan* Structural Biology and Biocomputing Lab, Department of Bioinformatics, Alagappa University, Karaikudi - 630 004, Tamil Nadu, India. *(Email:jjkanthan@gmail.com)**	**Accepted**
28.	**Modeling and Molecular Dynamics Simulation Studies on Aspartokinase (Wbm0441) Enzyme from Wolbachia Endosymbiont *Brugia Malayi*** **Mathimaran Amala, Sanjay Kumar Choubey,** Dhamodharan Prabhu, Surekha Kanagarajan, Mutharasappan Nachiappan and Jeyaraman Jeyakanthan* Structural Biology and Bio-Computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi – 630 004, Tamil Nadu, India. *(*Email:jjkanthan@gmail.com)*	**Accepted**
29.	**Identification of Potent PAK1 Antagonists Using E-Pharmacophore Based Mapping and Screening– an *In Silico* Approach.** **Jayashree Biswal[1]**, Suresh Kumar Rayala[2], Ganesh Venkatraman[3] and Jeyaraman Jeyakanthan[1*] [1]Structural Biology and Bio-Computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi - 630 004, Tamil Nadu, India [2] Department of Biotechnology, Indian Institute of Technology Madras, Chennai-600 036, Tamil Nadu [3] Department of Human Genetics, College of Biomedical Sciences, Sri Ramachandra University, Porur, Chennai-600 116, Tamil Nadu, INDIA. *(* Email: jjkanthan@gmail.com)*	**Accepted**
30.	**Computational Identification of Potent Inhibitors for Streptomycin 3″-Adenylyltransferase of *Serratia Marcescens*** **Dhamodharan Prabhu,** Ramasamy Vidhyavathi, Jeyaraman Jeyakanthan* [1]Structural Biology and Bio-Computing Laboratory, Department of Bioinformatics, Alagappa University, Karaikudi - 630 004, Tamil Nadu, India *(* Email: jjkanthan@gmail.com)*	**Accepted**
31.	**Exploration of Plant Bioflavonoids as Potential Matrix Metalloproteinase-9(MMP-9) Inhibitors for the Management of Rheumatoid Arthritis- a Computational Approach**	**Accepted**

	Pradiba D[1], Shunmuga Priya V[1], Aarthy M [2], Sanjeev Kumar Singh[2] and Vasanthi M*[1] [1]Department of Biotechnology, Kamaraj College of Engineering and Technology, Virudhunagar 626 001 [2]Computer Aided Drug Design and Molecular Modelling Lab, Department of Bioinformatics, Alagappa University, Karaikudi 630 004 *(*E-mail: vasanthimadurai@gmail.com)*	
32.	**Energy based Pharmacophore screening and molecular dynamics simulation studies in the discovery of potent inhibitors for Type II Diabetes** **J. Prajisha** and Jeyaraman Jeyakanthan* Structural Biology and Bio-Computing Lab,Department of Bioinformatics, Science Block, Alagappa University, Karaikudi - 630 004, Tamil Nadu, India *(* Email: jjkanthan@gmail.com)*	**Accepted**
33.	**Structural Insights on Binding mechanism of CAD Complexes (CPSase, ATCase and DHOase)** **Kanagarajan Surekha,** Dhamodharan Prabhu, Mutharasappan Nachiappan and Jeyaraman Jeyakanthan* Structural Biology and Biocomputing Lab, Department of Bioinformatics, Science Block, Alagappa University, Karaikudi - 630 004, Tamil Nadu, India *(* Email: jjkanthan@gmail.com)*	**Accepted**
34.	***In Silico* Based Network Pharmacology Approaches to Evaluate the Anti-Diabetic Potential of Poly-Herbal Formulation** **Vaishali. K**, Pradiba.D, Soundaryalakshmi.M and Vasanthi.M Department of Biotechnology, Kamaraj College of Engineering and Technology, Virudhunagar- 626 001 *(Email:kvs.vaishu@gmail.com)*	**Accepted**
35.	**Unraveling the Transcriptional Activation/Deactivation Mechanism of TRP-DNA Complex in Response to Exogenous Amino Acids Using Computational Approach** **Richard Mariadasse** and Jeyaraman Jeyakanthan* Structural Biology and Bio-Computing Lab, Department of Bioinformatics, Science Block, Alagappa University, Karaikudi - 630 004, Tamil Nadu, India *(* Email: jjkanthan@gmail.com)*	**Accepted**
36.	**Molecular modeling, Dynamics Studies and Density Functional Theory Approaches to Identify Potential Inhibitors of SIRT4 protein from Homo sapiens: a Novel Target for the Treatment of Type 2 Diabetes** **Sanjay K Choubey,** Dhamodharan Prabhu, Mutharasappan Nachiappan, Jayshree Biswal and Jeyaraman Jeyakanthan* Structural Biology and Bio-Computing Lab, Department of Bioinformatics, Science Block, Alagappa University, Karaikudi - 630 004, Tamil Nadu, India *(* Email: jjkanthan@gmail.com)*	**Accepted**
37.	**A Web-Based Database on the Fatty Acid Compound and Their Interactions in Protein Structures** **Santhosh Rajendran**[1], Sekar Kanagaraj[2] and Jeyakanthan Jeyaraman[1]* [1] Structural Biology and Bio Computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi - 630 004, Tamil Nadu, India [2] Department of Computational and Data Sciences, Indian Institute of Science, Bangalore - 560 012, Karnataka India *(*E-mail: jjkanthan@gmail.com)*	**Accepted**
38.	**Computational Analysisfor Drug Target Identification in Nautella Italica: Modelling, Docking and Simulation Studies of Target Protein, Rpob** **Rajasree Odumpatta**[a], Mohanapriya Arumugam[a]* Department of Biotechnology, School of Biosciences and Technology, Vellore Institute of Technology University	**Accepted**
39.	**Molecular Docking and Dynamic Studies of Bioactive Compounds from *Clematis gouriana* Roxb. ex DC Against Snake Venom**	**Accepted**

	Phospholipase (PLA$_2$) Protein **Sathishkumar Chinnasamy** and Karthikeyan Muthusamy* Department of Bioinformatics, Alagappa University, Science Block, Karaikudi – 630 004 *(*Email: mkbioinformatics@gmail.com*	
40.	**Molecular Docking and Molecular Dynamic Studies to Screen Inhibitors for Tissue transglutaminase: a Potential Drug Target to Combat Renal Fibrosis** ***Lakshmi Prasanna,*** *Arpita Devi, Madhava Reddy B A, PrakashPrabhu,* *A K Pasupulati** School of Life Sciences, University of Hyderabad *(*Email: pakumarsl@uohyd.ernet.in)*	**Accepted**
41.	**SCN5A Gene SNP's in Irritable Bowel Syndrome and Its Influence in Structural Variance** **Fathima Shifana S,** Aameena N and Vidhyavathi RM* Department of Bioinformatics, Alagappa University, Science Block, Karaikudi – 630 004. *(* Email: vidhyamiss@gmail.com)*	**Accepted**
42.	**Combined Structure and Ligand Based Virtual Screening to Identify New Potent Negative Allosteric Modulators of Mglur5 against CNS Disorders** **Sitrarasu Vijaya Prabhu** and Sanjeev Kumar Singh* Computer Aided Drug Design and Molecular Modelling Lab, Department of Bioinformatics, Alagappa University, Karaikudi-630004, Tamil Nadu, India *(*E-mail: skysanjeev@gmail.com*	**Accepted**
43.	**Deciphering the Binding Mode of Pyridine 1-Oxide Derivatives as PCAF BRD Inhibitors: a Docking And MM/PB(GB)SA Based Approach** **Venkatesan Suryanarayanan** and Sanjeev Kumar Singh* Computer Aided Drug Design and Molecular Modelling Lab, Department of Bioinformatics, Alagappa University, Karaikudi-630004, Tamil Nadu, India *(*Email: skysanjeev@gmail.com)*	**Accepted**
44.	**Flavonoids as Zika virus NS2B-NS3 protease inhibitors: A molecular docking and dynamics simulation study** **Rakhi Yadav,** Rajanish Giri* School of Basic Sciences, Indian Institute of Technology Mandi, Mandi, India, 175005 **E-mail: rajanishgiri@iitmandi.ac.in*	**Accepted**
45.	**An *In Silico* Approach Towards Inhibition of Precursor Membrane Protein (Prm) to Prevent Dengue Virus Maturation in Trans-Golgi network** **Avinash Ravichandran,** Suryanarayanan V, Vijay Prabhu S, Umesh Panwar and Sanjeev Kumar Singh* Computer Aided Drug Design and Molecular Modelling Lab, Department of Bioinformatics, Alag appa University, Karaikudi-630004, Tamil Nadu, India *(*E-mail: skysanjeev@gmail.com)*	**Accepted**
46.	**Molecular Mechanism Studies of HIV-1PR Resistance by Active and Inactive Site Mutations for Protease Inhibitors through *In Silico* Approach** **Chirasmita Nayak**, Ishwar Chandra and Sanjeev Kumar Singh* Computer Aided Drug Design and Molecular Modeling lab, Department of Bioinformatics, Alagappa University, Karaikudi – 630 004, Tamil Nadu, India. *(Email:skysanjeev@gmail.com)*	**Accepted**
47.	**Protein-Protein Docking Studies of RANKL-RANK and the Structural Transition Inducement of Hydroxyapatite for Bone Remodelling – *In Silico* Perspective**	**Accepted**

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48.	**Understanding the Molecular Evolution,Divergence and their Structural Impact of Selenoprotein P - A computational approach** **Aruna lakshmanan,** J. Josephsahayaran and J. Jeyakanthan Plant Bioinformatics Lab, Department of Bioinformatics, Science Block, Alagappa University, Karaikudi - 630 004 *(E. mail: jjsrbioinformatics2016@gmail.com)*	**Accepted**
49.	***In-silico* designing of potential inhibitors for HIV-1 integrase by E-Pharmacophore based Virtual Screening, Docking and Molecular Simulation approaches** **Umesh Panwar** and Sanjeev Kumar Singh* Computer Aided Drug Design and Molecular Modelling Lab, Department of Bioinformatics, Alagappa University, Karaikudi-630004, Tamil Nadu, India *(*Email: skysanjeev@gmail.com)*	**Accepted**