ALAGAPPA UNIVERSITY

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DEPARTMENT OF BIOINFORMATICS

(*UGC- INNO, DST-FIST-PURSE, DBT-BIC and RUSA 2.0 Sponsored Department*)

KARAIKUDI-630 004, TAMIL NADU, INDIA.

2nd International Conference cum Workshop on
"RECENT TRENDS IN STRUCTURAL BIOINFORMATICS AND COMPUTER AIDED DRUG DESIGN"
(ICSBCADD-2022)
November 21st – 25th, 2022

S.No.	Title of the Abstract	Talk / Posters
1.	**Mapping the protein binding site of the (pro)renin receptor using *in silico* 3D structural analysis** **Akio Ebihara** Faculty of Applied Biological Sciences, Gifu University, Tokai National Higher Education and Research System, 1-1 Yanagido, Gifu 501-1193, Japan	**Plenary Lecture**
2.	***In-silico* approaches to understand antibiotic resistance in clinically important bacterial pathogens** **Sravan Kumar Miryala, Sudha Ramaiah and Anand Anbarasu*** Medical & Biological computing laboratory, School of Biosciences & Technology,Vellore Institute of Technology, Vellore-632014, India	**Plenary Lecture**
3.	**The current status of computational screening of chemical libraries for druggability prediction : Accuracy and Speed** **N. Arul Murugan** Department of Computational Biology, Indraprastha Institute of Information Technology, New Delhi 110020	**Plenary Lecture**
4.	**Proteomics studies for biomarker discovery in head and neck squamous cell carcinoma treated with Radiotherapy** **Lipi Das [a,b] , Ashok K Varma [a,b,*]** a. Advanced Centre of Treatment, Research and Education in Cancer, Kharghar, Navi Mumbai. b. Homi Bhabha National Institute, Anushaktinagar, Mumbai - 400 094	**Plenary Lecture**
5.	**Structural biology using synchrotron radiation and cryo-electron microscopy** **Atsushi Nakagawa** Institute for Protein Research, Osaka University 3-2 Yamadaoka, Suita, Osaka 565-0861 Japan	**Plenary Lecture**
6.	**Genomic biomarkers for early detection of complex diseases** **Basant K. Tiwary** Department of Bioinformatics, School of Life Sciences, Pondicherry University,	**Plenary Lecture**

	Pondicherry-605014	
7.	**Translating bioinformatics for patient care in hospitals** **Chandra Verma** Atomistic Simulations and Design in Biology, Biomolecular modelling and Design Function,Bioinformatics Institute, A* STAR,Singapore-138671	**Plenary Lecture**
8.	**Structural Biology at NSRRC and recent applications** **Chun-Jung Chen*** Life Science Group, Scientific Research Division, National Synchrotron Radiation Research Center, Hsinchu 30076, Taiwan	**Plenary Lecture**
9.	**Modern Machine Learning Methods for Drug Design** **U. Deva Priyakumar** Center for Computational Natural Sciences and Bioinformatics, International Institute of Information Technology, Hyderabad 500 032	**Plenary Lecture**
10.	**Structure-based virtual screening for identification of novel greatwall kinase inhibitors** **A.Dinakara Rao, Anbumani Velmurugan Ilavarasi, Tulsi, Saswati Sarita Mohanty and Katike Umamahesh.** Department of Bioinformatics, School of Life Sciences, Pondicherry University, Puducherry	**Plenary Lecture**
11.	**QSAR Modeling approach in Virtual Screening of Active Compounds** **Feroz Khan** Computational Biology Unit, CSIR-Central Institute of Medicinal & Aromatic Plants, P.O.-CIMAP, Lucknow-226015 (U.P.), INDIA	**Plenary Lecture**
12.	**The Success story of PAK1-RUNX3** **Ganesh Venkatraman *and Suresh K Rayala** Department of Human Genetics, Sri Ramachandra Institute of Higher Education and Research, Chennai-600 116	**Plenary Lecture**
13.	**Plant Diseases in Guyana -Past, Present and Control Measures** **Gomathinayagam Subramanian and Rekha Gomathinayagam** University of Guyana Berbice Campus, Corentyne, Berbice, Guyana, South America	**Plenary Lecture**
14.	**Targeting pyruvate dehydrogenase kinase signalling in the development of effective cancer therapy: A combined computational and experimental approach** **Md. Imtaiyaz Hassan** Centre for Interdisciplinary Research in Basic Sciences, Jamia Millia Islamia, Jamia Nagar, New Delhi 10025, INDIA	**Plenary Lecture**
15.	**Dhanvantari-2022: Genome to Drug in silico - A country path today; A highway tomorrow** **B. Jayaram** Department of Chemistry, Kusuma School of Biological Sciences & Supercomputing Facility for Bioinformatics & Computational Biology, Indian Institute of Technology, Hauz Khas, New Delhi-110016, India	**Plenary Lecture**
16.	**Biomedical Text Mining and Applications in Drug Discovery**	**Plenary Lecture**

	Dr. N. Jeyakumar, Dept. of Bioinformatics, School of Life Sciences, Bharathiar University, Coimbatore 641 046	
17.	***Listeria Monocytogenes* High Temperature Requirement A (HtrA) Protease and Its Interaction with Extracellular Matrix Molecules** **Karthe Ponnuraj** Centre of Advanced Study in Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai 600025, India	**Plenary Lecture**
18.	**Designing and development of hybrid conjugates of commercial drugs and bioactive herbals a possible approach for novel efficacious nonresistant therapeutic agents** **Krishna Misra** Honorary Professor, Indian Institute of Information Technology, Allahabad	**Plenary Lecture**
19.	**Computational Explorations to Overcome the Anti-Microbial Resistance in Bacteria** **Lakshmi P.T.V** Department of Bioinformatics, School of Life Sciences, Pondicherry University, Puducherry-605014	**Plenary Lecture**
20.	**Structural intermediates in the assembly landscape of the human mitochondrial anion channel** **Radhakrishnan Mahalakshmi*** Molecular Biophysics Laboratory, Department of Biological Sciences, Indian Institute of Science Education and Research, Bhopal, India.	**Plenary Lecture**
21.	**Binding affinity of protein-carbohydrate complexes: database development, analysis and prediction** **M. Michael Gromiha** Department of Biotechnology, Indian Institute of Technology Madras Chennai 600036, INDIA	**Plenary Lecture**
22.	**Dissecting Hubs and Bottlenecks in a Protein-Protein Interaction Network** **Prof H. A. Nagarajaram** Department of Systems and Computational Biology, School of Life Sciences University of Hyderabad	**Plenary Lecture**
23.	**Exopolysaccharides and their functions in disease: The story in an oral bacterium** **N. Ramasubbu, C. Cugini and E. Shimizu** Oral Biology, Rutgers School of Dental Medicine, Newark, NJ 07101	**Plenary Lecture**
24.	**Structural characterization and engineering of a plasticizer-degrading enzyme** **Pravindra Kumar* and Jai Krishna Mahto** Department of Biosciences and Bioengineering, IIT Roorkee, Roorkee, India.	**Plenary Lecture**
25.	**Design, identification and evaluation of anti-cancer agents against Aurora kinases**	**Plenary Lecture**

	Punit Kaur[1] , Deepali Gupta [1] , Mukesh Kumar[1] , Mandeep Singh[1] , A.S. Ethayathulla[1] , Andrey E. Shchekotikhin[2] and Uddipan Das [1] [1]Department of Biophysics, All India Institute of Medical Sciences, New Delhi, Delhi 110029, India and [2]Gause Institute of New Antibiotics, Moscow, 11 B. Pirogovskaya Street, Moscow 119021, Russia	
26.	**Computer aided drug design for developing potential inhibitors of oncogene PELP1 for treating breast cancer** **Ratna K Vadlamudi** Professor, UT Health San Antonio, USA	**Plenary Lecture**
27.	**Role of sulfur-mediated chalcogen bonds in the structure and substrate specificity of proteins** **Saikrishnan Kayarat*, Vishal Adhav** Department of Biology, Indian Institute of Science Education and Research, Pune – 411008	**Plenary Lecture**
28.	**SciWhyLab tools for integrating machine learning, transcriptomics and lead generation** **Anuja Jain, Shruti Gupta, Ajay Kumar Verma, Ajay Arya, Manisha Kalsan, Dana Mary Varghese and Shandar Ahmad*** School of Computational and Integrative Sciences, Jawharlal Nehru University, New Delhi	**Plenary Lecture**
29.	**Inhibition Mechanism of Human Kidney Type Glutaminase to Arrest Cancer Cell Proliferation** **J. Sivaraman** Department of Biological Sciences, National University of Singapore, Singapore 117546	**Plenary Lecture**
30.	**PELP1 – a mediator for inflammation induced tumorigenesis** **Suresh K Rayala*and Ganesh Venkatraman [R1]** Department of Biotechnology, IIT Madras, Chennai-600 032	**Plenary Lecture**
31.	**Exploring the medicinally important secondary metabolites in fenugreek through transcriptome studies** **R. Sowdhamini** National Centre for Biological Sciences, Tata Institute of Fundamental Research, Bellary Road, Bangalore-560 065.	**Plenary Lecture**
32.	**Structure based understanding of the innate immunity proteins and their exploitation for therapeutic applications** **T.P. Singh** Department of Biophysics, All India Institute of Medical Sciences, New Delhi	**Plenary Lecture**
33.	**Potential Drug Resistance in SARS-CoV-2: Importance of Mutational Surveillance in Pandemics** **Timir Tripathi[1,2]** [1]Regional Director's Office, Indira Gandhi National Open University (IGNOU), Regional Centre Kohima, Kohima- 797001, Nagaland, India	**Plenary Lecture**

	[2]Molecular and Structural Biophysics Laboratory, Department of Biochemistry, North-Eastern Hill University, Shillong- 793022, Meghalaya, India.		
34.	**Molecular docking and Molecular dynamics simulations on various Marine Bioactive compounds against Neuro Degenerative Disorders** **Devadasan Velmurugan* and Anantha Krishnan Dhanabalan** Office of the Director, Research and Development Cell, AMET University, Kanathur 603112, Chennai.	**Plenary Lecture**	
35.	**Investigating enhancer reprogramming and 3D organisation in p53 deficient/mutant colorectal cancer cells** **Vijayalakshmi Mahadevan** Institute of Bioinformatics and Applied Biotechnology (IBAB),Bangalore, India	**Plenary Lecture**	
36.	**Gene expression and interaction biology reveals toll-like receptor signaling pathway as a major trigger in COPD pathogenesis** **Pavithra Dhamodharan [a] , Mohanapriya Arumugam [a*]** [a] Department of Biotechnology, School of Biosciences and Technology, Vellore Institute of Technology	**Plenary Lecture**	
37.	**Design of Peptidomimetic Ligands for the Inhibition of BACE1 of Alzheimer"s Disease: Computational and Chemical Biology Approach K. Muruga Poopathi Raja [1,2 *]** 1. Biophysical and Chemical Biology Laboratory, Department of Physical Chemistry, School of Chemistry, Madurai Kamaraj University, Palkalai Nagar, Madurai-625021. 2. Biophysical and Chemical Biology Laboratory, Department of Chemistry, School of Physical Sciences, Central University of Kerala, Periya, Kasaragod District, Kerala - 671 320.	**Plenary Lecture**	
38.	**Charge-Charge Repulsion: An instance from *Candida albicans* Pyruvate kinase** **Lukkani Laxman Kumar, Ayaluru Murali*** Department of Bioinformatics, Pondicherry University, Pondicherry – 605014	**Poster**	**Accepted**
39.	**An *in silico* Approach to Investigate the Interaction of Fe3+ ion with Ftr1p of Mucormycosis Causing *Rhizopus sp.*** **Ahana Roy Choudhury and Ayaluru Murali*** Department of Bioinformatics, School of Life Sciences, Pondicherry University, Puducherry- 605014	**Poster**	**Accepted**
40.	***In silico* Analysis of Red Seaweed *Gelideilla acerosa*** **Kirithiga. A[1], Anantha Krishnan. D[2], Velmurugan. D[2] and Ramakritinan. C.M[1*]** [1]Department of Marine Biotechnology, AMET Deemed to be University, Kanathur - 603112, Chennai, Tamil Nadu, India [2]Office of the Director, Research and Development Cell, AMET Deemed to be University, Kanathur - 603112, Chennai, Tamil Nadu, India	**Poster**	**Accepted**
41.	**A Machine Learning Application for Bioactivity Prediction of the Target Replicase Polyprotein 1ab of SARS-CoV-2** **Rajesh Das, Amouda Venkatesan***	**Poster**	**Accepted**

	Department of Bioinformatics, Pondicherry University, Kalapet, Puducherry-605014		
42.	**Screening of key genes involving in hormone signalling in a phytopathosystem (*Piper nigrum - Phytophthora capsici*) using transcript assembly** **B.Nagarathnam[1],Mohamed Shafi[1],Chidambareswaren Mahadevan[2], Manjula Sakuntala[2], R.Sowdhamini[1]** [1] National Centre for Biological Sciences, (TIFR),GKVK Campus,Bangalore-560065. India [2]Plant Disease Biology and Biotechnology, Rajiv Gandhi Centre for Biotechnology, Thycaud P.O, Thiruvananthapuram – 695014, Kerala.	**Poster**	**Accepted**
43.	**Big data analysis of *Rauwolfia serpentine* reveals the potency of indole alkaloids using *De-novo* Transcriptome studies** **Hithesh Kumar[1], Anand Anbarasu[1,2] and Sudha Ramaiah[3*]** [1]School of Bio-Sciences and Technology (SBST), Vellore Institute of Technology, Vellore, 632014 [2]Department of Biotechnology, SBST, Vellore Institute of Technology, Vellore [3]Department of Bio-sciences, SBST, Vellore Institute of Technology, Vellore	**Poster**	**Accepted**
44.	***In-silico* investigation of curcumin-indole-3-propionic acid diester Against the enzymes involved in Diabetes-associated cognitive decline** **Sidhambaram Jayanthi, Loganathan Chitra, Sakayanathan Penislusshiyan and Thayumanavan Palvannan*** Department of Biochemistry, Periyar University, Salem-636011*	**Poster**	**Accepted**
45.	**Proteoglycan signaling FN1 as a potential therapeutic target for pancreatic adenocarcinoma: A systems biology approach** **Gayathri Ashok, Anand Anbarasu and Sudha Ramaiah*** Medical and Biological Computing Laboratory, Department of Biosciences, School of Bio Sciences and Technology, Vellore Institute of Technology, Vellore, 632014	**Poster**	**Accepted**
46.	**Novel antimicrobial peptide mutants can potentially inhibit β-lactamase enzymes in Gram-negative clinically important bacterial pathogens** **Soumya Basu, Sudha Ramaiah, Anand Anbarasu*** Medical and Biological Computing Laboratory, School of Bio-Sciences and Technology (SBST), Vellore Institute of Technology, Vellore, India	**Poster**	**Accepted**
47.	**Novel curcumin derivative can inhibit MurC ligase to obstruct peptidoglycan biosynthesis in multi-drug resistant *Salmonella Typhi*: Evidence from Molecular Docking and Dynamics Simulations** **Reetika Debroy, Anand Anbarasu and Sudha Ramaiah*** Medical and Biological Computing Laboratory, School of Bio-Sciences and Technology, Vellore Institute of Technology (VIT), Vellore-632014, Tamil Nadu, India	**Poster**	**Accepted**
48.	**A Novel Ursodeoxycholic Acid Derivative can be a potential inhibitor for therapeutic target Parkin for Parkinson's Disease: Evidence from gene interaction network analysis, structure evaluation and molecular dynamics**	**Poster**	**Accepted**

	P. Priyamvada, Suvitha Anbarasu, Anand Anbarasu, Sudha Ramaiah* Medical and Biological Computing Laboratory, School of Bio-Sciences and Technology, Vellore Institute of Technology, Vellore-632014, Tamil Nadu.		
49.	**Two-component EvgS protein subdues both antimicrobial resistance and virulence in *Shigella flexneri* 2a str. 301: Evidence from Gene Interaction Network, Differential Gene Expression and Molecular Dynamics Simulation** **Aniket Naha, Anand Anbarasu, Sudha Ramaiah*** Medical and Biological Computing Laboratory, School of Bio-Sciences and Technology, Vellore Institute of Technology, Vellore-632014, Tamil Nadu, India	**Poster**	**Accepted**
50.	**Computational approach for the recognition of small molecule inhibitors for Toll-like receptor** **Shailya Verma and Ramanathan Sowdhamini*** National Centre for Biological Sciences, TIFR, Bangalore -560065, India	**Poster**	**Accepted**
51.	**Structural modelling of odorant receptors from *Aedes aegypti* and search for natural repellents** **Vikas Tiwari and R. Sowdhamini*** National Centre for Biological Sciences, Tata Institute of Fundamental Research, Bangalore 560065, India	**Poster**	**Accepted**
52.	**Integrative network analysis interweaves the missing links in cardiomyopathy diseasome** **Pankaj Kumar Chauhan & R. Sowdhamini*** National Centre for Biological Sciences (TIFR), Bangalore, IN 560065	**Poster**	**Accepted**
53.	**Structure analysis of HKT1;5 to understand the sodium transport affinity in wild rice species** **K. Mohamed Shafi[1], Gayatri Venkataraman[2] and Ramanathan Sowdhamini[1]** [1]National Centre for Biological Sciences (Tata Institute of Fundamental Research), Bangalore 560065 [2]Plant Molecular Biology Laboratory, M.S. Swaminathan Research Foundation (MSSRF), Chennai 600113	**Poster**	**Accepted**
54.	**A multi-epitope vaccine design against *Mycobacterium tuberculosis*: A subtractive proteomics and reverse vaccinology based immunoinformatics Approach** **Subhashree subhasmita Nayak, Ramadas Krishna*** Department of Bioinformatics, Pondicherry University, Pondicherry-605014	**Poster**	**Accepted**
55.	**The alteration of structural network by transient association between proteins** **Vasam Manjveekar Prabantu, Himani Tandon, Sandhya Sankaran, Ramanathan Sowdhamini, Narayanaswamy Srinivasnan** Molecular Biophysics Unit, Indian Institute of Science, Bangalore - 560012	**Poster**	**Accepted**
56.	***In-Silico* Identification of Hub Genes and their Regulatory Interaction Networks involved in Retinoic Acid Signaling Pathway of α-Synuclein in Parkinsons Diseases**	**Poster**	**Accepted**

	Kajal Abrol, Amutha Ramaswamy* Department of Bioinformatics, School of Life Sciences, Pondicherry University, Kalapet, Puducherry-605014		
57.	**Computational Analysis To Explore Possible Binding Between SIRT6 and PPARΓ** **Parvathy J, Himani Tandon, N Srinivasan, N Ravi Sundaresan** Interdisciplinary Mathematical sciences Initiative (IMI), IISc Bangalore, CV Raman Road, 560012	**Poster**	**Accepted**
58.	**Pseudokinases repurpose flexibility signatures associated with the protein kinase fold for noncatalytic roles** **Seemadri Subhadarshini, Anindita Paul, Narayanaswamy Srinivasan** Molecular Biophysics Unit, Indian Institute of Science, Bengaluru – 560012	**Poster**	**Accepted**
59.	**Microsecond molecular dynamics simulations probing the conformational landscape of LIMK1** **Hemavathy Nagarajan [a], Vetrivel Umashankar[b], Jeyaraman Jeyakanthan[a*]** [a]Structural Biology and Bio-Computing Lab, Department of Bioinformatics, Science Block, Alagappa University, Karaikudi, 630 003, Tamil Nadu, India, [b]Department of Bioinformatics, ICMR-National Institute of Traditional Medicine, Nehru Nagar, Belagavi, Karnataka-590 010, India	**Poster**	**Accepted**
60.	**Exploring the candidate genes encompassing the medicinal value of Athalakkai (*Momordica cymbalaria*) through transcriptomics approach** **Heyram Krishnakumar and Jeyaraman Jeyakanthan *** Structural Biology and Bio-Computing Lab, Department of Bioinformatics, Science Block, Alagappa University, Karaikudi, 630 003, Tamil Nadu, India.	**Poster**	**Accepted**
61.	**Comparative Studies on Bioactive Compounds of *Sphaeranthus amaranthoides* Against Parkinson's Disease: An *In-Silico* Approach** **Balasubramanian Sivaprakasam, Soundar Rajan Kulanthaivel, Priyanka Sappanimuthu, Joseph Sahayarayan Jesudass1* and Ramasamy Vidhyavathi** Department of Bioinformatics, Alagappa University, Karaikudi, Tamilnadu, India-630004	**Poster**	**Accepted**
62.	**Identification of Potent Lead Molecule against Serine/threonine-protein kinase B-raf receptor from *Endostemon viscosus* by using Computational approach** **Soundar Rajan Kulanthaivel, Balasubramanian Sivaprakasam, Priyanka Sappanimuthu, Jesudass Joseph Sahayarayan* and Ramasamy Vidhyavathi** Department of Bioinformatics, Alagappa University, Karaikudi, Tamilnadu, India-630004	**Poster**	**Accepted**
63.	**Consensus Secondary Structure Prediction (CSSP-2.0)** **Madhumathi Sanjeevi [a] , Ajitha Mohan [b] , Dhanalakshmi Ramachandran [b], Jeyakanthan Jeyaraman [a*] and Kanagaraj Sekar [b*]** [a] Structural Biology and BioComputing Laboratory, Department of Bioinformatics, Alagappa University, Karaikudi - 630 004, India and	**Poster**	**Accepted**

	[b] Department of Computational and Data Sciences, Indian Institute of Science, Bangalore - 560012, India		
64.	**Molecular Crosstalk between Sars-cov2 and Alzheimer's disease using Multi-Omics Datasets: A System Biology Approaches** **Premkumar T, Sajitha Lulu S*** Department of Biotechnology, School of Bio Sciences and Technology Vellore Institute of Technology, Vellore – 632014, Tamil Nadu	**Poster**	**Accepted**
65.	**Role of NF-KB Pathway Genes In Rheumatoid Arthritis: A Network Biology Approach** **Devi Soorya Narayana S, Vino S*** School of Bio Sciences and Technology, Vellore Institute of Technology, Vellore, 632014	**Poster**	**Accepted**
66.	**Evaluating Cell Surface Protein Liv1 as A Therapeutic Target In Triple-Negative Breast Cancer Patients** **Roshni S** Department of Human Genetics, Sri Ramachandra Institute of Higher Education & Research, Chennai.	**Poster**	**Accepted**
67.	**Purification, Crystallization and Preliminary X-ray Diffraction Analysis of Succinyl-diaminopimelate desuccinylase from *Wolbachia* endosymbiont of *Brugia malayi*** **P. Saritha[a], J. Jeyakanthan[a*] and Chun-Jung Chen[b*]** [a]Department of Bioinformatics, Alagappa University, Science Block, Karaikudi – 630004 [b]Life Science Group, Scientific Research Division, National Synchrotron Radiation Research Center, No. 101號, Hsin Ann Rd, East District, Hsinchu, 300, Taiwan.	**Poster**	**Accepted**
68.	**Identification of potential plant-based inhibitor against Scrub typhus through Computational approaches** **Sangavi P[1], Langeswaran K[2]*** [1]Department of Bioinformatics, Alagappa University, Karaikudi, Tamil Nadu, India [2*] Department of Biotechnology, Alagappa University, Karaikudi, Tamil Nadu, India	**Poster**	**Accepted**
69.	**Identification of unique biomarkers of non-alcoholic and alcoholic based Hepatocellular carcinoma** **Annadurai Priyadharshini and Arnold Emerson Issac*** Department of Biotechnology, School of Bio science and Technology, Vellore Institute of Technology, Katpadi, Vellore -632014.	**Poster**	**Accepted**
70.	**Development of novel amphiphilic drug-drug conjugates through the *in silico* approach against breast cancer** **S. Muthumanickam 1 , M.Manikandan 2 , P. Boomi 1* , J.Jeyakanthan 1 , M. Karunakaran** [1] Department of Bioinformatics, Alagappa University, Karaikudi, Tamil Nadu, India [2] Department of Industrial Chemistry, Alagappa University, Karaikudi, Tamil Nadu, India [3] Department of Physics, Alagappa Govt. Arts College, Karaikudi, Tamil Nadu, India	**Poster**	**Accepted**
71.	***In silico* molecular docking and Molecular Dynamic Simulation of designed twin drug against cancer**	**Poster**	**Accepted**

	M.Manikandan[1] , S. Muthumanickam[2] , P. Boomi[1,2*] , J. Jeyakanthan[2], H. Gurumallesh Prabu[1] [1]Department of Industrial Chemistry, Alagappa University, Karaikudi, Tamil Nadu, India [2]Department of Bioinformatics, Alagappa University, Karaikudi, Tamil Nadu, India		
72.	**Bioinformatic Analysis for Drug Discovery Against Esophageal Cancer** **C. N. Rahul[a], Vinod Jangid[c], Kanagaraj Sekar[b], Natarajan Aiswarya[b], Aarthi Rashmi B[c] & Jeyakanthan Jeyaraman[a]** [a]Structural Biology and Biocomputing Lab, Department of Bioinformatics, Alagappa University, Karaikudi, 630004, India and [b]Department of Computational and Data Sciences, Indian Institute of Science, Bangalore 560012, India and [c]Department of Bioinformatics, Sri Krishna Arts and Science College, Coimbatore 641038, India	**Poster**	**Accepted**
73.	**CAPS_protocol: A knowledge-driven approach to identify proteins of interest with an emphasis on biosynthetic pathways** **Adwait G. Joshi [a] , K. Harini [a] , Iyer Meenakshi [a] , K. Mohamed Shafi[a],[b] , Shaik Naseer Pasha [a] , Jarjapu Mahita[a] , Radha Sivarajan Sajeevan[a] , Snehal D. Karpe [a] , Pritha Ghosh [a] , Sathyanarayanan Nitish a,b , A. Gandhimathi a , Oommen K. Mathew [a] , Subramanian Hari Prasanna [a] , Manoharan Malini [a] , Eshita Mutt [a] , Mahantesha Naika [a] , Nithin Ravooru [a] , Rajas M. Rao [a], Prashant N. Shingate [a] , Anshul Sukhwal [a] , Margaret S. Sunitha [a] , Atul K. Upadhyay [a,c] , Rithvik S. Vinekar [a] and Ramanathan Sowdhamini [a,*]** [a:] National Centre for Biological Sciences (NCBS-TIFR), GKVK campus, Bellary road, Bangalore, 560065, Karnataka, India; [b:] The University of Trans-Disciplinary Health Sciences & Technology (TDU), Yelahanka, Bangalore, 560064, Karnataka, India; [c:] Department of Biotechnology, Thapar Institute of Engineering and Technology, Patiala, Punjab, 147004	**Poster**	**Accepted**
74.	**Antimicrobial Resistance (AMR) Profiling and Phylogenetic Analysis of *Neisseria gonorrhoeae* Clinical Isolates from Kenya** **Juma M [1] , Sankaradoss A [2] , Ndombi R [1] , Mwaura P [1] , Damodar T [2] , Nazir J [2] , Pandit A [2] , Khurana R [2] , Masika M [1] , Chirchir R [1] , Gachie J [1] , Krishna S [2,3] , Sowdhamini R [2] , Anzala O [1] , Meenakshi IS [1,*]** [1] KAVI Institute of Clinical Research, University of Nairobi, Nairobi, Kenya [2] National Centre for Biological Sciences, Tata Institute of Fundamental Research (TIFR), Bengaluru, India [3] School of Interdisciplinary Life Sciences, Indian Institute of Technology Goa, Ponda, India	**Poster**	**Accepted**
75.	**Identification of Critical Genes in Leukemia from Single-cell RNA Sequence Data: A Bioinformatics Approach** **Delsy Gnana Silvia D and Dr. Arnold Emerson[1]*** Department of Biotechnology, School of Bio Science and Technology, Vellore Institute of Technology (VIT). Katpadi, Vellore – 6320-14	**Poster**	**Accepted**
76.	**Characterization of obligate and non-obligate classes of domain-domain interactions in multi-domain proteins** **Sidhanta Swayam Prakash Das, R. Sowdhamini and N. Srinivasan** Molecular Biophysics Unit, Indian Institute of Science, Bangalore-560012	**Poster**	**Accepted**

	National Centre for Biological Sciences, Bangalore		
77.	**Influence of ms 2 ct 6 A37: enlightening tRNA Lys ASL folding dynamics with codon AAA/AAG** **Ms. Ambika S. Dound*, Dr. Vishwambhar V. Bhandare and Prof. Kailas D. Sonawane** Structural Bioinformatics Unit, Department of Biochemistry, Shivaji University, Vidyanagar, Kolhapur (MS), India– 416004	**Poster**	**Accepted**
78.	**Structural Refinement and Validation of Modelled Streptomycin Binding Protein from *Staphylococcus aureus*** **Ms. Shweta D. Dhumale* and Ms. Minakshee D. Devadkar* and Dr. Kailas D. Sonawane** Department of Microbiology, Shivaji University, Kolhapur 416004, India.	**Poster**	**Accepted**
79.	**Homology modelling and molecular docking studies of penicillin binding protein Transpeptidase from *Salmonella enterica* subspecies** **Ms. Shivani J. Kharade*, Nitin M. Naik and Kailas D. Sonawane** Shivaji University, Kolhapur (MS) 416004, India.	**Poster**	**Accepted**
80.	**Structural insights to the novel PSEN1 mutations in Alzheimer disease** **Sanghamitra Uttam Chopade* and Vishwambhar V. Bhandare** Department of Microbiology, Shivaji University, Kolhapur- 416 004, India	**Poster**	**Accepted**
81.	***In silico* studies of natural bioactives as a potential MAO-B and COMT inhibitors for the management of Parkinson's disease** **Pratibha Mali [a*] , Vishwambhar Bhandare [b] , Jyoti Jadhav [a]** [a] Department of Biochemistry, Shivaji University, Vidyanagar, Kolhapur, Maharashtra, India [b] Department of Microbiology, Shivaji University, Vidyanagar, Kolhapur, Maharashtra, India	**Poster**	**Accepted**
82.	**Intermolecular interactions between Aβ peptides and human CathD in Alzhimers using molecular modelling** **Subodh Kamble* and Kailas Sonawane** Structural Bioinformatics Unit, Department of Biochemistry, Shivaji University, Kolhapur, 416004, M.S., India	**Poster**	**Accepted**
83.	**Structural destabilization of Luteinizing hormone beta (LHB) heterodimeric subunit by novel variant *p.Cys46Arg*** **Vishwambhar Bhandare [1*] , Anurag Lila [2] and Ambarish Kunwar [3]** [1] Department of Microbiology, Shivaji University, Vidyanagar, Kolhapur, India - 416 004 [2] Department of Endocrinology, Seth G S Medical College & KEM Hospital, Mumbai, India - 400 012 [3] Department of Biosciences and Bioengineering, IIT Bombay, Powai, Mumbai, India - 400 076	**Poster**	**Accepted**
84.	**Computational search for potential COVID-19 drugs from FDA approved drugs and small molecules of natural origin identifies several anti-virals and plant products** **Abhishek Sharma, Vikas Tiwari and Ramanathan Sowdhamini*** National Centre for Biological Sciences, TIFR, Bangalore -560065, India	**Poster**	**Accepted**

85.	**Comprehensive *in silico* analysis of structural and functional SNPs of the human CYP27B1 protein** **John Marshal Jayaraj and Karthikeyan Muthusamy*** Department of Bioinformatics, Alagappa University, Karaikudi – 630 004, Tamil Nadu, India	**Poster**	**Accepted**
86.	**Hits Discovery on the NURR1 Receptor: Computational Approaches to Identify Agonist Compounds** **Thangam Nivethitha Saravanan, John Marshal Jayaraj, Swetha Subramanian and Karthikeyan Muthusamy*** Department of Bioinformatics, Alagappa University, Karaikudi – 630 004, Tamil Nadu, India	**Poster**	**Accepted**
87.	**HTNpedia: A Knowledgebase for Hypertension Research** **Lakshmanan Loganathan, Jeyanthi Sankar, Jeyaraman Jeyakanthan, Karthikeyan Muthusamy*** Department of Bioinformatics, Alagappa University, Karaikudi-630 003, Tamil Nadu, India.	**Poster**	**Accepted**
88.	**Identification of potential agonists for BDNF protein which involves in the pathogenesis of migraine and anxiety: an computational insights** **Sakthi Sasikala Sundaravel, and Karthikeyan Muthusamy*** Department of Bioinformatics, Alagappa University, Science Block, Karaikudi – 630004	**Poster**	**Accepted**
89.	**Computational approach on identification of inhibitors for SFRP1 protein: A potential target for colorectal cancer** **Muralidharan Jothimani, Vinitha Sivasubramaniyan, Karthikeyan Muthusamy*** Department of Bioinformatics, Alagappa University, Karaikudi-630 003, Tamil Nadu, India.	**Poster**	**Accepted**
90.	**Theoretical Investigation of PDGFRα Inhibition Using a Structure and Ligand Based Drug Design Approach"** **Vijay Nattan, Muralidharan Jothimani, Karthikeyan Muthusamy*** Department of Bioinformatics, Alagappa University, Karaikudi-630 003, Tamil Nadu, India.	**Poster**	**Accepted**
91.	**SYNERGISM OF THYMOQUINONE AND SWERTIANOLIN FOR ENHANCED THERAPEUTIC POTENTIAL AGAINST CLINICAL METHICILLIN RESISTANT *Staphylococcus aureus*** **J. Chitra[a], J. Jeba Mercy[a], SM. Rajendren[b*], Jemima Kingsly[c] and J. Jeyakanthan[d*]** [a]Department of Biotechnology, Dr. Umayal Ramanathan College for Women, Karaikudi–630003 [b]CSIR-Central Electrochemical Research Institute, Karaikudi – 630003 [c]Orbito Asia Diagnostics, Coimbatore – 641045 [d]Department of Bioinformatics, Alagappa University, Science Block, Karaikudi – 630004	**Poster**	**Accepted**
92.	***In silico* studies on protein based nanoparticles against colorectal cancer** **Muthulakshmi Muthumanickam[1], Rajaram Abhirami[2], Rameshthangam**	**Poster**	**Accepted**

	Palanivel[3*], Sanjeev Kumar Singh[4] [1]Department of Biotechnology, [2,4]Department of Bioinformatics, [3*]Department of Biotechnology (DDE), Alagappa University, Karaikudi.		
93.	***In Silico* and *in vitro* Bioactive Analysis of Traditionally important Herb Nerium Oleander** **SUNDARAM RAVIKUMAR[1], AGNIRAJ[1] AND RM. VIDHYAVATHI[2]** [1]Department of Biomedical Sciences, Alagappa University, Karaikudi-630 003, [2]Department of Bioinformatics, Alagappa University, Karaikudi 630 003	**Poster**	**Accepted**
94.	**BINDING PREDICTION AND INTERACTION ANALYSIS OF FIFTY ANTIBODIES WITH OMICRON BA1 AND BA2 PROTEIN: AN IN SILICO APPROACH** **Sandhya K. S.[a,b*], Arsha A Koshore[c], Arun Unni[a], Sunitha P. [a], Achuthsankar S. Nair[a]** [a]Department of Computational Biology and Bioinformatics, University of Kerala, Kerala [b]Malankara Catholic College, Mariagiri, Kalikkavilai, Tamil Nadu [c]Government College of Women, Trivandrum	**Poster**	**Accepted**
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98.	**Computational analysis of protein-protein interactions in two component systems** **Sneha Bheemireddy [1*] , Devendra Pratap Singh [2] , Narayanaswamy Srinivasan [1] , Ramanathan Sowdhamini [3] , Deepak Saini [2]** 1. Molecular Biophysics Unit, IISc Bangalore - 560012 2. Molecular Reproductive and Developmental Genetics, IISc Bangalore - 560012 3. National Center for Biological Sciences, Bangalore - 560065	**Poster**	**Accepted**
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	CAS in Crystallography and Biophysics department, University of Madras, Guindy Campus, Chennai 600025		
101.	**Identification of Alternative Transcripts in Retinoblastoma Progression through Meta Transcriptome Data Analysis** **Mohamed Hameed Aslam [1, 2] , Dr.D.Bharanidharan [1]** [1] Department of Bioinformatics, Aravind Medical Research Foundation, 1 Anna Nagar, Madurai-625020 [2] Department of Bioinformatics, Alagappa University Alagappa University, Science Block, Karaikudi – 630004.	**Poster**	**Accepted**
102.	***Lawsonia inermis* Flower Aqueous Extract Treatment Alleviates Diabetes associated cognitive Impairment** **Shahanaj. I & Natarajan. D** Natural Drug Research Laboratory, Department of Biotechnology, Periyar University, Salem- 636011 TN, INDIA.	**Poster**	**Accepted**
103.	**Identification of high affinity small molecule targeting 5-ALOX for the clinical treatment of pancreatic cancer** **Anushka Bhrdwaj[1], Anuraj Nayarisseri[2], Sanjeev Kumar Singh[1*]** [1] Department of Bioinformatics, Alagappa University, Science Block, Karaikudi – 630004, [2] In silico Research Laboratory, Eminent Biosciences, Indore - 452010	**Poster**	**Accepted**
104.	**Computational interpretations on HIV-1 Tat and human UHRF1 RING domain protein-protein interaction to reverse HIV-1 Latency** **Mohammad Aqueel Khan[1], Sanjeev Kumar Singh[1*]** [1]Computer Aided Drug Design and Molecular Modeling Lab, Department of Bioinformatics, Science block, Alagappa University, Karaikudi-630004, Tamil Nadu, India	**Poster**	**Accepted**
105.	**Structural Insights into the Molecular Design of NS2B/NS3 Phytochemical for the treatment of Dengue virus** **Khushboo Sharma[1], Anuraj Nayarisseri[2], Sanjeev Kumar Singh[1,*]** [1]Department of Bioinformatics, Alagappa University, Science Block, Karaikudi-630004, [2]In silico Research Laboratory, Eminent Biosciences, Indore-452010	**Poster**	**Accepted**
106.	**Structure elucidation of phytocompounds in blocking Protein-DNA interactions of sporulation mechanism in *Baccilus Cereus*** **Rajaram Abhirami[1], Chandrabose Selvaraj[1], Sanjeev Kumar Singh[1*]** [1]Computer Aided Drug Design and Molecular Modeling Lab, Department of Bioinformatics, Alagappa University, Karaikudi, India	**Poster**	**Accepted**
107.	**Structural analysis of Gp46 protein for exploring the HTLV-1 inhibitors using virtual screening, Quantum Mechanical and Molecular Dynamics analysis** **Gurunathan Rubha Shri[1], Chandrabose Selvaraj[1], Sanjeev Kumar Singh[1*]** [1]Computer Aided Drug Design and Molecular Modeling Lab, Department of Bioinformatics, Alagappa University, Karaikudi, India	**Poster**	**Accepted**

108.	**Virtual Screening and Molecular Dynamics Study of Novel ORAI1 agonist for Autism treatment.** **Rudhra Ondippili[1], Chandrabose Selvaraj[1], Sanjeev Kumar Singh[1*]** [1]Computer Aided Drug Design and Molecular Modeling Lab, Department of Bioinformatics, Alagappa University, Karaikudi, India	**Poster**	**Accepted**
109.	**Antibacterial and Anti-oxidant Activity of *Haloplegma duperreyi* Extracts** **Priyanka Sappanimuthu, Ahila mathimaran , Jeyaraman Jeyakanthan *, Vidhyavathi Ramasamy *** Department of Bioinformatics, Alagappa University, Karaikudi-630 003, Tamil Nadu, India.	**Poster**	**Accepted**
110.	**Structural and Functional Annotation of Hypothetical Proteins in *Acinetobacter baumannii*** **Raji Rajmichael and Jeyakanthan Jeyaraman*** Structural Biology & Bio-Computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi-630004, Tamil Nadu, India	**Poster**	**Accepted**
111.	**Structural and Functional Stability Analyses of SpeB from *Thermus thermophilus* HB8 – A Computational Approach** **Malaisamy Veerapandiyan, Nagarajan Hemavathy, Alagesan Karthika, Jayaraman Manikandan, and Jeyaraman Jeyakanthan** Structural Biology and Biocomputing Lab, Department of Bioinformatics, Alagappa University, Karaikudi – 630004, Tamil Nadu, India.	**Poster**	**Accepted**
112.	**A Compendious study of Dengue NS1 protein and its interaction with Human RPL18 using Network Analysis and Drug Discovery approach** **Muthuraja Arun Pravin, Chandrabose Selvaraj and Sanjeev Kumar Singh*** Computer Aided Drug Design and Molecular Modelling Lab, Department of Bioinformatics, Alagappa University, Karaikudi-630 004, Tamil Nadu, India	**Poster**	**Accepted**
113.	**Mechanistic Insights on Allosteric Regulation of Aspartatae kinase from *Wolbachia* Endosymbiont of *Brugia Malayi*** **Mathimaran Amala and Jeyaraman Jeyakanthan*** Structural Biology and Biocomputing Lab, Department of Bioinformatics, Alagappa University, Karaikudi – 630004, Tamil Nadu, India.	**Poster**	**Accepted**

114.	**Exploration of novel target from central metabolic pathway of Mycobacterium tuberculosis a protein involved in organism survival** **Sneha Subramaniyan and Jeyakanthan Jeyaraman*** Structural Biology & Bio-Computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi-630004, Tamil Nadu, India	**Poster**	**Accepted**
115.	**Decoding the whole genome sequence of a clinical isolate of *Pseudomonas aeruginosa*** **Bhuvaneswari Narthanareeswaran and Jeyaraman Jeyakanthan*** Structural Biology and Biocomputing Lab, Department of Bioinformatics, Alagappa University, Karaikudi – 630004, Tamil Nadu, India.	**Poster**	**Accepted**
116.	**Whole Genome Sequencing identified a genetic variant rs20360548 of *GPRC6A* gene is associated with T2DM and DR: A case-control study and *in silico* analysis** **Rizza A N[a,b], PavithraJanarthanan[a], Nagarajan Hemavathy[c], Rajiv Raman[d], Lucia Sobrin[e], Ricky Chan[f], Sudha K Iyengar[f], Sinnakaruppan Mathavan[a*]** [a]SN ONGC Department of Genetics and Molecular Biology, Vision Research Foundation, Chennai, 600 006, India [b]Department of Biotechnology, Alagappa University, Karaikudi, 630 003, Tamil Nadu, India [c]Structural Biology and Bio-Computing Lab, Department of Bioinformatics, Science Block, Alagappa University, Karaikudi, 630 003, Tamil Nadu, India [d]ShriBhagwanMahavir Department of Vitreo Retinal Services, Medical Research Foundation, Chennai, 600 006, India [e]Massachusetts Eye and Ear, Mass General Brigham, Boston, Massachusetts, 02114, United States [f]Department of Population and Quantitative Health Sciences, School of Medicine, Cleveland, Ohio, 44106, United State	**Poster**	**Accepted**
117.	**Structure based design of anti-bacterial drugs using mammalian heme peroxidases as potential drug targets.** **V. Viswanathan [1,2] , J. Jeyakanthan [1] , P. Sharma [2] , S. Sharma [2] and T. P. Singh [2]** [1] Department of Bioinformatics, Alagappa University, Karaikudi, Tamil Nadu. [2] Department of Biophysics, All India Institute of Medical Sciences, New Delhi.	**Poster**	**Accepted**
118.	**Major Phytoconstituents of Momordica cymbalaria seed extract against vancomycin resistant Enterococcus faecium** **Ahila Mathimaran, Jeyakanthan Jeyaraman a*** Department of Bioinformatics, Algappa University, Kararikudi, Tamil Nadu, India**.**	**Poster**	**Accepted**
119.	**Computational insights into the conformational dynamics of drug resistance mutation in the pncA gene of Mycobacterium tuberculosis** **Manikandan Jayaraman and Jeyakanthan Jeyaraman*** Structural Biology and Biocomputing Lab, Department of Bioinformatics, Alagappa University, Karaikudi – 630004, Tamil Nadu, India.	**Poster**	**Accepted**

120.	**Identification of potential inhibitor against Hepatocellular Carcinoma through *in silico* approach** **Srinithi R[1] , Nachammai KT[2] , Sangavi P[1] , Langeswaran K[2]*** [1]Department of Bioinformatics, Science Campus, Alagappa University, Karaikudi, Tamil Nadu, India [2]Department of Biotechnology, Science Campus, Alagappa University, Karaikudi, Tamil Nadu, India	**Poster**	**Accepted**
121.	**Whole Genome Sequencing and annotation studies of Nocardia farcinica** **N.Shaslinah, Chitra jeyaraj pandian, Jemima D kingsley, and Jeyakanthan Jeyaraman*** Structural Biology & Bio-Computing Lab, Department ofBioinformatics, Alagappa University, Karaikudi-630004, Tamil Nadu, India	**Poster**	**Accepted**
122.	**Potent Inhibitors for Tetracycline Repressor Family of Transcription Regulator protein in Tetracycline-resistant strain of Acinetobacter baumannii** **Karthika Alagesan[1] , Chitra Jeyaraj Pandian[2] , Jemima Kingsley[3] , Jeyaraman Jeyakanthan[1] *** [1] Structural Biology and Bio-Computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi 630004, Tamil Nadu, India. [2] Department of Biotechnology, Dr. Umayal Ramanathan College for Women, Karaikudi 630003, Tamil Nadu, India.	**Poster**	**Accepted**
123.	**In-silico analysis of Structure and Functional of Glucose-6-phosphate Dehydrogenase through Molecular Dynamics Simulation** **Karthika Alagesan [1] , Chun Jung Chen [2] , Jeyaraman Jeyakanthan [1] *** [1] Structural Biology and Bio-Computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi 630004, Tamil Nadu, India. [2] Life Science Group, Scientific Research Division, National Synchrotron Radiation Research Center, Hsinchu 30076, Taiwan.	**Poster**	**Accepted**
124.	**Unravelling the functional mode/mechanism of streptomycin adenylyltransferase from *Serratia marcescens*** **D. Prabhu[1], S. Rajamanikandan[1], J. Jeyakanthan[2], P. Ramasamy[1]** [1] R & D Wing, Sree Balaji Medical College and Hospital-BIHER, Chennai-600 044, India, [2] Department of Bioinformatics, Alagappa University, Karaikudi-630 003, India E-mail:jjeyakanthan@alagappauniversity.ac.in	**Poster**	**Accepted**

125.	**Computational screening of potent phytochemicals from medicinal plants as SARS-CoV-2 NSP1 inhibitors** **S. Rajamanikandan[1], D. Prabhu[1], J. Jeyakanthan[2], P. Ramasamy[1]** [1] R & D Wing, Sree Balaji Medical College and Hospital-BIHER, Chennai-600 044, India, [2] Department of Bioinformatics, Alagappa University, Karaikudi-630 003, India E-mail:jjeyakanthan@alagappauniversity.ac.in	**Poster**	**Accepted**