



**DEPARTMENT OF BIOINFORMATICS**  
(UGC-INNO, DST-FIST & PURSE Sponsored Department)



**ALAGAPPA UNIVERSITY**

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**International Conference on  
"RECENT TRENDS IN STRUCTURAL BIOINFORMATICS AND COMPUTER AIDED DRUG  
DESIGN" (ICSBCADD-2019)**

December 11<sup>th</sup> – 13<sup>th</sup>, 2019

**LIST OF PARTICIPANTS**

S.No	Title of Abstract	Presentation	Status
1.	<b>Computational insights into the inhibitory mechanism of resveratrol and clioquinol hybrid against amyloid-<math>\beta_{42}</math> aggregation and protofibril destabilization in Alzheimer's disease</b> Dr. Bhupesh Goyal* School of Chemistry & Biochemistry, Thapar Institute of Engineering & Technology (Deemed to be University), Patiala-147004, Punjab, India	Oral	Accepted
2.	<b>Alkaloids as potential drug lead for fighting against multi drug resistant: a case study of NDM-1 from <i>Klebsiella pneumonia</i> as drug target</b> Dr. Ved Vrat Verma* Informatics System & Research Management (ISRM) Division, Indian Council of Medical Research (ICMR), Ansari Nagar, New Delhi – 110029, INDIA	Oral	Accepted
3.	<b>Exploring the Selectivity of SIK2 families using a Molecular modeling studies</b> Prajisha Jayaprakash and Jeyaraman Jeyakanthan* Structural Biology & Bio-Computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India	Poster	Accepted
4.	<b>A systems pharmacology approach to decipher the mechanism of action of Parangichakkai chooranam, a Siddha therapy for psoriasis</b> Dr. A. Mohana Priya* School of Biosciences and Technology, Vellore Institute of Technology, Vellore – 632014.	Oral	Accepted
5.	<b>Role of Hydration sites in Binding Affinity of Pak1 inhibitors using Water mapping and scoring approaches</b> Jayashree Biswal <sup>1</sup> , Suresh Kumar Rayala <sup>2</sup> , Ganesh Venkatraman <sup>3</sup> and Jeyaraman Jeyakanthan <sup>1*</sup> <sup>1</sup> Structural Biology & Bio-Computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi - 630004, Tamil Nadu, India <sup>2</sup> Department of Biotechnology, Indian Institute of Technology Madras, Room No. BT 306, Chennai- 600036, Tamil Nadu, India <sup>3</sup> Department of Human Genetics, Sri Ramachandra University, Porur, Chennai-600116, Tamil Nadu, India	Poster	Accepted
6.	<b>The target validation using structure-based targeting of orthologous pathogen proteins (STOPP) approach</b> Dr. Yogavel Manickam and Amit Sharma Molecular Medicine – Structural Parasitology Group, International Centre for Genetic Engineering and Biotechnology (ICGEB), ArunaAsaf Ali Marg, New Delhi – 110067, India	Oral	Accepted

7.	<p><b>Cloning, Expression and Purification of N1 Aminopropyl Agmatine Ureohydralase (SpeB) protein from <i>Thermus thermophilus</i> HB8</b></p> <p>Veerapandiyan Malaisamy and Jeyaraman Jeyakanthan* Structural Biology &amp; Bio-Computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India</p>	Poster	Accepted
8.	<p><b>Molecular modeling investigations on Life-Threatening diseases</b></p> <p>Dr. R. Balajee and Jeyaraman Jeyakanthan* Structural Biology &amp; Bio-Computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India</p>	Oral	Accepted
9.	<p><b>Understanding the mode of action of active compounds from Chyawanprashin modulating AKT1 gene in Aging: An <i>in silico</i> analysis</b></p> <p>Swathika Praveen<sup>1</sup>, Arjun A.R<sup>1</sup>, Sajitha Lulu S<sup>2</sup>, Girinath G Pillai<sup>3</sup> <sup>1</sup>Department of Integrative Biology, <sup>2</sup>Department of Biotechnology, School of Life Sciences and Technology, Vellore Institute of Technology, Vellore-632014, Tamil Nadu, India <sup>3</sup>Zastra innovations Pvt. Ltd, Bengaluru.</p>	Oral	Accepted
10.	<p><b>Tangeretin – A novel inhibitor against Hepatocellular carcinoma</b></p> <p>Sangavi P and Langeswaran K* Cancer Genetics &amp; Molecular Biology Laboratory, Department of Bioinformatics, Science Campus, Alagappa University, Karaikudi-630004, Tamil Nadu, India</p>	Poster	Accepted
11.	<p><b>Computational understanding on molecular mechanism of hypertensive drug metabolizing enzymes and its implication on developing personalized drugs</b></p> <p>Lakshmanan Loganathan and Karthikeyan Muthusamy* Pharmacogenomics and CADD Laboratory, Department of Bioinformatics, Science Campus, Alagappa University, Karaikudi-630004, Tamil Nadu, India</p>	Oral	Accepted
12.	<p><b>Insight into structural and functional analysis of the impact of missense mutation in Cytochrome P450 oxidoreductase protein</b></p> <p>Rajalakshmi Kumar<sup>1</sup>, Manikandan Jayaraman<sup>2</sup>, Adithan Chandrasekaran<sup>1*</sup> and Ramadas Krishna<sup>2*</sup> <sup>1</sup>Central Inter-Disciplinary Research Facility (CIDRF), Sri Balaji Vidyapeeth (Deemed to be University), Puducherry – 607402, India. <sup>2</sup>Centre for Bioinformatics, School of Life Sciences, Pondicherry University, Pondicherry – 605014, India.</p>	Poster	Accepted
13.	<p><b>Experimental Characterization of Streptomycin adenylyltransferase from <i>Serratia marcescens</i></b></p> <p>Dhamodharan Prabhu, Mathimaran Amala, Poopandi Saritha, Malaisamy Veerapandiyan and Jeyaraman Jeyakanthan* Structural Biology &amp; Bio-Computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India</p>	Poster	Accepted
14.	<p><b><i>In silico</i> identification of common cancer biomarkers among heterogeneous types of cancer</b></p> <p>H. Lalremmawia and Basant K. Tiwary* Centre for Bioinformatics, Pondicherry University, Kalapet- 605014</p>	Oral	Accepted

15.	<p><b>Deleterious nsSNPs screening and molecular dynamics study on human Klotho for their effects on protein structure, stability and function.</b></p> <p>John Marshal Jayaraj and Karthikeyan Muthusamy* Pharmacogenomics and CADD Laboratory, Department of Bioinformatics, Science Campus, Alagappa University, Karaikudi-630004, Tamil Nadu, India</p>	Poster	Accepted
16.	<p><b>Eigen Value ANalysis (EVANS)- A “universal” QSPR formalism for addressing pharmacodynamics, pharmacokinetics and toxicity issues in drug development</b></p> <p>Blessy Joseph, <u>Anish Gomatam</u>, Mushtaque Shaikh, Vijay Khedkar, Elvis Martis, Poonam Advani, Evans Coutinho* Department of Pharmaceutical Chemistry, Bombay College of Pharmacy, Kalina, Mumbai, India</p>	Oral	Accepted
17.	<p><b>Molecular Cloning and Structural Studies on FCMS from <i>Pyrococcus horikoshii</i> OT3</b></p> <p>R. Guru Raj Rao<sup>1</sup>, K. Sekar<sup>3</sup>, Chun-Jung Chen<sup>2</sup>, J. Jeyakanthan<sup>1*</sup> <sup>1</sup>Structural Biology &amp; Bio-Computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India. <sup>2</sup>Life Science Group, Scientific Research Division, National Synchrotron Radiation Research Centre, Hsinchu, 30076, Taiwan. <sup>3</sup>Department of Computational and Data Sciences, Indian Institute of Sciences, Bangalore – 560012, India.</p>	Poster	Accepted
18.	<p><b>Structural insight into conformational dynamics of non-active site mutations in KsaA: A Mycobacterium tuberculosis target protein</b></p> <p>Manikandan Jayaraman, Savita Kumari Rajendra, Krishna Ramadas* Centre for Bioinformatics, School of Life Sciences, Pondicherry University, Puducherry-605014, India</p>	Poster	Accepted
19.	<p><b>Insights into molecular modeling of SH3BP2-Tankyrase protein complex structure and molecular docking studies</b></p> <p>Muralidharan Jothimani, Lakshmanan Loganathan, and Karthikeyan Muthusamy* Pharmacogenomics and CADD Laboratory, Department of Bioinformatics, Science Campus, Alagappa University, Karaikudi-630004, Tamil Nadu, India</p>	Poster	Accepted
20.	<p><b>Identification of peptide based vaccine candidates against <i>Staphylococcus epidermidis</i>: A Subtractive genomics and proteomics approach</b></p> <p>Guneswar Sethi<sup>1</sup>, Satyanarayan Sethi<sup>2</sup>, Ramadas Krishna<sup>1</sup> <sup>1</sup>Centre for Bioinformatics, School of Life Sciences, Pondicherry University, Puducherry-605014, India <sup>2</sup>Central Institute of Brackish water Aquaculture, CIBA, 75, (ICAR), Chennai-28 India</p>	Poster	Accepted
21.	<p><b>Molecular Evolution, Binding Site Interpretation and Functional Divergence of Aspartate Semialdehyde Dehydrogenase</b></p> <p>Mathimaran Amala, Mariadasse Richard, Poopandi Saritha, Dhamodharan Prabhu, Malaisamy Veerapandiyan, Kangarajan Surekha and Jeyaraman Jeyakanthan* Structural Biology &amp; Bio-Computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India</p>	Poster	Accepted

22.	<p><b>Comparison of Machine Learning classifiers in miRNA target prediction</b></p> <p>Sherin K. and Achuthsankar S. Nair  Department of Computational Biology and Bioinformatics, University of Kerala, Thiruvananthapuram, Keralam-695581</p>	Oral	Accepted
23.	<p><b><i>In silico</i> perceptive into the stereochemical necessities of the bradykinin receptor and its antagonist molecules.</b></p> <p>Manikandan Selvaraj, Lakshmanan Loganathan, and Karthikeyan Muthusamy*  Pharmacogenomics and CADD Laboratory, Department of Bioinformatics, Science Campus, Alagappa University, Karaikudi-630004, Tamil Nadu, India</p>	Poster	Accepted
24.	<p><b>Optimization framework for identification of dysregulated module in Breast Cancer Data</b></p> <p>Suma L.S. and Vinod Chandra S.S.  Department of Computational Biology and Bioinformatics, University of Kerala, Thiruvananthapuram, Keralam-695581</p>	Oral	Accepted
25.	<p><b>Expression and Purification of Succinyl-diaminopimelatede succinylase (dapE) from Wolbachia endosymbiont of <i>Brugia malayi</i></b></p> <p>Poopandi Saritha<sup>1</sup>, Mathimaran Amala<sup>1</sup>, Kangarajan Surekha<sup>1</sup>, Jayashree Biswal<sup>1</sup>, Yen-Chieh-Huang<sup>2</sup>, Chun-Jung-Chen<sup>2</sup> and Jeyaraman Jeyakanthan<sup>1*</sup>  <sup>1</sup>Structural Biology &amp; Bio-Computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi- 630 004, Tamil Nadu, India.  <sup>2</sup>Life Science Group, Scientific Research Division, National Synchrotron Radiation Research Centre, Hsinchu, 30076, Taiwan.</p>	Poster	Accepted
26.	<p><b><i>In silico</i> identification of blood biomarkers for Schizophrenia using Machine Learning</b></p> <p>T Sayamsmruiti Panda and Basant K. Tiwary*  Centre for Bioinformatics, School of Life Sciences, Pondicherry University, Puducherry-605014, India</p>	Poster	Accepted
27.	<p><b>Structural and Functional Characterization of SIRT4 protein from <i>Homo sapiens</i></b></p> <p>Dr. M. Nachiappan and Jeyaraman Jeyakanthan*  Structural Biology &amp; Bio-Computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India</p>	Oral	Accepted
28.	<p><b>A gene expression and structural dynamics study on AccA1: A potential drug target for antituberculosis activity</b></p> <p>Chandra Jyoti Singha<sup>a</sup> and Ramadas Krishna*  <sup>a</sup>Centre for Bioinformatics, School of Life Sciences, Pondicherry University, Puducherry-605014, India</p>	Poster	Accepted
29.	<p><b>Purification and <i>in vitro</i> characterization of PH0140 from <i>Pyrococcus horikoshii</i> OT3</b></p> <p>G. Kohila and Jeyaraman Jeyakanthan*  Structural Biology &amp; Bio-Computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India</p>	Poster	Accepted

30.	<p><b>Understanding the mechanism of Domain swapping in Human Cellular Retinol Binding Protein II (hCRBP II)</b></p> <p>Sankaran SV. *, Nahren Manuel Mascarenhas  Department of Chemistry, Sacred Heart College (Autonomous),  Tirupattur (Vellore Dt.)635601</p>	Oral	Accepted
31.	<p><b>A novel search engine for the proteins involved in the Notch crosstalk signaling pathways</b></p> <p>Madhumathi Sanjeevi<sup>1</sup>, Santhosh Rajendran<sup>1</sup>, Sanjay K Choubey<sup>1</sup>, Sekar Kanagaraj<sup>2</sup>, and Jeyakanthan Jeyaraman<sup>1*</sup>  <sup>1</sup>Structural Biology &amp; Bio-Computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India.  <sup>2</sup>Department of Computational and Data Sciences, Indian Institute of Sciences, Bangalore – 560012, India.</p>	Poster	Accepted
32.	<p><b>The Combined Use of <i>in vitro</i> and <i>in silico</i> analyses to assess anti-cancerous potential of a bioactive compound Naringenin and its derivatives</b></p> <p>Dr. Beutline Malgija M, Host Antony David and Joyce Priyakumari C  Bioinformatics Centre of BTISnet, Madras Christian College, Chennai 600 059</p>	Poster	Accepted
33.	<p><b>Role of substituents on Copper (II) tetrapyridine complexes towards redox chemotherapy through experimental and computational approaches</b></p> <p>Dr. Manikandamathavan and Jeyaraman Jeyakanthan*  Structural Biology &amp; Bio-Computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India</p>	Oral	Accepted
34.	<p><b>Understanding the role of serine proteases of <i>Trichophyton rubrum</i>, a dermatophytes, as potential virulence factors</b></p> <p>Chitra Latka<sup>1,2</sup> and Bhupesh Taneja<sup>1,2*</sup>  <sup>1</sup>Genome Informatics and Structural Biology Unit, CSIR-Institute of Genomics and Integrative Biology, New Delhi, India  <sup>2</sup>Academy of Scientific and Innovative Research, New Delhi, India</p>	Poster	Accepted
35.	<p><b>Computational identification of potent anti-bacterial drug molecules for Gram Negative Pathogens</b></p> <p>R. Raji and Jeyaraman Jeyakanthan*  Structural Biology &amp; Bio-Computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India</p>	Poster	Accepted
36.	<p><b>Molecular dynamic simulation of BACE1 with small molecular inhibitor and peptide based inhibitor</b></p> <p>Arokia Anto Royan M, S. Muneeswaran and K. Muruga Poopathi Raja*  Department of Physical Chemistry, School of Chemistry, Madurai Kamaraj University, Palkalai Nagar, Madurai-625021.</p>	Poster	Accepted
37.	<p><b>Insights on Exogenous Tryptophan-mediated Allosteric communication and Helical Transition of TRP protein for Transcription Regulation</b></p> <p>Richard Mariadasse, Sanjay Kumar Choubey and Jeyaraman Jeyakanthan*  Structural Biology &amp; Bio-Computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India</p>	Oral	Accepted

38.	<p><b>Synthesis, Characterization and Computational studies of peptide based inhibitors for BACE1 of Alzheimer's disease</b></p> <p>S. Muneeswaran, M. Thamaraiselvam and K. MurugaPoopathi Raja*  Department of Physical Chemistry, School of Chemistry, Madurai Kamaraj University, Palkalai Nagar, Madurai-625021.</p>	Poster	Accepted
39.	<p><b>MRPC: missing regions in polypeptide chains - A knowledgebase</b></p> <p>Rajendran Santhosh, Namrata Bankoti, Padmashri Adgonda Malgonnavar, Daliah Michael, Jeyaraman Jeyakanthan* and K. Sekar*  <sup>1</sup>Structural Biology &amp; Bio-Computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India.  <sup>2</sup>Department of Computational and Data Sciences, Indian Institute of Sciences, Bangalore - 560012, India.</p>	Poster	Accepted
40.	<p><b>Achromobacter Xylosoxidans induced Bacteremia in premature neonates: Case report</b></p> <p>Chitra J<sup>2</sup>, Jeba Mercy<sup>2</sup>, Viji R<sup>2</sup>, Jeyaraman Jeyakanthan<sup>1*</sup>  <sup>1</sup>Structural Biology &amp; Bio-Computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India.  <sup>2</sup>Department of Biotechnology, Dr. Umayal Ramanathan College for Women, Karaikudi-630002</p>	Oral	Accepted
41.	<p><b>In silico discovery of Cassia fistula as a potential inhibitor for ovarian cancer</b></p> <p>Kaviya Kabilan and Jeyaraman Jeyakanthan*  Structural Biology &amp; Bio-Computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India</p>	Poster	Accepted
42.	<p><b>Unraveling the Structural dynamics of Chikungunya Helicase</b></p> <p>Prateek Kumar, Deepak Kumar, Rajanish Giri*  School of Basic Sciences, Indian Institute of Technology Mandi, VPO Kamand, Himanchal Pradesh 175005, India</p>	Poster	Accepted
43.	<p><b>Antidepressant activity of nutraceutical compounds from wheat seedlings</b></p> <p>P. Ravikumar and M. Jeyam*  Department of Bioinformatics, Bharathiar University, Coimbatore- 641046, Tamil Nadu, India</p>	Oral	Accepted
44.	<p><b>Identification of potential inhibitor for Jaundice from Nigella sativa - an in silico analysis</b></p> <p>Komatha Malarvizhi and Jeyaraman Jeyakanthan*  Structural Biology &amp; Bio-Computing Lab, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India</p>	Poster	Accepted
45.	<p><b>An in silico approach for identifying the molecular level interaction of Chemotherapy drugs Crizotinib and Temozolomide in Glioblastoma and Lung Cancer targets</b></p> <p>Saleena Y, Vinod Chandra S.S. and Achuthsankar S. Nair  Department of Computational Biology and Bioinformatics, University of Kerala, Thiruvananthapuram, Kerala-695581</p>	Oral	Accepted

46.	<p><b>Pharmacoinformatic exploration of MMP inhibitor for the treatment of Diabetic Retinopathy from <i>Pinus pinaster</i> phytoligands</b></p> <p>T. Indhumathi, S. Muthumanickam and P. Boomi* Chemoinformatics and Nano drug delivery Lab, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India</p>	Poster	Accepted
47.	<p><b>Identification of genes and pathways responsible for resistance of glioblastoma to antiVEGF therapy-A Bioinformatics approach</b></p> <p>Arya K.R., Bharath Chand R.P, Achuthsankar S. Nair, P.R. Sudhakaran Department of Computational Biology and Bioinformatics, University of Kerala, Thiruvananthapuram, Keralam-695581</p>	Oral	Accepted
48.	<p><b>A computational study to analyze the potent inhibitor against Cardiovascular disease (CVD) from <i>Salix tetrasperma</i></b></p> <p>Soundarya Soundarapandian, Abinaya Karthikeyan, Joseph Sahayarayan Jesudoss and Vidhyavathi Ramasamy* Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India</p>	Poster	Accepted
49.	<p><b>Asparagine and Glutamine Repeats: Aggregations to Diseases</b></p> <p>K. Muruga Poopathi Raja* Chemical Biology and Biophysics Laboratory, Department of Physical Chemistry, School of Chemistry, Madurai Kamaraj University, Palkalai Nagar, Madurai-625021.</p>	Oral	Accepted
50.	<p><b>Identification of potent novel antiviral compound through the computational methods</b></p> <p>S. Muthumanickam, T. Indhumathi and P. Boomi* Chemoinformatics and Nano drug delivery Lab, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India</p>	Poster	Accepted
51.	<p><b>Identifying novel targets and their inhibitory Phytocompounds in <i>H.pylori</i>-mediated infection - An <i>in silico</i> approach</b></p> <p>Priya Venugopal, Abhinand C.S., Athira T., Achuthsankar S. Nair Department of Computational Biology and Bioinformatics, University of Kerala, Thiruvananthapuram, Keralam-695581</p>	Oral	Accepted
52.	<p><b>Development of the potent anti-protozoan inhibitors against enzymes involved in cysteine biosynthetic pathway of <i>Entamoeba histolytica</i></b></p> <p>Ramachandran Vijayan, Sudhaker Dharavath, Khushboo Kumari, Priya Tomar and Samudrala Gourinath* School of Life Sciences, Jawaharlal Nehru University, New Delhi-110067, India</p>	Poster	Accepted
53.	<p><b>Role of ADME and Toxicity in the Drug Candidate Selection using Multi Parameter Optimization</b></p> <p>Girinath G. Pillai Zastra Innovations, Bengaluru-560043.</p>	Oral	Accepted
54.	<p><b>Screening for novel agonists for ATF6 to alleviate ER stress induced disease pathogenesis</b></p> <p>M. Shoufia Jabeen, Hemamalini Vedagiri* Molecular Genomics Lab, Department of Bioinformatics, Bharathiar University, Coimbatore-641046</p>	Oral	Accepted

55.	<p><b>Subtractive proteomics approach for identifying putative drug targets and elucidating inhibitors from <i>Balanites aegyptiaca</i> for <i>Microsporium gypseum</i> – A computational study</b></p> <p>Syed Abuthakir Mohamed Husain, Sharmila Velusamy and Jeyam Muthusamy*</p> <p>Biochematics Lab, Department of Bioinformatics, Bharathiar University, Coimbatore-641046, Tamil Nadu, India</p>	Oral	Accepted
56.	<p><b>Epitope identification from virulence proteins of <i>Staphylococcus aureus</i> and <i>Streptococcus pyogenes</i> for Vaccine development – An <i>in silico</i> approach</b></p> <p>Sharmila Velusamy, Syed Abuthakir Mohamed Husain and Jeyam Muthusamy*</p> <p>Biochematics Lab, Department of Bioinformatics, Bharathiar University, Coimbatore-641046, Tamil Nadu, India</p>	Oral	Accepted
57.	<p><b>A Review on Lipoxygenase Structure and its Role in Plant and Mammals Physiology</b></p> <p>Tulsi, Lakshmi Priya, Sampath R, Ishwar Patidar, Anbu V and A. Dinakara Rao*</p> <p>Department of Bioinformatics, School of Life Sciences, Pondicherry University, Puducherry-605014.</p>	Poster	Accepted
58.	<p><b>A Biochemical, molecular and computational approach to characterize lipoxygenase from flax (<i>Linum usitatissimum</i>)</b></p> <p>P. Lakshmi Priya and A. Dinakara Rao*</p> <p>Centre for Bioinformatics, School of Life Sciences, Pondicherry University, Puducherry-605014.</p>	Poster	Accepted
59.	<p><b>Virtual Screening approaches to identify potent inhibitors against Obesity causing protein in PCOS</b></p> <p>Abinaya Karthikeyan, Soundarya Soundarapandian, Vidhyavathi Ramasamy and Joseph Sahayarayan Jesudoss*</p> <p>Plant Molecular Biology and Bioinformatics Laboratory, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India</p>	Poster	Accepted
60.	<p><b>Investigations on the interaction between PTNP14 with high and low risk HPV types 16 and 11</b></p> <p>Aarthy Murali and Sanjeev Kumar Singh*</p> <p>Computer Aided Drug Design and Molecular Modeling Laboratory, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India</p>	Oral	Accepted
61.	<p><b>Computational study on 5-substituted 2-acylaminothiazoles class of compounds to activate the Tat-mediated HIV-1 transcription</b></p> <p>Mohammad Aqueel Khan and Sanjeev Kumar Singh*</p> <p>Computer Aided Drug Design and Molecular Modeling Laboratory, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India</p>	Poster	Accepted
62.	<p><b>Structural insights into the inhibition of TasA enzyme targeting spore and biofilm forming mechanism in <i>Bacillus cereus</i></b></p> <p>Rajaram Abhirami, Chandrabose Selvaraj and Sanjeev Kumar Singh*</p> <p>Computer Aided Drug Design and Molecular Modeling Laboratory, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India</p>	Poster	Accepted

63.	<p><b>Integrated microarray meta-analysis unveiled a panel of diagnostic biomarkers of Glioblastoma</b></p> <p>Chirasmita Nayak and Sanjeev Kumar Singh*</p> <p>Computer Aided Drug Design and Molecular Modeling Laboratory, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India</p>	Oral	Accepted
64.	<p><b>Structure based screening of anti HIV-1 inhibitors by targeting V3 loop in the envelope protein gp120</b></p> <p>Ishwar Chandra and Sanjeev Kumar Singh*</p> <p>Computer Aided Drug Design and Molecular Modeling Laboratory, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India</p>	Poster	Accepted
65.	<p><b>In silico studies of phytochemicals as the potent inhibitors against the E protein of Dengue Virus</b></p> <p>Karthikeyan M and Sanjeev Kumar Singh*</p> <p>Computer Aided Drug Design and Molecular Modeling Laboratory, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India</p>	Poster	Accepted
66.	<p><b>Atomistic Intuitions on Enzymatic reaction mechanism and protein-protein interaction of MDH and MMo from <i>Methylococcus capsulatus</i></b></p> <p>Chandrabose Selvaraj and Sanjeev Kumar Singh*</p> <p>Computer Aided Drug Design and Molecular Modeling Laboratory, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India</p>	Poster	Accepted
67.	<p><b>In silico strategies to disrupt the protein-protein interaction between integrase and LEDGF/p75</b></p> <p>Umesh Panwar and Sanjeev Kumar Singh*</p> <p>Computer Aided Drug Design and Molecular Modeling Laboratory, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India</p>	Oral	Accepted
68.	<p><b>Virtual Screening to identify novel potential inhibitors for AChE of Alzheimer's disease by an <i>in silico</i> approach</b></p> <p>Mohd. Babu Khan<sup>1</sup>, Bhagath KP<sup>1</sup>, Tuleshwori DS<sup>1</sup>, Lakshmi PK<sup>1</sup>, Tulsi Yadav<sup>1</sup>, Naidu Subbarao<sup>2</sup> &amp; A. Dinakara Rao<sup>1*</sup></p> <p><sup>1</sup>Centre for Bioinformatics, School of Life Sciences, Pondicherry University, Puducherry-605 014.</p> <p><sup>2</sup>SCIS, Jawaharlal Nehru University, New Delhi 110067, India.</p>	Oral	Accepted
69.	<p><b>Investigation of Dual negative allosteric modulator to predict correct pose and unraveling the binding mode between mGluR1 and mGluR5 through binding pose metadynamics and molecular dynamics simulations</b></p> <p>Sitrarasu Vijaya Prabhu and Sanjeev Kumar Singh*</p> <p>Computer Aided Drug Design and Molecular Modeling Laboratory, Department of Bioinformatics, Alagappa University, Karaikudi- 630004, Tamil Nadu, India</p>	Oral	Accepted
70.	<p><b>Mapping the interaction of Zika virus NS4B with NS3 Helicase protein</b></p> <p>Taniya Bhardwaj, Prateek Kumar, Rajanish Giri*</p> <p>School of Basic Sciences, Indian Institute of Technology Mandi, VPO Kamand, Himanchal Pradesh 175005, India</p>	Poster	Accepted

71.	<p><b>Evolution and Structural Basis of the Surface Protein Hemagglutinin in the Indian Influenza A (HIN1) Strains of 2017</b></p> <p>Shilpa Sri Pushan, Mahesh Samantaray, Ramaswamy Amutha* Centre for Bioinformatics, Pondicherry University, R.V. Nagar, Kalapet, Puducherry-605 014, India</p>	Poster	Accepted
72.	<p><b><i>In silico</i> approach for biomarker identification and Phytochemicals screening of potent inhibitor for Polycystic ovary syndrome (PCOS) targets</b></p> <p>Nirmaladevi Ponnusamy, Pavithra Damodharan, Rajasree Odumpatta, Mohanapriya Arumugam* Department of Biotechnology, Vellore Institute of Technology, Vellore, India-632 014</p>	Oral	Accepted
73.	<p><b>Assembly strategy of the trimeric polymerase complex of Indian Influenza A virus: A computational approach</b></p> <p>Mahesh Samantaray, Shilpa Sri Pushan, Ramaswamy Amutha* Centre for Bioinformatics, Pondicherry University, R.V. Nagar, Kalapet, Puducherry-605 014, India</p>	Poster	Accepted
74.	<p><b>Targeting Cancer Stem Cells: Role of Hedgehog Signalling Pathway in Tumorigenesis and Tumor resistance</b></p> <p>Jesu Castin. E, Karthik. S, Pooka. B and Sherlin Rosita. A* Department of Biotechnology &amp; Bioinformatics, Bishop Heber College (Autonomous), Tiruchirappalli-620017</p>	Poster	Accepted
75.	<p><b>An in silico approach for the identification of anti HIV-1 reverse transcriptase phytoconstituents through Molecular modelling</b></p> <p>L. Abibarath and Dr. P. Manogar* PG and Research Department of Botany, Nehru Memorial College (AUTONOMOUS) (Nationally Accredited with "A" Grade by NAAC), Puthanampatti-621 007, Trichy Dt.</p>	Poster	Accepted