



Alagappa University

Department of Bioinformatics

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S. No	Title of the abstract	Status
1	<i>In silico anticancer studies of bioactive compounds in <i>Tephrosia purpurea Pers.</i></i> Keerthana M.*, Rajaram K.*, Dinesh K., Sureshkumar P. <i>Bharathidasan Institute of Technology, Anna University-Chennai, Tiruchirappalli- 620024, Tamil nadu, India</i>	Accepted
2	Molecular Dynamics simulation of β-melanotropin stimulating hormone (β-MSH) docked onto the receptor MC4R. Mutangana Dieudonne, Ramesh K. V.* <i>Department of Biotechnology, Center for Postgraduate Studies, Jain University, 18 /3, 9th Main, Jayanagar 3rd block, Bangalore – 560011, Karnataka, India.</i>	Accepted
3	Investigating the structural impact of T174M and M235T mutations of Angiotensinogen by molecular dynamics simulation. Karthikeyan Muthusamy* and Kh. Dhanachandra Singh <i>Department of Bioinformatics, Alagappa University, Science Block, Karaikudi – 630004</i>	Accepted
4	An insight on Transcription Regulation of Leucine Responsive Regulatory Protein (PH0140) from <i>Pyrococcus horikoshii</i> OT3. Richard. M ¹ , Renganayaki. M ¹ , Velmurugan. D ² and Jeyakanthan. J ¹ <i>¹Structural Biology and Bio-Computing Lab, Department of Bioinformatics, Science Block, Alagappa University, Karaikudi- 630 004.</i> <i>²Centre of Advanced Study in Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai – 600 025.</i>	Accepted
5	<i>In silico validation of anti-diabetic properties of <i>Aegle marmelos.</i></i> Ramkumar S., Ravikumar P., Sharanya, Jeyam M.* <i>Department of Bioinformatics, Bharathiar Univeristy, Coimbatore-46</i>	Accepted
6	Improving the stability of human GM-CSF using molecular dynamic simulation.	Accepted

	<p>Shrinath N., G.Senthamizhan S., Nagavignesh S., Sulochana Somasundaram, Sivanandham M.</p> <p><i>Department Of Biotechnology, Sri Venkateswara College of Engineering (Affiliated to Anna University) , Post Bag No.3, Pennalur , Sriperumbudur-602105</i></p>	
7	<p>Molecular modeling and virtual screening approaches for identification of <i>Candida albicans</i> CYP51 inhibitors.</p> <p>Karnati Konda Reddy, Sanjeev Kumar Singh*</p> <p><i>Computer-Aided Drug Design and Molecular Modeling Lab, Department of Bioinformatics, Alagappa University, Karaikudi-630 004, Tamil Nadu, India</i></p>	Accepted
8	<p><i>In silico</i> screening of 3, 4 dihydro pyrimidones as Anti HIV agent.</p> <p>Gopinathan N., Chitra K.</p> <p><i>Department of Pharmaceutical Chemistry, Faculty of Pharmacy Sri Ramchandra University Porur Chennai- 600116</i></p>	Accepted
9	<p>Crystal structure and docking analysis of (2E, 4E)-ethyl 5-(phenyl sulfonyl)penta-2,4-dienote, (2E,4E)-ethyl 5-(3-bromophenylsulfonyl)penta-2,4- dienoateenoate and (2E,4E)-ethyl 5-(2,4-dichlorophenylsulfonyl)penta-2,4-dienoateenoate.</p> <p>Sabari V., Aravindhyan S.</p> <p><i>Department of Physics, Presidency College, Chennai-600005, Tamil Nadu, India.</i></p>	Accepted
10	<p>TNAU Proteome database for Green gram proteome – Construction and utilization.</p> <p>Janani R¹. Cayalvizhi B¹. Nagarajan P¹. Raveendran M¹. Rabindran R². Kannan Babu J.R³. Jagadeesh Selvam N.,¹ Senthil N.¹</p> <p><i>¹Centre for Plant Molecular Biology and Biotechnology, Tamil Nadu Agricultural University, Coimbatore 641003, Tamil Nadu, India</i></p> <p><i>²Department of Plant Pathology, Tamil Nadu Agricultural University, Coimbatore 641003, Tamil Nadu, India</i></p> <p><i>³Department of Pulses, Tamil Nadu Agricultural University, Coimbatore 641003, Tamil Nadu, India</i></p>	Accepted

11	<p>Molecular insights of λphage derived plyG enzyme towards SrtA inhibition in <i>Bacillus anthracis</i> through Protein-Protein docking and Molecular dynamics simulations.</p> <p>Chandrabose Selvaraj and Sanjeev Kumar Singh*</p> <p><i>Computer-Aided Drug Design and Molecular Modeling Lab, Department of Bioinformatics, Alagappa University, Karaikudi-630 004, Tamil Nadu, India</i></p>	Accepted
12	<p><i>In-silico</i> study on embelin and its metal complexes as human pancreatic alpha amylase inhibitors for diabetes mellitus.</p> <p>Gnanamani Arumugam ¹, Radhakrishnan Narayanaswamy², Lam Kok Wai,³ Saba Maanvizhi.^{4*}</p> <p>¹<i>Senior Scientist, Microbiology Division, Central Leather Research Institute, Adyar, Chennai, Tamil Nadu,India.</i></p> <p>²<i>Laboratory of Natural Products, Institute of Bioscience (IBS), Universiti Putra Malaysia (UPM), Serdang, Selangor, Malaysia.</i></p> <p>³<i>Faculty of Pharmacy, UniversitiKebangsaan Malaysia (UKM), Jalan Raja Muda Abdul Aziz, Kuala Lumpur, Malaysia.</i></p> <p>^{4*}<i>Assistant Professor, Faculty of Pharmacy, Sri Ramachandra University, Porur, Chennai, Tamil Nadu, India</i></p>	Accepted
13	<p><i>Insilico</i> studies of Carbamoyl Phosphate Synthetase (CPSase) Large (TTHA0612) and Small Chains (TTHA0280) from <i>Thermus thermophilus</i> HB8.</p> <p>Sureka K., Prabhu D and Jeyakanthan J.*</p> <p><i>Structural Biology and Biocomputing Lab, Department of Bioinformatics, Alagappa University, Karaikudi - 630 003, Tamil Nadu, India.</i></p>	Accepted
14	<p>Comparative molecular docking studies of novel piperazine derivatives and Alzheimer's drugs with human acetylcholinesterase.</p> <p>Kavitha Raj V.¹, Kumar J.R.¹, Lingappa Mallesha², Mohana³ K.N.</p> <p>¹<i>Postgraduate Department of Biochemistry, JSS College, Ooty Road, Mysore, India</i></p> <p>²<i>Postgraduate Department of Chemistry, JSS College, Ooty Road, Mysore, India</i></p> <p>³<i>Department of Chemistry, University of Mysore, Manasagangothri, Mysore, India</i></p>	Accepted
15	<p>TNAU PDB - Tamil Nadu Agricultural University Proteome Database - Maize</p>	Accepted

	<p>Proteome</p> <p>Sreemol G.¹, VeeraRanjani R.¹, Thangavelu A.U.¹, Saranya S.¹, Kashmiri P. Jadhav¹, Senthil N.¹, Tamilarasi P.M.², Sumathi K.², Ganesan K. N.², Paranidharan V.³ and Raveendran M.¹</p> <p>¹<i>Centre for Plant Molecular Biology and Biotechnology, Tamil Nadu Agricultural University Coimbatore 641003, Tamil Nadu, India.</i></p> <p>²<i>Centre for Plant Breeding and Genetics, Tamil Nadu Agricultural University, Coimbatore, Tamil Nadu, India.</i></p> <p>³<i>Department of Plant Pathology, Centre for Plant Protection studies, Tamil Nadu Agricultural University, Coimbatore 641003, Tamil Nadu, India</i></p>	
16	<p>Prediction of catalytic triad by <i>in-silico</i> approach in Hepatitis B virus target protein – HBx.</p> <p>Sweta Kumari, Sudharsana S., Mohana Priya A.</p> <p><i>Bioinformatics Division, SBST, VIT University, Vellore</i></p>	Accepted
17	<p><i>In silico</i> investigation of piperine’s male contraceptive effect: Docking & molecular dynamic studies on Androgen Receptor.</p> <p>Ramya Chandar Charles M¹., Gopichand Chinta,² Latha P²., Mohane Selvaraj Coumar^{1,*}</p> <p>¹<i>Centre for Bioinformatics, Pondicherry University.</i></p> <p>²<i>Department of Biochemistry and Molecular biology, Pondicherry University.</i></p>	Accepted
18	<p>Molecular Dynamic, Screening and Docking Studies of Translation Initiation Factor (PH0702) from <i>Pyrococcus horikoshii</i> OT3.</p> <p>Prajisha J. ¹, Naga soundarya R.¹, Shankar Prasad Kanaujia J., ² and Jeyakanthan J.^{1,*}</p> <p>¹<i>Structural Biology and Bio-Computing Lab, Department of Bioinformatics, Science Block, Alagappa University, Karaikudi - 630 004, Tamil Nadu, India.</i></p> <p>²<i>Department of Biotechnology, Indian Institute of Technology, Guwahati - 781 039, Assam, India.</i></p>	Accepted
19	<p>Expression, purification and preliminary crystallization efforts of the Non-receptor Tyrosine Kinase, PTK6.</p> <p>Manish Kumar Thakur^{1,2*}, Srinivasan Swaminathan², Rajiv Tyagi,² Ramachandraiah Gosu^{1,2}.</p>	Accepted

	<p>¹Department of Biochemistry, University of Mysore, ²Structural Biology Division, Jubilant Biosys Ltd, #96 Industrial Suburb, 2nd Stage Yeshwanthpur, Bangalore 560022, India</p>	
20	<p>Enhanced antibacterial activity of chlorocuprate of sulphanililide An Experimental and theoretical approach.</p> <p>Elangovan A¹, Arivazhagan G², Shanmugam R¹, Thamarachelvn A¹, Padmavathy S³, Ramu A.⁴</p> <p>¹ Department of Chemistry, Thiagarajar College, Madurai-9. ²Department of Physics, Thiagarajar College, Madurai-9. ³ Department of Zoology and Microbiology, Thiagarajar College, Madurai-9. ⁴ School of Chemistry, Madurai Kamaraj University, Madurai-20</p>	Accepted
21	<p>Identification of specific gene locus to study the molecular epidemiology of Dengue virus.</p> <p>Muruganandam N., Anwesh M., Jeeva Bharathi G.S., Vijayachari P. Regional Medical Research Centre (ICMR), Port Blair, Andaman & Nicobar Islands, India.</p>	Accepted
22	<p>Some insights into structure, function and evolution of neuropilins.</p> <p>Navina Panneerselvan*, Malathi Ragunathan*. Department of Genetics, Dr. A.L.M.P.G.I.B.M.S, University of Madras, Sekkihar Campus, Taramani, Chennai – 600113.</p>	Accepted
23	<p>Structure function approach for mining functionally superior alleles: a case study in family-79 beta glucuronidase in plants.</p> <p>Sivaranjani V., Hindumathi V., Jayakanthan M*, Srividhya V., Arul L. Centre for Plant Molecular Biology and Biotechnology. Department of Plant Molecular Biology and Bioinformatics. Tamil Nadu Agricultural University, Coimbatore-641003. *Centre for Cellular and Molecular Biology, Hyderabad</p>	Accepted
24	<p>Insilico analysis of dietary phytochemical effects on obesity associated protein FTO.</p> <p>Reshma Radhakrishnan^{1*}, Preethy Paul¹, Shanmuga Sundari I², Sudharsana S. ¹Vivekanandha College of Engineering for Women, Tiruchengode, India,</p>	Accepted

	² VIT University, Vellore, India	
25	<p>Inhibitor design for Dengue virus protease.</p> <p>Subasri S.*¹, Timiri Ajay Kumar², Barji Nayan Sinha², Venkatesan Jayaprakash², Velmurugan D.^{1,3}</p> <p>¹ CAS in Crystallography and Biophysics, University of Madras, Guindy Campus, Chennai.</p> <p>² Department of Pharmaceutical Science, Birla Institute of Technology, Mesra, Ranchi.</p> <p>³ Bioinformatics Infra structure Facility, University of Madras, Guindy Campus, Chennai</p>	Accepted
26	<p>Docking studies of thrombin and factor Xa dual inhibitors.</p> <p>Vardhini V.^{1*}, Velmurugan D.^{1,2}</p> <p>¹CAS in Crystallography and Biophysics</p> <p>²Bioinformatics Infrastructure Facility, University of Madras, Guindy Campus, Chennai – 6000259</p>	Accepted
27	<p>Surfactant-like amphiphilic peptides and their role in heavy metal removal.</p> <p>Praveen Bhai Patel,* Arpita Yadav.</p> <p>Department of Chemistry, University Institute of Engineering and Technology Chhatrapati Shahu Ji Maharaj University, Kanpur-208024</p>	Accepted
28	<p>Protein Prototype Comparison: Glutathione S-Transferase (GST)of <i>Wuchereria bancrofti</i>.</p> <p>Rama M. ¹, Balaji S. ^{2*}, Anil Kumar N.V. ¹</p> <p>¹Department of Chemistry, ²Department of Biotechnology, Manipal Institute of Technology, Manipal University, Manipal – 576104.</p>	Accepted
29	<p>Ig 4 domain does not promote homodimerization: an binding interface study on members of protein family with Horseshoe conformation.</p> <p>Ravi Kanth J*, Ramesh K V</p> <p>Department of Biochemistry, CPGS Jain University, Bangalore</p>	Accepted
30	<p>Role of metals in the ligand binding of snake venom metalloproteinase (SVMPs): a molecular dynamics approach.</p> <p>Sathishkumar Chinnasamy and Karthikeyan Muthusamy*</p> <p>Department of Bioinformatics, Alagappa University, Science Block, Karaikudi – 630004</p>	Accepted

31	<p>The structure of NIP1 β-sheet fold:No more novel.</p> <p>Balaji. S <i>Department of Biotechnology, Manipal Institute of Technology, Manipal University, Manipal 576 104, India</i></p>	Accepted
32	<p>Exploring the antagonist property of allicin against cysteine proteinase from <i>Entamoeba histolytica</i>.</p> <p>Raghavendran R.*, Kavitha B and Arun Jyothi Mathias <i>DBT - Bioinformatics Infrastructure Facility, Maharani's Science College for Women Bengaluru</i></p>	Accepted
33	<p>Screening of Bioactive Compounds against Nonreceptor Fyn Kinase: Virtual screening and Network approach.</p> <p>Sudharsana Sundarrajan^{1*}, Thabitha Amalraj¹, Swetha Kumari¹, Sajitha Lulu¹, Mohana Priya Arumugam¹ ¹<i>School of Biosciences and Technology, VIT University, Vellore 632014, India</i></p>	Accepted
34	<p>Homology modeling, molecular dynamics, virtual screening and ADME prediction studies on LukS subunit protein from <i>Staphylococcus aureus</i>.</p> <p>Periyasamy Vijayalakshmi, Pitchai Daisy* <i>Department of Biotechnology and Bioinformatics, Holy Cross College (Autonomous), Tiruchirapalli</i></p>	Accepted
35	<p>Polypharmacology potential of natural bio active molecules by docking on MAPK, mTOR, Wnt signaling pathways.</p> <p>Barathkumar T.R., Jeganathan Manivannan, Subaashini Sekar, Muthusamy Thangaraj <i>CAS in Marine Biology, Faculty of Marine Sciences, Porto novo, Annamalai University, Parangipettai 608 502, Tamilnadu, India</i></p>	Accepted
36	<p>In-silico analysis on antiviral activities of Myricetin against Dengue 2 virus.</p> <p>Lavanya P., Sudha Ramaiah and Anand Anbarasu <i>Medical & Biological Computing Laboratory, School of Biosciences and Technology. VIT University, Vellore – 632014, Tamil Nadu, India</i></p>	Accepted
37	<p>Molecular Docking and Dynamics Study of Aminoimidazole Ribonucleotide (AIR) synthetase from <i>Pyrococcus horikoshii</i> OT3.</p> <p>Guru Raj Rao R. ¹, Sekar K. ² and Jeyakanthan J. ^{1*} ¹<i>Department of Bioinformatics, Science Block, Alagappa University, Karaikudi-630 004,</i></p>	Accepted

	<p>Tamil Nadu, India</p> <p>²Supercomputer Education and Research Center, Indian Institute of Science, Bangalore 560012, India</p>	
38	<p>Network and polymorphic analysis of obesity candidate gene-plin1: A bioinformatics approach.</p> <p>Susmita Bag*, Shilpa Gupta, Vikram Prakash, Sudha Ramaiah and Anand Anbarasu <i>Medical & Biological Computing Laboratory School of Biosciences and Technology VIT University, Vellore Tamilnadu-632014</i></p>	Accepted
39	<p>Molecular docking study of catechins compounds from Camellia sinensis against UPPS in Staphylococcus aureus.</p> <p>Anitha P.*, Lavanya P., Anand Anbarasu, Sudha Ramaiah <i>Medical & Biological Computing Laboratory, School of Biosciences and Technology. VIT University, Vellore – 632014, Tamil Nadu, India</i></p>	Accepted
40	<p>Molecular docking study on Ceftobiprole and its derivatives with Penicillin binding proteins.</p> <p>Kumar K.M.*, Anand Anbarasu, Sudha Ramaiah <i>Medical & Biological Computing Laboratory, School of Biosciences and Technology. VIT University, Vellore – 632014, Tamil Nadu, India</i></p>	Accepted
41	<p>Development and evaluation of 3D-QSAR pharmacophore to screen the potential CDK2 inhibitor.</p> <p>Karthiga Arumugasamy and Sanjeev Kumar Singh* <i>Computer-Aided Drug Design and Molecular Modeling Lab, Department of Bioinformatics, Alagappa University, Karaikudi-630 004, Tamil Nadu, India</i></p>	Accepted
42	<p>Crystal Structure Analysis and Molecular Docking Studies on a Schiff base derivative.</p> <p>Ranjith B¹., Karunakaran², Selvaraju C² and Gunasekaran K¹. ¹<i>Centre of Advanced Study in Crystallography and Biophysics, Guindy Campus</i> ²<i>National Centre for Ultrafast Process, Taramani Campus University of Madras, Chennai-25</i></p>	Accepted
43	<p>In silico expression analysis and Mechanism of the hypoglycemic effect of glycoside (stevioside).</p>	Accepted

	<p>Stalin A¹, Stephen Irudayaraj S². and Ignacimuthu S.*^{1, 2}</p> <p><i>¹Division of Bioinformatics, Entomology Research Institute, Loyola College, Chennai-600034, India</i></p> <p><i>²Division of Ethnopharmacology, Entomology Research Institute, Loyola College, Chennai-600034, India)</i></p>	
44	<p>Molecular Docking of Flindersine with some targets related to β-cells Protection.</p> <p>Stephen Irudayaraj S¹., Stalin A²., Duraiyadiyan V¹. Ignacimuthu S. *^{1, 2}</p> <p><i>¹Division of Ethnopharmacology, Entomology Research Institute, Loyola College, Chennai-600034, India</i></p> <p><i>²Division of Bioinformatics, Entomology Research Institute, Loyola College, Chennai-600034, India</i></p>	Accepted
45	<p>Single Nucleotide Polymorphisms in microRNA binding sites of Oncogenes: Implications in Cancer and Pharmacogenomics.</p> <p>Manikandan M. and Munirajan A. K.</p> <p><i>Department of Genetics, Dr. ALM PG Institute of Basic Medical Sciences, University of Madras, Taramani campus, Chennai – 600113, Tamil Nadu, India.</i></p>	Accepted
46	<p>HDACIDB: A Database for Histone Deacetylase Inhibitors.</p> <p>Sangeetha Shanmugasamy, Ranjitha Shanmugasamy and Gopal Ramesh Kumar</p> <p><i>Bioinformatics Lab, AU-KBC Research Centre, Anna University, M.I.T Campus, Chennai, India</i></p>	Accepted
47	<p>Characterization of Hypothetical Proteins of <i>Geobacter sulfurreducens</i> PCA Related to Electricity Production.</p> <p>Ashok Selvaraj, Chinnasamy Perumal Rajadurai, Nupoor Chowdhary, Kandavel Palani Kannan, Gopal Ramesh Kumar*</p> <p><i>Bioinformatics Lab, AU-KBC Research Centre, Anna University, M.I.T Campus, Chennai, India</i></p>	Accepted
48	<p>Identification of Potential Inhibitors Against Human Influenza A Viruses Based on CPSF30 binding and RNA Binding Domain of NS1 Protein: An E-Pharmacophore Approach.</p> <p>Ishwar Chandra, Abhisek K Behera, Sarah S Cherian*</p> <p><i>Bioinformatics and Data Management Group, National Institute of Virology, Pune 411001, India.</i></p>	Accepted

49	<p>Designing of agonist and antagonist for Alpha 2A Adrenoceptor through structure based and pharmacophore based screening.</p> <p>Krishnasamy Gopinath, A. Joseph Arul Rayan, Kh. Dhanachandra Singh and Muthusamy Karthikeyan *</p> <p><i>Department of Bioinformatics, Alagappa University, Science Block, Karaikudi – 630004</i></p>	Accepted
50	<p>Modeling and interaction energy analysis of some substituted phenyl thiazolyl derivatives with Quadrapole mutant PFDHFR enzyme and their synthesis.</p> <p>J.M.Kalita*, S.K.Ghosh, S.Sahu, M.Dutta</p> <p><i>Department Of Pharmaceutical Sciences, Dibrugarh University, Dibrugarh Assam, 786004</i></p>	Accepted
51	<p>Evaluation and Effectiveness Studies for Different Binding Sites of CDK2 Inhibitors.</p> <p>Sunil Kumar Tripathi, Sekar Elakkiya, Sanjeev Kumar Singh*</p> <p><i>Computer Aided Drug Design and Molecular Modelling Lab, Department of Bioinformatics, Alagappa University, Karaikudi-630004, Tamil Nadu, India</i></p>	
52	<p>Molecular mechanism of the interactions between TNKS1/TNKS2 and IWR1 inhibitor.</p> <p>P. Kirubakaran and M. Karthikeyan*</p> <p><i>Department of Bioinformatics, Science Block, Alagappa University, Karaikudi 630 004, Tamilnadu, India</i></p>	
53	<p>Structural insights of fluoroquinolone derivatives targeting the LPXTG signal cleave peptide receptors in <i>Streptococcus mutans</i>.</p> <p>Bharathi Priya Ramanathan, Chandrabose Selvaraj and Sanjeev Kumar Singh*</p> <p><i>Computer Aided Drug Design and Molecular Modeling Lab, Department of Bioinformatics, Alagappa University, Karaikudi-630 004, Tamil Nadu, India</i></p>	
54	<p>Identification of potential FXR agonists using pharmacophore based virtual screening, QM/MM docking and molecular dynamics studies.</p> <p>Sindhu. T and P. Srinivasan*</p> <p><i>Department of Bioinformatics, Science Block, Alagappa University, Karaikudi -630004, Tamilnadu, India.</i></p>	
55	<p>Discovery of small molecule inhibitors of GacA using molecular modeling and virtual screening approach.</p> <p>S. Rajamanikandan and P. Srinivasan*</p> <p><i>Department of Bioinformatics, Science Block, Alagappa University, Karaikudi -630004, Tamilnadu, India.</i></p>	

56	<p><i>In-Silico</i> Molecular Docking and QSAR Studies of 5-HT_{2A} Serotonin receptor with Antipsychotic Risperidone derivatives.</p> <p>Kiran Bhargava^{1*}, Rajendra Nath¹, Prahlad Kumar Seth², Kamlesh Kumar Pant¹, Rakesh Kumar Dixit¹ <i>¹Department of Pharmacology and Therapeutics, King George's Medical University, Erstwhile CSMMU, Lucknow 226003, UP, India</i> <i>²Biotech Park, Lucknow 226021, UP, India</i></p>	
57	<p>Identification of novel TNF-α inhibitors using e-Pharmacophore based virtual screening approach.</p> <p>A. Sudha and P. Srinivasan* <i>Department of Bioinformatics, Science Block, Alagappa University, Karaikudi -630004, Tamilnadu, India</i></p>	
58	<p>Ligand based pharmacophore mapping and virtual screening for identification of potential DDR1 inhibitors.</p> <p>Ramar Vanajothi and Pappu Srinivasan* <i>Department of Bioinformatics, Science Block, Alagappa University, Karaikudi -630004, Tamilnadu, India</i></p>	