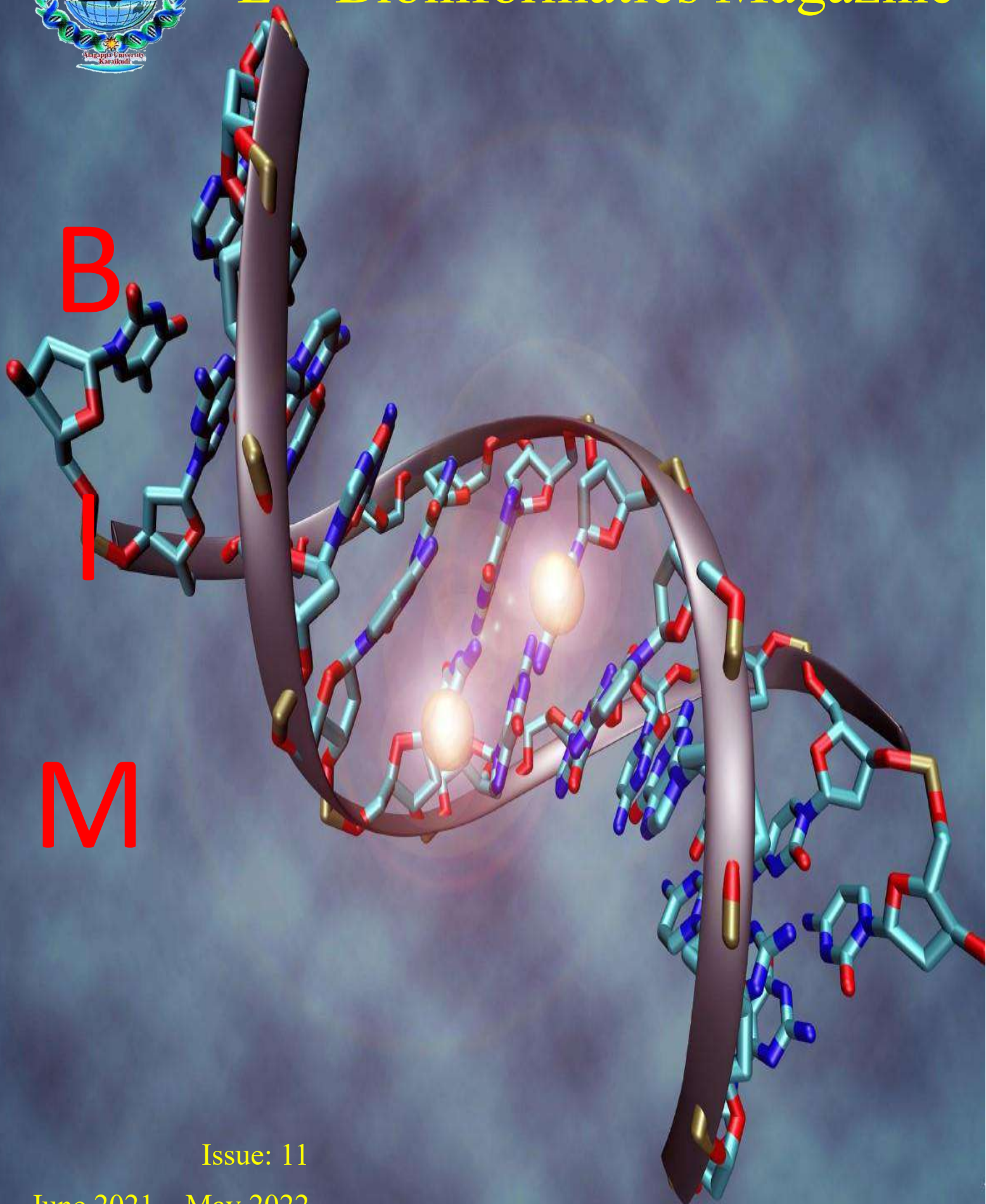




E – Bioinformatics Magazine



Issue: 11

June 2021 – May 2022

About the DBI – BIM

The e-magazine delivers simple, concise, and relevant information of the happenings at Department of Bioinformatics. This is a periodical magazine published for June 2021 – May 2022.

The magazine is sent free of charge to all alumni of DBI, as well as to faculties, staffs, and students.

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Message From the Chief Editor

Dear all,

It is with immense delight that I write this editorial for the current issue of “e-Bioinformatics Magazine” (e-BIM). Our department was found in 2008, since then it has achieved exponential growth and stardom among the other departments of Alagappa University, Karaikudi as well as other institutions. The tireless efforts by the faculty members in research and teaching in various fields have paved way to attain greater heights. Our department is funded by several funding agencies like DST, DBT, CSIR, ICMR, UGC and TNSCST. It is also sponsored by UGC Innovative programme, DST-FIST and DST-PURSE. Our faculty members believe that teaching and research are like two eyes that look far into wider horizons with a view to broadening the frontiers of knowledge. Besides this, extension activities have become imperative today and the department cannot isolate themselves from this responsibility. It is these extension activities that carry the fruits of research and knowledge to the society at large. Research scholars and students have always been noteworthy in their contributions for our department e-BIM highlights various Departmental events, Invited talks by Eminent Scientists, Student activities, Publications, Achievements, Recognitions, Contributions, Conference related activities, etc., during Academic year of June 2021 to May 2022. It also highlights the Department of Biotechnology (DBT), New Delhi approved the Establishment of Bioinformatics and Computational Biology Centre at the Department of Bioinformatics, Alagappa University, Karaikudi.

e-BIM is believed to provide platform to look back our achievements and to bring our merits into limelight that would give us enormous passion and boost to scale the heights of Bioinformatics.

Chief Editor

(Mr. Lakshmanan L)

Department Events (June 2021 to May 2022)

Orientation for First year M.Sc., Students

The Department of Bioinformatics, Alagappa University has organized an orientation programme for First Year Post Graduate Students on October 6, 2021 (2021 – 2022). Prof. J. Jeyakanthan, Professor and Head of the Department, elucidated the objectives of the programme that empower students by providing numerous resources like library, instrumentation, computational and student assistance facilities. He also presented a quick overview of the ongoing research projects and development prospects in the Department. Prof. Sanjeev Kumar Singh briefed the roles of each faculty member, responsibilities of students in contributing to research progress and significance of participating in research studies Dr. M. Karthikeyan introduced about the importance of the orientation programme. Dr. R M. Vidhyavathi, Dr. J. Joseph Sahayarayan, Dr. P. Boomi, and Dr. K. Langeswaran elucidated the infrastructure and resources available in the Department.



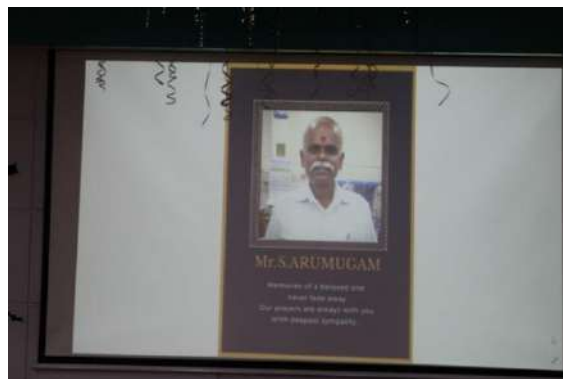
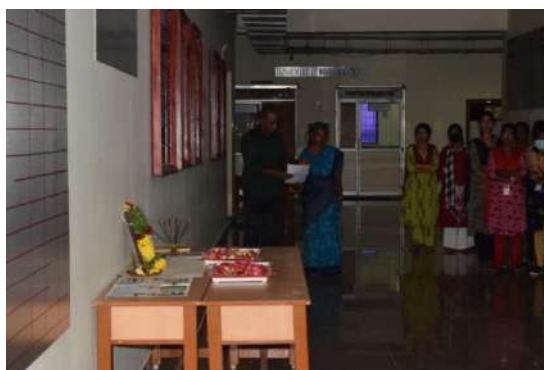
Ayutha Pooja and Saraswathi Pooja Celebrations

On 13th October, 2021, the Department of Bioinformatics celebrated Ayutha pooja. All the faculty members and students participated in this event to commemorate this devotional ceremony that serves as a reminder to all students in preserving our heritage and culture.



Mr. S. Arumugam, Office Assistant – Condolence Meeting

One of our office staff, Mr. S. Arumugam, started his carrier at our university on September 27, 1991, and has worked as an Office Assistant in the Department of Bioinformatics since 2011. Unfortunately, he suddenly passed away on 5th November, 2021. He was well-known among faculty, scholars, and students as a committed and honest worker during his tenure in the university. A condolence gathering was held in the Department of Bioinformatics on 11-11-2021, at 4 p.m. Dr. J. Jeyakanthan, Professor and Head, expressed his condolences for Mr. S. Arumugam and stated that Mr. Arumugam will be remember forever as a warm-hearted, *honest* and straightforward person. The Professors, Faculty Members, Office Staffs, Students, and Research Scholars participated in the condolence meet and prayed to rest Mr. S. Arumugam's *soul* in *peace*.



RUSA-Weekly Online Workshop- Cryptozens

RUSA sponsored weekly online Workshop (Cryptozens) was organized in the Conference Hall of Department of Bioinformatics on 16th November, 2021 at 3 p.m. (online). Mr. V. Nandakumar, IRS, Department of Revenue, Ministry of Finance, Government of India, delivered a special address about crypto currency, block chain and the ways people achieved prosperity by using digital currency. He also detailed about the government regulations in purchasing, selling, and transferring crypto currency.





Fresher's Day Celebration (Offline)

Second year M.Sc students (2020-2022) organized a Fresher's Day celebration to the fresher's (2021-23 Batch students) in the Conference Hall of Department of Bioinformatics on 19th November, 2021. Fresher's Day is intended to welcome newcomers with positive, accepting environment, encouraging them to show their creative potential, build confidence, and avoid ragging. It's a great day for seniors, juniors and research scholars to get-together and socialise with freshers. Dr. J. Jeyakanthan, Professor & Head, delivered the welcome address, and Prof. Dr. Sanjeev Kumar Singh offered the presidential address. Seniors shared the department activities and Fresher's discussed about their memorable experiences in UG as well as their course expectations in the Department for their future. Several cultural programmes and games were conducted to make freshers more comfortable.





Department of Biotechnology (DBT), New Delhi approved the Establishment of Bioinformatics and Computational Biology Centre at the Department of Bioinformatics, Alagappa University, Karaikudi.

Recently, DBT has approved Department of Bioinformatics, Alagappa University to establish Bioinformatics and Computational Biology (BIC) Centre with the objectives to create and maintain sophisticated Bioinformatics resources for the benefit of Researchers and aspiring students especially from rural backgrounds. This is a pride to Department of Bioinformatics as Alagappa University is the first University among the State Universities in Tamil Nadu to establish the BIC Centre. The credit goes to Dr. J. Jeyakanthan, Professor & Head with faculty members, Prof. Sanjeev Kumar Singh, and Asst. Prof. Dr. M. Karthikeyan who proposed in obtaining the BIC centre for research theme on “Identification of Potent Drug for Life-Threatening Diseases” to develop multivariate drugs through computational and experimental approaches.

Usually, a drug discovery process takes about 20 years to get expedited and approved. Bioinformatics tools applied in BIC Centre is a straight forward approach to decipher the Structural and Functional aspects of targeted proteins with respect to disease escalation through Structural Biology and Protein Crystallography techniques. Also, the Mechanism of Action (MoA) between the targeted proteins and the identified leads will be unravelled by Computer Aided Drug Discovery (CADD) approach that reduces the constraints of time, manpower and cost. The developed drugs will be targeted against several Life-Threatening diseases such as Cancer, Virus and Bacterial infectious diseases. In this current scenario where, effective drugs are the only requirement to completely curb the progression of diseases and facilitated by effective research collaboration originating from BIC Centre.

DBT-BIC has been granted to Department of Bioinformatics, Alagappa University for 5 years with a tune of Rs. 350 lakhs. The BIC and National Networking Project (NNP) is initiated under the stewardship of Prof. J. Jeyakanthan as the Project Coordinator & Principal

Investigator (PI) including Prof. Sanjeev Kumar Singh as PI and Dr. M. Karthikeyan as the Co-PI. Also, one of the outcomes of the BIC Centre is to produce highly skilled manpower trained in the area of Bioinformatics, Computational Biology and Computer Aided Drug Design.

Science Day

The science day was celebrated by Alagappa University on 28 Feb 2022. As a part it, Students and Teachers from various schools and colleges visited various labs in the Department of Bioinformatics and interacted with the faculties and Scholars. Teachers explained about the Bioinformatics and Computer Aided Drug Design to the students and also explained the ongoing research in Department of Bioinformatics.



Women's Day celebration

International Women's Day was celebrated in department of Bioinformatics on 8th March 2022 at Conference Hall. In this occasion, Dr. J. Jeyakanthan Professor & Head and all other faculties appreciated the roles and responsibilities of women. Women faculty, staff and students shared their views about the hurdles faced by women in daily life and how they overcome their struggles. The faculties have motivational speech to encourage and inspire the young minds to achieve higher as part of the celebration gifts and sweets were distributed.

Parents Teachers Alumni Meet (PTAM)

Parents-Teachers and Alumni Meet (PTAM) was conducted by Department of Bioinformatics, Alagappa University, Karaikudi on 06th March, 2022 through online (Meeting ID: meet.google.com/xpm-sgia-osq) at 11.00 am.

During the occasion Alumni shared their experiences and views about the Department. The occasion was graced by more than 15 Alumni across various batches and family members of the current batch students.

Speaking on the occasion, Prof. J. Jeyakanthan underlined and praised the achievements of Alumni in all walks/spheres of life. He felt that it was matter of great pride for Department of Bioinformatics, Alagappa University that its Alumni are holding prestigious positions in various Government organizations, Private sector and Academic Institutions. He praised the contribution of the Alumni towards the growth of the Department and emphasized on the need for further strengthening the linkage between the Alumni and current students of Alagappa University.

Alumni shared their experiences and views about the department in the gathering during the meeting. Many of the current students also interacted with the passed-out seniors and learned from their experiences. Parents gave very good feedback about the Department and the Faculty members. Parents were much satisfied on seeing the activities and facilities of the Department and assured their support to the growth and wellness of the Department.

The main purpose of this meet is to create a common platform, where teacher and parents come together to enrich the student's educational experiences and discuss variety of issues, regarding all round development of students.



ALAGAPPA UNIVERSITY
(A State University Accredited with "A" Grade by NMAC
 CUCPA, 3.64 in the Third Cycle and
 Graded as Category A by AIIBD-UGC, 2020; QS India Rank: 24,
 QS ASIA Rank: 222, NIRF Rank: 23)
 Karaikudi-630 004, Tamil Nadu, India.

DEPARTMENT OF BIOINFORMATICS

Cordially invite you to the

**Parents-Teachers-Alumni Meet
 (PTAM) – 2020-2021**

On 6th March, 2022 (Sunday) at 11.00 AM

Dr. M. KARTHIKEYAN
 Assistant Professor
Delivers Welcome Address

Dr. J. JEYAKANTHAN
 Professor and Head
Presides

Dr. SANJEEV KUMAR SINGH
 Professor
Delivers Special Address

EXPERIENTIAL SHARING
Parents, Students and Alumni

Dr. J. JOSEPH SAHAYARAYAN
 Assistant Professor
Delivers Vote of Thanks

Dr. J. JOSEPH SAHAYARAYAN Dr. J. JEYAKANTHAN
 Assistant Professor Professor and Head

PROGRAMME

Invocation : Tamizhrai Vazhthu and
 Vallai Vazhthu

Presidential Address : **Dr. J. JEYAKANTHAN**
 Professor and Head

Special Address : **Dr. SANJEEV KUMAR SINGH**
 Professor

Felicitation Address : **Dr. RM. VIDHYAVATHI**
 Assistant Professor
Dr. P. BOOMI
 Assistant Professor
Dr. K. LANGESWARAN
 Assistant Professor

Delivers Appreciation : **Parents, Students & Alumni**
 Address

Discussion : **Parents, Teachers, Alumni
 & Students**

National Anthem

Meeting ID: meet.google.com/xpm-sgja-osq

Membership

Prof. Sanjeev Kumar Singh, Department of Bioinformatics was nominated by Honourable Governor of Tamil Nadu as Member of Planning Board Alagappa University On 25.03.2022 for the period of three years.

Invited Talks/Address

- **Dr. J. Jeyakanthan** delivered memorable lecture on “High-throughput crystallography and Biocomputing” as a Resource Person in the “Online Faculty Development Programme on Tools and technique in characterization of compounds” organized jointly by CSIR-Central Electro Chemical Research Institute and Dr. Umayal Ramanathan College for Women, Karaikudi (17th – 21st, January 2022).
- **Dr. J. Jeyakanthan** gave outstanding lecture on “Structural and Functional Studies on Transcriptional Regulatory Protein from *Pyrococcus horikoshii* OT3 – *In silico* and *in vitro* approach” in the International Virtual Conference on “Biological Innovations & Computational Exploration for Pandemic Challenges (BICPAC’22)” organized by Department of Biotechnology and Bioinformatics, Bishop Heber College (Autonomous), Trichy (24th -25th, February 2022).
- **Dr. J. Jeyakanthan** delivered a special lecture on “High–Throughput Structural Biology & Bio-Computing” in the “Theme based Activities (5D10TBA) Programme” organized by Department of Industrial Chemistry, Alagappa University, Karaikudi (24th, March 2022).
- **Dr. RM. Vidhyavathi** was invited as a Resource Person for one-day state level seminar on “Programming Aspects of Machine Learning and its Applications” at Vidhya Giri College of Arts and Science on 31st March 2022.



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RESEARCH ARTICLE

Journal of Cellular Biochemistry | WILEY

Molecular dynamics simulation of Toxin-Antitoxin (TA) system in *Acinetobacter baumannii* to explore the novel mechanism for inhibition of cell wall biosynthesis: Zeta Toxin as an effective therapeutic target

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Abstract

The majority of bacteria and archaea contains Toxin-Antitoxin system (TA) that codes for the stable Toxin and unstable Antitoxin components forming a complex. The Antitoxin inhibits the catalytic activities of the Toxin. In general, the Antitoxin will be degraded by the proteases leading to the Toxin activation that subsequently targets essential cellular processes, including transcription, translation, replication, cell division, and cell wall biosynthesis. The Zeta Toxin-Epsilon Antitoxin system in ESKAPE pathogen stabilizes the resistance plasmid and promotes pathogenicity. The known TA system in *Acinetobacter baumannii* are known to be involved in the replication and translation, however, the mechanism of Zeta Toxin-Epsilon Antitoxin in cell wall biosynthesis remains unknown. In the present study, molecular docking and molecular dynamic (MD) simulations were employed to demonstrate whether Zeta Toxin can impair cell wall synthesis in *A. baumannii*. Further, the degradation mechanism of Antitoxin in the presence and absence of adenosine triphosphate (ATP) molecules are explained through MD simulation. The result reveals that the cleavage of Antitoxin could be possible with the presence of ATP by displaying its response from 20 ns, whereas the Zeta Toxin/Epsilon was unstable after 90 ns. The obtained results demonstrate that Zeta Toxin is “temporarily favorable” for ATP to undergo phosphorylation at UNAG kinase through the substrate tunneling process. The study further evidenced that phosphorylated UNAG prevents the binding of MurA, the enzyme that catalyzes the initial step of bacterial peptidoglycan biosynthesis. Therefore, the present study explores the binding mechanism of Zeta Toxin/Epsilon Antitoxin, which could be beneficial for preventing cell wall biosynthesis as well as for unveiling the alternative treatment options to antibiotics.

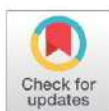
RESEARCH ARTICLE

In silico identification of natural product inhibitors against Octamer-binding transcription factor 4 (Oct4) to impede the mechanism of glioma stem cells

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**OPEN ACCESS**

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Data Availability Statement: All data are fully available in the MS.

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Abstract

Octamer-binding transcription factor 4 (Oct4) is a core regulator in the retention of stemness, invasive, and self-renewal properties in glioma initiating cells (GSCs) and its overexpression inhibits the differentiation of glioma cells promoting tumor cell proliferation. The Pit-Oct-Unc (POU) domain comprising POU-specific domain (POU_S) and POU-type homeodomain (POU_{HD}) subdomains is the most critical part of the Oct4 for the generation of induced pluripotent stem cells from somatic cells that lead to tumor initiation, invasion, posttreatment relapse, and therapeutic resistance. Therefore, the present investigation hunts for natural product inhibitors (NPIs) against the POU_{HD} domain of Oct4 by employing receptor-based virtual screening (RBVS) followed by binding free energy calculation and molecular dynamics simulation (MDS). RBVS provided 13 compounds with acceptable ranges of pharmacokinetic properties and good docking scores having key interactions with the POU_{HD} domain. More Specifically, conformational and interaction stability analysis of 13 compounds through MDS unveiled two compounds ZINC02145000 and ZINC32124203 which stabilized the backbone of protein even in the presence of linker and POU_S domain. Additionally, ZINC02145000 and ZINC32124203 exhibited stable and strong interactions with key residues W277, R242, and R234 of the POU_{HD} domain even in dynamic conditions. Interestingly, ZINC02145000 and ZINC32124203 established communication not only with the POU_{HD} domain but also with the POU_S domain indicating their incredible potency toward thwarting the function of Oct4. ZINC02145000 and ZINC32124203 also reduced the flexibility and escalated the correlations between the amino acid residues of Oct4 evidenced by PCA and DCCM analysis. Finally, our examination proposed two NPIs that can impede the Oct4 function and may help to improve overall survival, diminish tumor relapse, and achieve a cure not only in deadly disease GBM but also in other cancers with minimal side effects.

Structural and functional insights on vitamin D receptor and CYP24A1 deleterious single nucleotide polymorphisms: A computational and pharmacogenomics perpetual approach

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The development of chronic kidney disease (CKD) drugs remains a challenge due to the variations in the genes. The vitamin D receptor (VDR) and Cytochrome 24A1 (CYP24A1) genetic variants might affect the drug potency, efficacy and pathway. Here we have to analyse and determine the deleterious single-nucleotide polymorphisms (nsSNPs) of VDR and CYP24A1 genes and their different population's drug responses in different populations to understand the key role in CKD. Among that the large scale of nsSNP, we used certain computational tools that predicted six missense variants are observed to be significantly damaging effect and SNP variability with large differences in various populations. Molecular docking studies were carried out by clinical and our screened compounds to VDR and CYP24A1. Docking results revealed all the compounds have a good binding affinity (Score). The screened compounds (TCM_2868 and UNPD_141613) show good binding affinity when compared to known compounds. The QM/MM study revealed that the compounds have electron transfer ability and act as a donor/acceptor to mutated proteins. The structural and conformational changes of protein complexes were analysed by molecular dynamics study. Hence, this study helps to identify suitable drugs through drug discovery in CKD treatment. The abovementioned compounds have more binding affinity, efficacy, and potency of both wild and mutant of VDR and CYP24A1.

KEYWORDS

CYP24A1, molecular docking, nsSNPs, QM/MM and molecular dynamics, VDR

1 | INTRODUCTION

Chronic kidney disease (CKD) is recognized as a non-communicable disease that steadily increases mortality and morbidity around worldwide.¹ The abnormalities in vitamin D metabolism and the gradual decline of vitamin D lead to the pathogenesis of CKD.² Vitamin D is a secosteroid prohormone that biologically plays an important role in calcium and phosphate regulation, bone mineralization and a variety of physiological functions for instance immune response, immune inflammation, cell differentiation, growth and proliferation. The endocrine circulating level of 25-hydroxyvitamin D or 25(OH)D is a

common biomarker to felicitate the vitamin D status.³ The metabolism of vitamin D is high up or downregulation of the expression disparity might cause by several key proteins activity which alters its effects or level.⁴ The key metabolic proteins comprise Cytochrome 24A1 (CYP24A1) enzyme is referred to as 25-hydroxyvitamin D3-24-hydroxylase which can catalyse the bi-functional conversion of 25-OH-D₃ and 1, 25-(OH) 2D₃ (Vitamin D₂) into 24 and 25 hydroxylated products and vitamin D receptor (VDR) is a nuclear receptor family, which acts as a vitamin D inducible factor exert calcium and phosphate homeostasis.⁵⁻⁹ Genetic factors such as single nucleotide polymorphisms (SNPs) or genetic variation play a crucial role in the



Contents lists available at ScienceDirect

Journal of Infection and Public Health

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Essential oils as an effective alternative for the treatment of COVID-19: Molecular interaction analysis of protease (M^{Pro}) with pharmacokinetics and toxicological properties

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ABSTRACT

Background: The current health concern to the entire world is the chronic respiratory disease caused by coronavirus 2 (COVID-19). A specific treatment or proper therapy is still lacking, and the investigations from across the world for proper drug/vaccine development towards disease control are in progress. The Coronavirus replication takes place by the conversion of the polypeptide into functional protein and this occurs due to the key enzyme Main protease (M^{Pro}). Therefore, identification of natural and effective M^{Pro} inhibitors could be a safe and promising approach for COVID-19 control.

Methods: The present *in silico* study evaluates the effect of bioactive compounds found in *Eucalyptus* and *Corymbia* species essential oil on M^{Pro} by docking. Molecular docking of the major seven compounds of essential oil (citronellol, alpha-terpineol, eucalyptol, D-limonene, 3-carene, o-cymene, and alpha-pinene) with M^{Pro} was studied by AutoDock 4.2, and the properties were analysed by PreADMET and Biovia Discovery Studio visualizer.

Results: The calculated parameters such as binding energy, hydrophobic interactions, and hydrogen bond interactions of 6LU7 (M^{Pro}) with *Eucalyptus* and *Corymbia* volatile secondary metabolites represented its scope as an effective therapy option against covid-19. Among the docked compounds, eucalyptol shows the least binding energy without toxicity.

Conclusions: The outcome of this study reported that the essential oil of *Eucalyptus* and *Corymbia* species, mainly eucalyptol can be utilized as a potential inhibitor against COVID-19 and also it can be used in its treatment. Hence, further analysis was required to explore its potential application in medicine.

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Introduction

Public health has always been a prime issue due to the continuous emerging of pandemics in last two decades. There were

outbreaks of SARS-CoV-1, MERS-CoV, and now the current pandemic Coronavirus disease of 2019 (COVID-19) has become an extreme threat to human life, the livelihood, and also has brought about relentless social-economical along with political issues in the tainted countries [1]. The WHO has categorized COVID-19 as a pandemic [2]. The International Committee on Taxonomy of Viruses (ICTV) gave the name for this virus as severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) [3]. COVID-19 causes ARDS-Acute Respiratory Distress Syndrome, a condition in which

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***In silico* approach of naringin as potent phosphatase and tensin homolog (PTEN) protein agonist against prostate cancer**

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Communicated by Ramaswamy H. Sarma

ABSTRACT

Prostate cancer (PC) is one of the major impediments affecting men, which leads approximately 31,620 deaths in both developing and developed countries. Although some chemotherapy drugs have been reported for prostate cancer, they are not effective due to the lack of safety, efficacy and low selectivity. Hence, the novel alternative anticancer agents with remarkable effect are highly appreciable. Natural plants contain several bio-active compounds which have been traditionally used for the various medical treatments. Particularly, naringin is a natural bio-active compound commonly found in the citrus fruits, which have shown numerous biological activities. Phosphatase and tensin homolog (PTEN) is a tumor suppressor gene, which activates both lipid phosphates and protein phosphates. The PTEN gene is negative regulator of PI3K/AKT/mTOR pathways, since, this signaling pathway play an essential role in the cell survival, proliferation and migration. In the present *in silico* investigation, structure based virtual screening, molecular docking, molecular dynamics simulation and Adsorption, Distribution, Metabolism, Excretion (ADME) prediction were employed to determine the binding affinity, stability and drug likeness properties of top ranked screened compounds and naringin, respectively. The results revealed that the complex has good molecular interactions, binding stability (peak between 0.3 and 0.4 nm) and no violations in the Lipinski Rule of 5 in naringin, but the screened compounds violated the drug likeness properties. From the *in silico* analyses, it is identified that naringin compound might assist in the development of novel therapeutic candidate against prostate cancer.

Abbreviations: ADME: adsorption, distribution, metabolism, excretion; BOILED: Brain or intestinal EstimateD; GROMACS: GROningin MACHine for Chemical Simulations; MDS: molecular dynamics simulation; MM-GBSA: molecular mechanics-generalized born surface area; OPLS: optimized potentials for liquid simulations; PC: prostate cancer; PTEN: phosphatase and tensin homolog; PDB: Protein Data Bank; RMSD: root mean square deviation; RMSF: root mean square fluctuation

ARTICLE HISTORY

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KEYWORDS

ADME profiles; molecular docking; molecular dynamics; naringin; PTEN protein

1. Introduction

Prostate cancer (PC) is the most common non-cutaneous cancer and fifth leading cause of cancer related death affecting men globally (Ishizuya et al., 2020; Naveed et al., 2016). In 2019, approximately 174,650 new cases were identified and 31,620 people were died (Chen et al., 2019; Kohaar et al., 2019). The PC of metastatic behaviors has promoted by the voltage-gated sodium channel, which stimulates the various cellular processes (Gumushan Aktas & Akgun, 2018). It is a hereditary disease and genetic risk factor of PC may be passed from parent to child (Osanyinpeju et al., 2018). Currently, several significant treatments such as androgen deprivation therapy (Ferroni et al., 2017), surgery (Hensbergen et al., 2020),

radio ligand therapy (Wang et al., 2018) and hormonal therapy (Tony et al., 2015;) have been undertaken to improve the patient outcomes. Due to adverse side effects such as peripheral neuropathy, high-frequency hearing loss and affecting normal healthy cell, it is very difficult to eradicate. Hence, it is evident that there is a need to develop new anticancer agent that hinder the metastatic potential and cause the cell death response of prostate cancer cells.

PTEN is a lipid phosphatase of PI 3-Kinase and directly opposing the activation of the PI3K signaling by converting the PIP3 produced by PI3K back to PIP2 (Álvarez-García et al., 2019). Accordingly, loss of PTEN tumor suppressor gene result in the deficiency of regulation of PIP3 levels leads to promote prostate cancer development (Zhou et al., 2019).

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HOME COIMBATORE TAMIL NADU INDIA WORLD BUSINESS

TRENDING NOW Tamil Nadu reports 15,759 new cases, 378 deaths and 29,243 recoveries today, active c

COIMBATORE Her

Alagappa University professor collaborates for target-specific and r targeting organics for COVID-19

Covai Post Network January 6, 2021



The COVID-19 outbreak is spreading alarmingly and the number of deaths is also increasing every day in the world.

Collaborative research and mobilization of scientific skills is needed to address the COVID-19 challenge. In collaborative research culture, Professor J. Jeyakanthan, Professor and Head, Department of Bioinformatics University, has jointly collaborated with Dr. Doc. N. Anul Murugan Docent in Theoretical Chemistry and Bio Department of Theoretical Chemistry and Biology, School of Engineering Sciences in Chemistry, Biotechno



மென்மேகங்கள் நவந்தது சென்றது. இதை கிராம மக்கள் ஆச்சரியத்துடன் பார்த்து ரசித்தனர்.

கணினி பகுப்பாய்வு ஆராய்ச்சியில் உறுதி

கீழாநெல்லி, வெற்றிலை, கபசுர குடிநீர் நோய் எதிர்ப்பாற்றலை அதிகரிக்கிறது

அழுகப்பா பல்கலைக்கழக பேராசிரியர் துகவல்

காரைக்குடி, நவ. 3: கீழா நெல்லி, வெற்றிலை மற்றும் கபசுர குடிநீர் நோய் எதிர்ப்பாற்றலை அதிகரித்து சிறந்த முறையில் செயல்படுவது கணினி பகுப்பாய்வு ஆராய்ச்சியில் உறுதி செய்யப்பட்டிருக்கிறது என, அழுகப்பா பல்கலைக்கழக உயிரிதகவலியல் துறை தலைவர் தெரிவித்தார்.

சிலகளை மாவட்டம், காரைக்குடி அழுகப்பா பல்கலைக்கழக உயிரிதகவலியல் துறை தலைவர் பேராசிரியர் ஜெயகாந்தன் கூறியதாவது

கொரோனா வைரஸின் பரவலைத் தடுப்பதற்காக மருந்துகளின் மூலம் நோய் தொட்டியு புரதங்களை அழிக்கும் மருந்துகள் குறித்து, உடந்தி ஆண்டுக் களம் தொடர் ஆராய்ச்சியில் ஈடுபட்டு வருகிறோம். கொரோனா விற்கு எதிரான ஆற்றல் மருந்துகளை உருவாக்க ஒலினை தாயரங்களை கொண்டு

உயிர் தகவலியல் துறை மற்றும் கணினி அமைப்புகளின் மூலம் கணினி அமைப்புகளின் மூலம் நோய் எதிர்ப்பாற்றலை அதிகரித்து முனைவர் துகவல் தலைமையில் செயல்பட்டுள்ளதில் உறுதி செய்து கொடுத்தார்.



ஆக வு களம் பேராசிரியர் ஜெயகாந்தன், இக்கவலைக்குறிக்க முட்டி அண்டு மூலம் அடமீலிட்டிரேசனல் (எபிடி) அங்கீகரிக்கப்பட்ட டெக்னாலஜியோன் அகாலாபுட்டுட்டி, நாமேச்ட்டாட், மருந்துகளை காட்டிலும், ஆய்வுகள் பரிந்துரைக்கப்பட்ட கீழா நெல்லி, வெற்றிலை மற்றும் கபசுர குடிநீர் சிறப்பாக செயல்படுகிறது.

42 சிறிய மூலக்கூறுகள் சேர்ந்த கவலை வைரஸ்க்கு எதிராக ஆண்டி வைரஸாகவும், நோய் எதிர்ப்பாற்றலை அதிகரித்து சிறந்த முறையில் செயல்படுவது கணினி பகுப்பாய்வு மூலம் நோய் எதிர்ப்பாற்றலை அதிகரிக்கப்பட்ட தண்டமுறையில் உள்ள மருந்துகளுடன் ஒப்பிடுகையில் இந்த மருந்து கவலை கொரோனா வைரஸை தொற்றுக்கு சிறந்த மருந்துகளாக செயல்படும் என ஆராய்ச்சி மூலம் கண்டறியப்பட்டுள்ளது. இந்த மூலக்கூறுகள் புரத பிணைப்பை பலவீனப்படுத்தி வைரஸ், மனித செய்வீனுள் நுழைவதை தடுக்கிறது. கபசுர குடிநீர், கீழாநெல்லி மற்றும் வெற்றிலை ஆகியவற்றின் மருந்துவக குணங்கள் குறித்து தொடர்ந்து பய் வேறு வகையான ஆராய்ச்சிகள் கணினி மூலம் மேற்கொள்ளப்பட்டு வருகிறது.

இக்கவலைக்குறிக்க முட்டி அண்டு மூலம் அடமீலிட்டிரேசனல் (எபிடி) அங்கீகரிக்கப்பட்ட டெக்னாலஜியோன் அகாலாபுட்டுட்டி, நாமேச்ட்டாட், மருந்துகளை காட்டிலும், ஆய்வுகள் பரிந்துரைக்கப்பட்ட கீழா நெல்லி, வெற்றிலை மற்றும் கபசுர குடிநீர் சிறப்பாக செயல்படுகிறது.

இவ்வாறு கூறினார்.

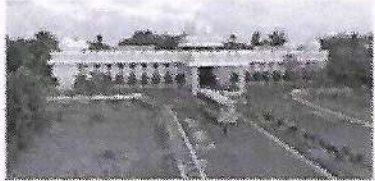
துணைகளின் சீரமைப்பு

மாண்புமிகு பேரவை அமைச்சர் சி. வி. வி. சுவாமிநாதன்

Mayadavarasu recently. Collector addressed the students. ... President of the Mayiladuthurai ... and students from various colleges ... organized by the State Minorities Union Committee Mrs. Kamatchi attended the function.

DBT sanctions Rs. 350 lakh to Algappa University to set up BIC

Kataikudi, May 14: The Department of Biotechnology (DBT), New Delhi has approved and sanctioned some of Rs. 350 lakhs to the Department of Bioinformatics, Alagappa University, Karaikudi, to establish a Bioinformatics and Computational Biology Centre (BIC) for a period of 5 years. The objectives of the BIC centre is to create and maintain sophisticated Bioinformatics resources and conduct workshops / hands-on training programmes for the benefit of researchers and aspiring students and teachers, especially from rural background. It is the first state University in Tamilnadu to establish this BIC centre. Both, the BIC Centre and National Networking Project (NNP), were proposed and initiated by the Project Coordinator and Principal Investigator (PI), Prof. Dr. Jayakanthan, HOD of Bioinformatics, Prof. Sanjeev Kumar Singh and Asst. Prof. Dr. M. Karthikeyan are the other Co-Principal investigator.



on the research theme of "Identification of Potent Drug for Life-Threatening Diseases". A typical drug discovery cycle takes about 15 years with an approximate cost of \$80 million to get approval for marketing. However, the BIC Centre in the Department of Bioinformatics, Alagappa University, will employ rapid and cost-effective Bioinformatic methods to decipher the Structural and Functional aspects of therapeutic protein targets in various infectious diseases and human disorders using various Structural Biology and Protein Crystallography techniques. Besides, the

Mechanism of Action (MoA) of the targeted proteins and their interactions with the identified leads can also be unravelled by Computer-Aided Drug Discovery (CADD) approach. The developed drugs will be targeted against several life-threatening diseases such as Cancer, Virus and Bacterial Infectious diseases. Especially the research in BIC will focus on identifying potent leads for viral fever caused by mosquito-borne diseases such as Dengue, Malaria and Chikungunya. In addition, Crystallography studies on major druggable proteins

responsible for human life-threatening diseases such as Cancer, Hypertension and Diabetes will also be deciphered besides identifying novel therapeutics against the targets. The convenor of the Vice-Chancellor Officiating Committee of Alagappa University, Dr. D. Karthikeyan IAS, Principal Secretary, Department of Higher Education, Government of Tamilnadu, and Members Dr. R. S. Swaminathan, Prof. S. Karuppachamy, Syndicate Members Prof. K. Sankaranarayanan, Dr. K. Gunasekaran, Dr. M. L. Raja and the Registrar Mr. Prof. S. Raja Mohan congratulated the Professors and research students on their richly deserved honour for doing outstanding research for many years that contributed to this noteworthy achievement.

The main work of the BIC Centre is to produce highly skilled manpower trained in the area of Bioinformatics, Computational Biology and Computer Aided Drug Design. The BIC Centre will also develop multi drugs through computational and experimental approaches.

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15/01/1985, Residing at No

MISSING
I. Periyannan (S/o) S/o
Periyannan, had lost my
original document of Kovilpatti
Village to survey No 117 by
land Heirship D 28 9 Document
No 244/2004 and my wife
document of Kovilpatti Village
to survey No 2597 Document
No. 3084/2002. Both
documents were no used when
I take copy of them. If
anybody found and the
above documents please
contact my below address.
Thavamani, S/o
Periyannan
Mannakalipuram Village
A. Kovilpatti Taluk
Valluvar, Tk.
Madurai District

அறிவிப்பு
பெரியண்ணன் (ச/ச) ச/ச
பெரியண்ணன், தனது
கொழும்புத்தூர் கிராம
சுவாமிநாதர் கிராம
சுவாமிநாதர் கிராம
சுவாமிநாதர் கிராம

Department Profile

DEPARTMENT PROFILE

Objectives

Department of Bioinformatics established in the year 2008 is one of the pioneer Departments in India facilitates learning in the interdisciplinary area of Structural Bioinformatics, Computational Genomics and Proteomics as well as to make the learners competent in Computational and Experimental aspects of their research interests.

Special Features

- Focusing on multidisciplinary areas to converge at a point of bringing out an effective drug using Computational sources against dreadful diseases.
- Unique blend of fundamental sciences, practical application with computational programs and insight into medicinal perspective.

Programs Offered

- **M.Sc.** Bioinformatics (Two year)
- **M.Phil.** Bioinformatics (One year)
- **Ph.D.** Full-time/Part-time
- **P.G. Diploma** in Structural Pharmacogenomics (One Year) – UGC Innovative Program
- **P.G. Diploma** in Bioinformatics (One Year)

Faculty Members

Name	Qualification	Area of Research
Dr. J. Jeyakanthan Professor & Head	M.Sc., M.Phil., Ph.D.	Structural Biology and Bio-Computing
Dr. Sanjeev Kumar Singh Professor	M.Sc., Ph.D.	Structural Bioinformatics and Computer Aided Drug Design
Dr. M. Karthikeyan Assistant Professor	M.Sc., Ph.D.	Pharmacogenomics and Computer Aided Drug Design
Dr. RM. Vidhyavathi Assistant Professor	M.Sc., M.Phil., M.Tech., Ph.D	Data Mining and Data Warehousing, Database Management System
Dr. J. Joseph Sahayarayan Assistant Professor	M.Sc., Ph.D.	Plant Bioinformatics and Biotechnology
Dr. P. Boomi Assistant Professor	M.Sc., Ph.D.	Nanoparticles synthesis and Nano drug delivery
Dr. V. K. Langeswaran Assistant Professor	M.Sc., Ph.D.	Molecular Oncology and Environmental Toxicology

Research Focus on

- Small and Macro Molecule X-ray crystallography, Biological and Macromolecular Database Development, Computer Aided Drug Design.
- Computer Aided Drug Designing, Molecular Modelling, Structural Bioinformatics, Quantum Mechanics, QSAR Studies, Database and Tool Development
- Human Molecular Genetics, Pharmacogenomics and Computer Aided Drug Discovery, Cell Signaling, Database Creation & Management.
- Data Mining and Data Warehousing, Database Management System, Networking and Image Processing

- Antimicrobial and anticancer activity studies, Quantification and Purification of Bioactive compounds, Structural Elucidation of Compounds, Genotoxicity studies, Transgenic Tissue Engineering and *In silico* studies
- Polymer synthesis, Nanoparticles synthesis, Bioinorganic chemistry, Nano drug delivery, Electrochemistry, Biomedical applications (Antimicrobial, Anticancer activities) using nano, micro and macromolecules
- Molecular Oncology, Environmental Toxicology and Reproductive Toxicity

Funding Agencies

DBT	UGC	DST	CSIR	AURF	TNSCST	ICMR	BRNS	UGC-Innovative Program [#]	DST INDO-TAIWAN	MHRD -RUSA 2.0	DST-FIST Level-I
296.90	92.15	160.75	32.00	07.44	01.89	54.59	30.33	54.00	227.29	69.39	62.00
Total									1088.73		

[#] Plus, two assistant professor's salary for a period of five years

Award/ Recognition

- The Department of Bioinformatics has been recognized for its innovation programme under UGC scheme of Innovation and DST-FIST for the Improvement of S & T Infrastructure
- Faculty members have been conferred with the UGC-Research and ICMR Lala Ram Khandhari Award(s) for their contribution towards drug development for Diabetes and Sexually transmitted diseases.

Research Collaborating Organizations/ Institutes

Ongoing	
National	
N. Rama Varier Ayurveda Foundation (NRAF), Madurai	2019-.*
Bishop Heber College (Autonomus), Tiruchirappalli	2018-23
GE Healthcare Pvt. Ltd., Karnataka	2017-19
Indian Institute of Technology- Madras, Chennai	2017-22
Sri Ramachandra University, Chennai	2016-21
CSIR-Central Drug Research Institute, Lucknow	2014-17
International	
National Synchrotron Radiation Research Center, Taiwan	2017-20
University of Manchester, Manchester, United Kingdom	2016-21
National Institute of Health, United States of America	2016-21
Institute of Experimental Medicine, Czech Republic	2016-21
School of Science, Osaka University, Japan	2010-15
RIKEN, Kanagawa, Japan	2010-15
Institute of Protein Research, Osaka University, Japan	2010-15
Bio-Metal Science Lab, RIKEN, Harima Institute, SPring-8, Japan	2010-15
National Collaboration	
Anna University, Tiruchirappalli	Bharathiar University, Coimbatore
Bharathidasan University, Tiruchirappalli	Chhatrapati Shahu Ji Maharaj University, Kanpur
CSIR - Central Drug Research Institute, Lucknow	CSIR - Central Electrochemical Chemical Research Institute, Karaikudi

CSIR - Centre for Cellular and Molecular Biology, Hyderabad	CSIR-National Chemical Laboratory, Pune
Indian Institute of Technology, BHU, Varanasi	Indian Institute of Technology-Delhi
Indian Institute of Technology-Kanpur, Uttar Pradesh	Indian Institute of Technology-Madras, Chennai
Indian Institute of Technology-Mandi, Himachal Pradesh	Indian Institute of Technology-Guwahati, Assam
Indian Institute of Science, Bangalore	Indian Institute of Science Education and Research, Bhopal
Indian Institute of Science, Education and Research, Pune	Institute of Life Sciences, Bhubaneswar
Integral University, Lucknow	International Centre for Genetic Engineering and Biotechnology, New Delhi
Jawaharlal Nehru Tropical Botanic Garden and Research Institute, Kerala	Jawaharlal Nehru University, New Delhi
King George Medical University, Lucknow	Madurai Kamaraj University, Madurai
National Institute of Immunology, New Delhi	North-Eastern Hill University, Shillong
Noorul Islam University, Nagercoil	Pondicherry University, Puducherry
SASTRA University, Thanjavur	Sri Ramachandra University, Chennai
University of Madras, Chennai	University of Mysore, Mysuru
VIT University, Vellore	
International Collaboration	
Konkuk University, South Korea	Loma Linda University, USA
Nanyang Technological University, Singapore	National Synchrotron Radiation Research Center, Taiwan
Osaka University, Japan	RIKEN, Harima Institute, SPring-8, Japan
Other Collaboration	
Eminent Biosciences, Indore	Schrödinger, USA

Infrastructure Facilities in the Department

- Total area of the Department: 28.38 x 40.88 mts
- Smart Classrooms
- Well-equipped laboratory facilities for Practical and Research works
- Good stock of Library books and Journals
- INFLIBNET facility to access e-journals
- E-Library facility to access e-books

Resources

- AKTA™ protein purification system with cold cabinet
- AMBER & Geneious Pro
- Bio safety cabinets
- Bio photometer Plus
- Cambridge Structural Database
- Cold Room
- Deep Freezers (-80°C and -20°C)
- ELISA Reader and Washer
- Electrophoresis and Western Blot Units
- Ice Flakers
- In-house protein database
- Kinetics Spectrophotometer
- Microscope
- Milli-Q Integral Water Purification System
- Multiplate Reader
- Nano Spectrophotometer
- Orbital Shaker
- Power backup (20, 10 and 5 KVA UPSs)

- Gel Documentation system
- Gradient PCRs
- High End Servers and workstations
- High Performance Computing cluster system
- High Speed Cooling Centrifuges
- Protein Crystallization Facility
- Smart Class Room Facilities
- Ultra Sonicator
- UV - VIS - Spectrophotometer





Contact Us

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ALAGAPPA UNIVERSITY PLACEMENT CELL

Alagappa University, Karaikudi 630 003

1.1 Details required the preparation of department profile for the Academic Year 2021-22

CORE COMPETENCY

The **Department of Bioinformatics** have been focusing to develop novel and potent drug candidates against human disorders (Cancer, Diabetes, Hypertension and Chronic Kidney disease) and infectious diseases including bacterial infections (Malaria, Filariasis, TB and Nosocomial infections namely ESKAPE pathogens) and viral infections (Influenza, Dengue, Chikungunya, HIV, ZIKA and COVID-19) through streamlining of both computational and experimental techniques to hasten the discovery of novel drug candidates against various human diseases. The generated data are compiled, stored and maintained in the form of user-friendly databases which can be retrieved easily and will be resourceful for the Scientific Community. The industry-academia collaboration brought about in the DBT approved BIC Centre and National Network Projects (NNP) will certainly enhance the training opportunities for the students, research scholars and faculty members. Apart from the training, the Centre will also refine and take lead molecules to the next phase of clinical evaluations leading to product-oriented outcomes and Patents.

HALLMARKS

- ★ More than **58** Publications, **12** books and **1** monograph were published during this year.
- ★ **2** Patents were filled and published.
- ★ Completed **DAE-BRNS** Projects (**Rs.30.33 lakhs** - 2018-2021)
- ★ Ongoing research projects during this year include **DST INDO-TAIWAN**, **TANSCHE** Govt. of Tamil Nadu and **ICMR**.
- ★ Research Competency of the department was further enhanced with generous funding by National and International agencies.
- ★ Organized Hands-on Training (Workshop) has been conducted for the students and other participant's to get familiar with the recent developments in the area of Computer Aided Drug Design.
- ★ Conducted Career guidance for the M.Sc students to enlighten them of various job prospects and opportunities available at different sectors.
- ★ Outstanding scholars were given opportunity to visit sophisticated laboratories to carry out their research work at premier institutes.

Collaborative research work with the following leading Institutions:

- Department of Biology, College of Science in **Zulfi, Majmaah University**, Majmaah, Saudi Arabia.
- IIT Madras-**69.38**, NSRRC, Taiwan-**73.72**,
- **DST INDO-TAIWAN** collaborative research project, Taiwan.
- Nanyang Technological University, Singapore.
- University of Manchester, U.K National Institute of Health, USA and Institute of Experimental Medicine, Czech Republic.
- International Centre for Genetic Engineering and Biotechnology, Delhi.

- IISC Bangalore, IIT –Madras, Guwahati, Delhi and Mandi University of Madras, and Chhatrapati Shahuji Maharaj University, Kanpur, CSIR-NCL, Pune, CSIR-CDRI, Lucknow and CSIR-CECRI, Karaikudi.
- OrbitO Asia Diagnostics, Coimbatore, Sree Balaji Medical College and Hospital, Chennai, Sastra Deemed University, Thanjavur, KTH Royal Institute of Technology, Sweden and Indian Institute of Food Processing Technology(NIFTEN – T), Thanjavur.

DEEDS & DEVELOPMENTS

- ❖ **Five days** International Conference cum Workshop on “Recent Trends in Structural Bioinformatics and Computer Aided Drug Design”**ICSBCADD’2022** from 21st November to 25th November 2022
- ❖ **38** distinguished scientists and eminent academicians from across India and countries like the USA, Singapore, Taiwan, and Japan participated
- ❖ More than **200** participants from various countries across the world
- ❖ It helped participants to develop technical Proficiency in handling computational tools to respond to biological issues
- ❖ **DBT-BIC** has been granted BIC and National Networking Project (NNP) to Department of Bioinformatics, Alagappa University for **5 years** with a tune of **Rs. 350 lakhs**.
- ❖ **The Broad-Based Board of Studies (BBBOS)** was held on July 28th, 2022 at 11.00 am through hybrid mode in the Department of Bioinformatics, Alagappa University
- ❖ **RUSA-Weekly online workshop- Cryptozens** was conducted on November 16, 2021.
- ❖ Special address on crypto currency and block chain was organized in the department for efficient use of digital currency.

AWARDS & ACHIEVEMENTS

Faculty Achievements/Awards:

- ✚ Patent was received during the year 2021-22.
- ✚ Faculties delivered invited lectures in National and International conferences.

Students/Scholars:

- ✚ **Five** research scholars got Post-Doctoral Fellow positions in world class universities.
- ✚ **17** Research scholars received prestigious fellowships [**ICMR,ICMR-SRF, JRF, DST-INDO -TAIWAN and TANSICHE**].
- ✚ Research scholars also won prizes for Best Presentation of papers at various National and International conferences.



WHO WE SERVE

- Academicians
- Scientists
- Research Scholars
- Industrialists
- Students

WHAT WE DO



- Conference's
- Symposium & Workshop
- Awards
- Recognizing scientific contributions



WHAT WE CAN DO

- Provide an opportunity to develop scientific network
- Foster and conduct collaborative research
- Platform to bring out research ideas
- Promote research training



WHAT YOU GET



- Knowledge from Eminent Scientists
- Discussion with Experts
- Recognition of research works



WHO WE ARE

Bioinformatics and Drug Discovery Society (BIDS) is an Indian academic society for the development of Bioinformatics and Computational Biology with a mission to develop the application of Bioinformatics in India.

Since 2017

Serve as a platform for dissemination of scientific knowledge and function as a central hub between Bioinformatics, Biological sciences and other allied Life Sciences.

Helps in discovering the scientific and academic efforts throughout the globe and recognizes the researchers and scientist bestowed with the awards and credits.

JOIN US

Web link : <http://www.bids.org/>

Google form link: <https://rb.gy/bxwed>

- 1.Registration Fee for BIDS Life membership for Faculties/PDF/- INR. 3000/-.
- 2.Registration Fee for BIDS Life membership for Students- INR. 500/-.
- 3.Registration Fee for Corporate Individuals - INR. 10,000/-
- 4.Registration Fee for Overseas candidate- \$ 100

Bank Name	: State Bank of India (SBI), Karaikudi
Account name	: Bioinformatics and Drug Discovery Society
Account number	: 36993002251
IFSC Code	: SBIN0000855

Scan & Register



CONTACT US

President

Prof. D. Velmurugan , SRMIST, Chennai

Secretary General

Prof. Sanjeev Kumar Singh

Email: secretary.bids@gmail.com

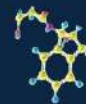
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**Bioinformatics and
Drug Discovery Society**

An Academic Society for Connecting People Worldwide
(Registered under Tamil Nadu Act 27 of 1975 with Sl. No. 42/2017)

BIDS REGISTRATION



Membership Details

• **Eligibility for Membership:**

B.Sc., M.Sc., Ph.D. or equivalent degree in science and actively engaged in research or teaching in the field of Life science.

• **Registration Fee:**

Registration Fee for BIDS Life membership for Faculties - INR. 3000/-

Registration Fee for Student Membership - INR. 500/-

Registration Fee for Corporate Individuals - INR. 10,000/-



• **Online Electronic Transfer Details:**

Name of the Bank	: State Bank of India (SBI)
Branch	: Karaikudi
Branch Code	: 855
Address	: Subramaniapuram 1 st Street, Sekkalai Karaikudi-630002, Tamil Nadu
Account name	: Bioinformatics and Drug Discovery Society
Account number	: 36993002251
IFSC Code	: SBIN0000855
CIF	: 89869362836



• **Demand Draft Details:**

The Demand Draft should be in favour of	: "Bioinformatics and Drug Discovery Society"
Payable at	: Karaikudi

Contact

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