E – Bioinformatics Magazine

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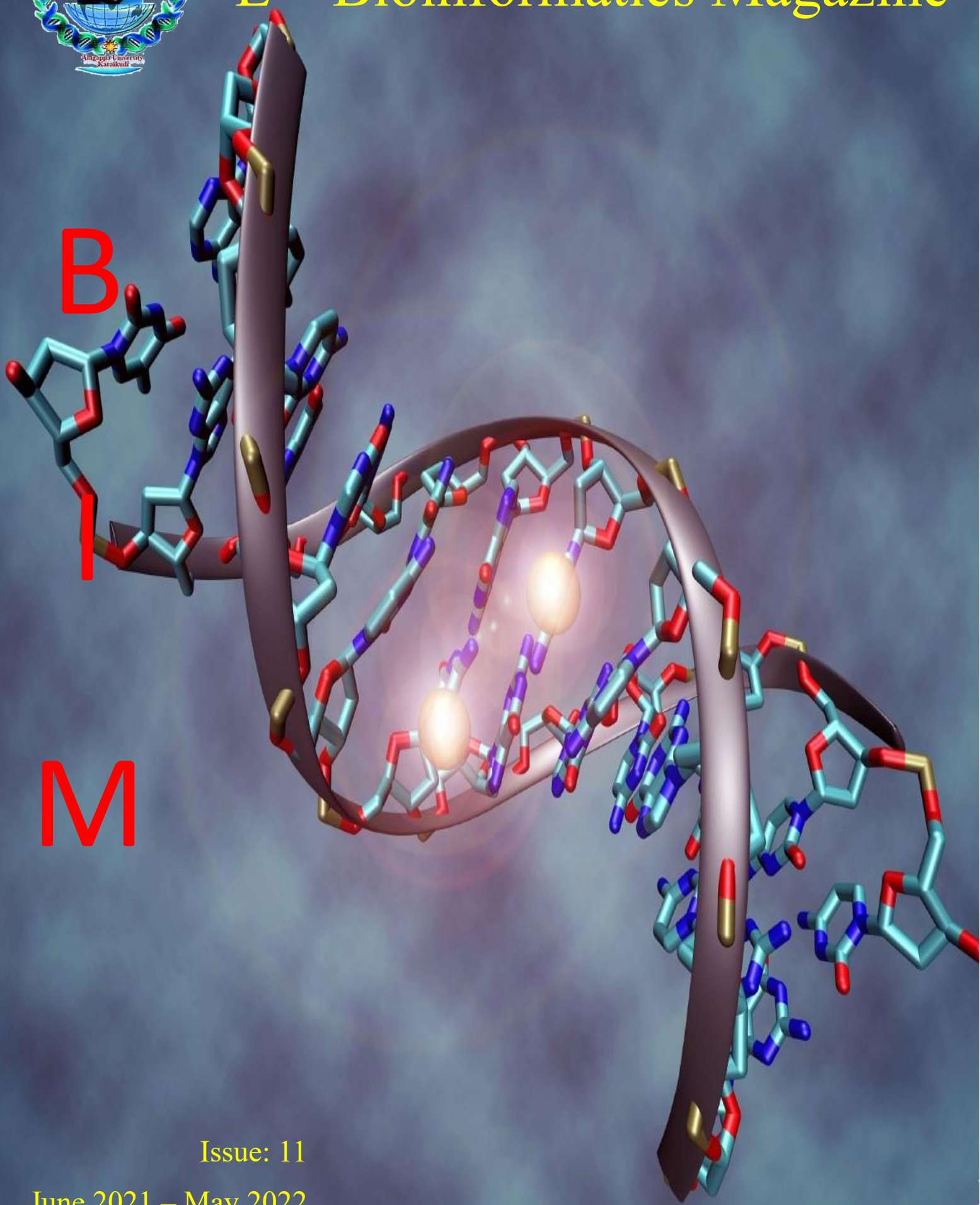

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June 2021 – May 2022

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.

ADVISORY COMMITTEE

Dr. J. Jeyakanthan
Professor & Head

Dr. Sanjeev Kumar Singh
Professor

Dr. M. Karthikeyan
Assistant Professor

Dr. RM. Vidhyavathi
Assistant Professor

Dr. J. Joseph Sahayarayan
Assistant Professor

Dr. P. Boomi
Assistant Professor

Dr. V. K. Langeswaran
Assistant Professor

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.

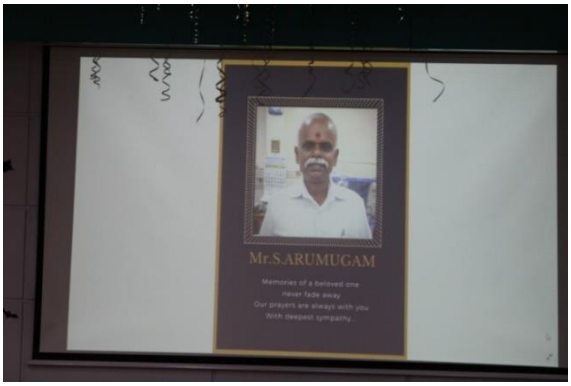
Ayutha Pooja and Saraswathi Pooja Celebrations

On 13thOctober, 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 5thNovember, 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-sgja-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 NAAC (CGPA: 3.64) in the Third Cycle and Graded as Category-I by MHRD-UGC, 2020: QS India Rank: 24, QS ASIA Rank: 222, NIRF Rank: 53)

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
Assistant Professor

Dr. J. JEYAKANTHAN
Professor and Head

PROGRAMME

Invocation	: Tamilthai Vazhthu and Vallal 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 Address	: Parents, Students & Alumni
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 0n 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 (17^{th} – 21^{st}, 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 (24^{th} -25^{th}, 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 ($24^{th,}$ 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 31^{st} March 2022.

Recent and Key Publications

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DOI: 10.1002/jcb.30137

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.

PLOS ONE

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.

Funding: The author(s) received no specific funding for this work.

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.

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RESEARCH ARTICLE

CELL BIOCHEMISTRY & FUNCTION WILEY

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-D_3 and 1, 25-(OH) $2D_3$ (Vitamin D_3) 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

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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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M^{pro}

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.

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: GROningen 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

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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 (Tonry 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-Garcia 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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Press Release

தினகரன்

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மனித செல்களின் நோய் எதிர்ப்பு ஆற்றலை அதிகரிப்பதால்

கொரோனாவை விரட்ட நிலவேம்பும் கைகொடுக்கும்

அழகப்பா பல்கலை பேராசிரியர் தகவல்

காரைக்குடி, ஜூலை 11: மனித செல்களின் நோய் எதிர்ப்பு ஆற்றலை அதிகரிப்பதால் கொரோனா வைரசை கட்டுப்படுத்த நிலவேம்பையும் பயன்படுத்தலாம் என, அழகப்பா பல்கலைக்கழக பேராசிரியர் தெரிவித்துள்ளார்.

சிவகங்கை மாவட்டம், காரைக்குடி அழகப்பா பல்கலைக்கழக உயிர்தகவலியல்துறை தலைவர் பேராசிரியர் ஜெயகாந்தன் கூறியதாவது:

கோவிட் 19க்கு சிகிச்சையளிப்பதற்கான ஆராய்ச்சிகள் அழகப்பா பல்கலைக்கழகத்தில் நடந்து வருகிறது. பாரம்பரிய முறையில் தாவரங்களில் இருந்து பைட்டோ கெமிக்கல்களை பிரித்து, ரசாயன சேர்மங்களை சேர்த்து ஊட்டச்சத்து மருந்துகளை கண்டுபிடிப்பதன் மூலம் கோவிட் 19 பாதிப்பிலிருந்து நிவாரணம் பெறுவது குறித்து ஆராய்ச்சி நடக்கிறது.

பேராசிரியர் ஜெயகாந்தன்.

காய்ச்சல், வயிற்றுப் போக்கு மற்றும் சளி போன்றவற்றுக்கு சிகிச்சையளிக்க பொதுவாக பாரம்பரிய மூலிகையான நிலவேம்பு (ஆன்ட்ரோகிராபிஸ் பானிகியுலட்டா) பயன்படுத்தப்படுகிறது. நிலவேம்பு கசப்பு சுவையின் ராஜா என்றழைக்கப்படுகிறது. நிலவேம்பில் 10க்கும் மேற்பட்ட பிளாவனாய்டுகள், 20 டைட்டர்பெனாய்டுகள் போன்ற மருத்துவ குணங்கள் உள்ளன. இந்த பைட்டோ கெமிக்கல்கள் மற்ற தாவரத்தின் பகுதிகளுடன் ஒப்பிடும்போது நிலவேம்பின் இலைகளில் அதிகம்.

நிலவேம்பில் உள்ள மூலக்கூறுகளை எடுத்து கோவிட் 19 வைரஸ்புரோட்டின் உடன் பிணைப்பு செய்து பார்த்ததில், பாக்டீரியா, வைரசுடன் எதிர்த்து போராடும் என கண்டறியப்பட்டுள்ளது. கணினி மூலம் நிலவேம்பு புரத மூலக்கூறை வடிவமைத்து தற்போது பயன்பாட்டில் உள்ள மருந்துகளுடன் பிணைப்பு செய்து பார்த்ததில், அந்த மருந்துகளை விட இதில் மனித செல்களில் நோய் எதிர்ப்பு சக்தியை கூட்டும் திறன் அதிகமாக உள்ளது. மேலும் மருத்துவ ரீதியில் விரிவான முறையில் ஆய்வு செய்து பயன்பாட்டுக்கு கொண்டு வருவதற்கான ஆய்வுகள் நடக்கிறது.

இவ்வாறு தெரிவித்தார்.

சிவகா

DINAKARAN – 06.01.2021

கொரோனா வைரசை அழிக்கும் மருந்து சேர்மங்கள் கண்டுபிடிப்பு

அழகப்பா – ஸ்வீடன் பல்கலை. பேராசிரியர்கள் வடிவமைப்பு

காரைக்குடி, ஜன. 6: கொரோனா வைரஸின் முக்கிய மூலக்கூறுகளை அழிக்கும் மருந்துகள் மற்றும் அதற்கான சாத்தியக்கூறுகள் கணினி முறையில் கண்டுபிடிக்கப்பட்டுள்ளது என அழகப்பா பல்கலைக்கழக பேராசிரியர் ஜெயகாந்தன் தெரிவித்துள்ளார்.

சிவகங்கை மாவட்டம், காரைக்குடி அழகப்பா பல்கலைக்கழக உயிர் தகவலியல் பேராசிரியர் ஜெயகாந்தன் கூறியதாவது:

ஸ்வீடன் ஸ்டாக்ஹோம் கே.டி.எச். ராயல் இன்ஸ்டியூட் ஆப் டெக்னாலஜி வேதியியல் மற்றும் உயிரியியல் துறையின் டாக்டர் அருள்முருகனுடன் இணைந்து, மருந்து சேர்மங்கள் கணினி முறையில் கண்டுபிடிக்கப்பட்டுள்ளது. வைரஸ் புரத மூலக்கூறுகளை பொறுத்தவரை அதிகளவில் பல மூலக்கூறுகள் இருக்கும். இதற்கு ஒரு மருந்து அளிக்கும்பட்சத்தில் அனைத்தையும் சரி செய்யாது. மீதம் உள்ள வைரஸ் மூலக்கூறுகளை கண்டுபிடித்து, உருமாறும் வைரஸ்களின் பல புரதங்களைகுறிவைத்து அழிப்பதற்கு தேவையான மருந்துகள் கணினி முறையில் கண்டுபிடிக்கப்பட்டுள்ளது.

பேராசிரியர் ஜெயகாந்தன்

இம்மருந்து வைரஸின் உருமாற்றங்களை சுற்றி செயல்பட உதவும். கொரோனா வைரஸ் அதன் புரதங்களை மாற்றியமைத்து விரைவாக உருமாறுகிறது. பல புரதங்களை குறிவைத்து தாக்கக்கூடிய மருந்து இருந்தால், ஒன்று உருமாறினாலும் மற்றவைகளுக்கும் அது பயனுள்ளதாக செயல்படும்.

பாலோக்சாவீர் மார்பாக்சில், நடமைசின், ஆர்யூ 85053 ஆகிய மருந்துகள் மூன்று வைரஸ் புரதங்களை குறிவைத்து தாக்குவதுடன், வைரஸ் மூலம் பரவும் நோய்களுக்கு சிகிச்சையளிப்பதில் திறம்பட செயல்படுகிறது. தவிர திவாண்டினிப், ஓலாபரிப், சோலிப்ளோடசின், கோல்வாடினிப், சோனிடேகிப், ரெகோராபெனிப் மற்றும் பி.சி.ஓ. 371 ஆகியவைகளும் சோதனைக்குப் பரிந்துரைக்கப்பட்டுள்ளன. தவிர பைதாலோசையனின், டாடாலாப்பில் போன்ற மருந்துகள் விரைவாக உருமாறும் கொரோனா வைரஸை எதிர்ப்பதில் பயனுள்ளதாக இருக்கும் என ஆராய்ச்சியில் கண்டுபிடிக்கப்பட்டுள்ளது. இவ்வாறு அவர் கூறினார்.

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Searching for target-specif and multi-targeting organi for Covid-19 in the Drugba database with a double sc approach

Natarajan Arul Murugan[1], Sanjiv Kumar[2], Jeyaraman Jeyakanthan[3]

The current outbreak of Covid-19 infection due to SARS-CoV-2, a virus from has become a major threat to human healthcare. The virus has already infect and the number of deaths reported has reached more than 1.1 M which may of medicine. The traditional drug discovery approach involves many years of development and demands for a huge investment which cannot be adopted infection. Rather we need a swift and cost-effective approach to inhibit and With the help of computational screening approaches and by choosing appr is possible to identify lead drug-like compounds for Covid-19. In this study, w database to screen compounds against the most important viral targets nam (3CLpro), papain-like protease (PLpro), RNA-dependent RNA polymerase (R protein. These targets play a major role in the replication/transcription and h therefore, are vital for the viral reproduction and spread of infection. As the computational screening approaches are more reliable, we used the crystal s protease and spike protein. For the remaining targets, we used the structure modeling. Further, we employed two scoring methods based on binding free in AutoDock Vina and molecular mechanics—generalized Born surface area a these results, we propose drug cocktails active against the three viral target and RdRp. Interestingly, one of the identified compounds in this study i.e. Ba been under clinical trial for the treatment of Covid-19 infection. In addition, compounds such as Phthalocyanine, Tadalafil, Lonafarnib, Nilotinib, Dihydr can bind to all three targets simultaneously and can serve as multi-targeting included calculation of binding energies for various compounds currently un these compounds, it is found that Remdesivir binds to targets, 3CLpro and R affinity. Moreover, Baricitinib and Umifenovir were found to have superior ta while Darunavir is found to be a potential multi-targeting drug. As far as we where the compounds from the Drugbank database are screened against fou

அரசின் விதிமுறைகளை கடைபிடிப்பதே பாதுகாப்பானது

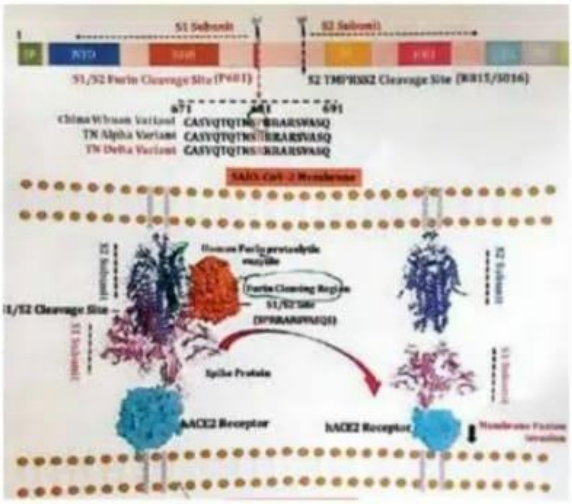
கொரோனா வைரஸ் பரவல் நீண்ட காலத்திற்கு இருக்கும்

அழகப்பா பல்கலைக்கழக பேராசிரியர் தகவல்

காரைக்குடி, அக். 7: கொரோனா வைரசின் முக்கிய புரதங்களை அழிக்கும் மருந்துகள் மற்றும் சாத்தியக்கூறுகள் குறித்து சிவகங்கை மாவட்டம், காரைக்குடி அழகப்பா பல்கலைக்கழக உயிரி தகவலியல் துறை தலைவர் ஜெயகாந்தன் தலைமையில் ஆராய்ச்சி மாணவர்கள் ரிசாட் மரியதாஸ், ராஜு ஆகியோர் ஸ்பைக் புரதங்களை அடிப்படையாககொண்டு ஆராய்ச்சி மேற்கொண்டனர்.

இதுகுறித்து பேராசிரியர் ஜெயகாந்தன் கூறுகையில், ''இந்தியாவில் பரவும் டெல்டா வகை கொரோனா வைரஸின் நோய்த்தொற்று தொடர்பான புரதங்களையும் அதன் மாறும் தன்மையையும் கணினி முறையில் கண்டுபிடிக்கும் ஆராய்ச்சி மேற்கொள்ளப்பட்டது. இந்நோய் பரவலுக்கு முக்கிய பங்காற்றும் ஸ்பைக் புரதம் 1,273 அமினோ அமிலங்களை கொண்டது. மற்ற வைரஸ்களை போன்றே கோவிட் 19 வைரஸ் பல்வேறு வகையான மரபணு மாற்றங்களுக்கு உட்படும் தன்மை கொண்டவை. ஸ்பைக் புரதத்தில் ஏற்படும் மாற்றங்கள் நோயின் தீவிரம் மற்றும் தொற்று பரவுதலை அதிகரிக்கும்.

உலகளவில் பல்வேறு ஆராய்ச்சி ஆய்வகங்களில் 3,60,009 கோவிட் தரவுகள் பதிவேற்றம் செய்யப்பட்டுள்ளது. அவற்றிலிருந்து 47 ஆயிரம் இந்திய ஸ்பைக் புரதங்களை மட்டும் எடுத்துக்கொண்டு ஆராய்ச்சி மேற்கொள்ளப்பட்டது. ஒவ்வொரு புரத மூலக்கூறுகளும் ஒவ்வொரு விதமான வேலை செய்யும். இதில் ஸ்பைக் புரத மூலக்கூறு கோவிட் வைரஸ் தாக்குதலுக்கு முக்கியமான புரதமாகும். இதில் உள்ள 1,273 அமினோ அமிலங்களில் 681வது அமினோ அமிலமாக புரோலின் உள்ளது. இந்த அமினோ அமிலம், அரிஜினைன் அமினோ அமிலமாக மாறி டெல்டா வைரஸ் என பெயரிடப்பட்டுள்ளது. இதில் வேறுவிதமான அமினோ அமில மாற்றங்கள் ஏற்படலாம். அவ்வாறு ஏற்படும்போது டெல்டாவை விட அதி தீவிர பாதிப்பை ஏற்படுத்தும் என கணினியின் மூலம் மேற்கொள்ளப்பட்ட ஆய்வின் முடிவில் அறியப்பட்டுள்ளது. சரியான தடுப்பு மருந்து கண்டுபிடிக்காத வரையில் கோவிட் 19 என்பது முற்று பெறாமல் மாற்றங்கள் நடந்துகொண்டே இருக்கும். எனவே அரசு அறிவித்துள்ள அனைத்து வழிகாட்டு விதிமுறைகளையும் கடைபிடிப்பதே நம்மை பாதுகாத்துக் கொள்ள சரியான தீர்வு'' என்றார்.



▶ ஸ்பைக் புரத அமைப்பு மற்றும் பிளவு ஏற்படுத்தும் பகுதியை பற்றி கணினி மூலம் கண்டறியப்பட்ட படம்.

பேராசிரியர் ஜெயகாந்தன்

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COIMBATORE Hor

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 s the world.

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

தினகரன்

2/12

வெண்மேகங்கள் தவழ்ந்து சென்றது. இதை கிராம மக்கள் ஆச்சர்யத்துடன் பார்த்து ரசித்தனர்.

கணினி பகுப்பாய்வு ஆராய்ச்சியில் உறுதி

கீழாநெல்லி, வெற்றிலை, கபசுர குடிநீர் நோய் எதிர்ப்பாற்றலை அதிகரிக்கிறது

அழகப்பா பல்கலைக்கழக பேராசிரியர் தகவல்

காரைக்குடி, நவ. 3: கீழா நெல்லி, வெற்றிலை மற்றும் கபசுர குடிநீர் நோய் எதிர்ப்பாற்றலை அதிகரித்து சிறந்த முறையில் செயல்படுவது கணினி பகுப்பாய்வு ஆராய்ச்சியில் உறுதி செய்யப்பட்டுள்ளது என, அழகப்பா பல்கலைக்கழக உயிரி தகவலியல் துறை தலைவர் தெரிவித்தார்.

சிவகங்கை மாவட்டம், காரைக்குடி அழகப்பா பல்கலைக்கழக உயிரி தகவலியல்துறை தலைவர் பேராசிரியர் ஜெயகாந்தன் கூறியதாவது:

கொரோனா வைரஸின் ஸ்பைக் புரதத்தில் ஏற்படும் மாற்றங்கள் மற்றும் நோய் தொடர்பு புரதங்களை அழிக்கும் மருந்துகள் குறித்து, கடந்த 2 ஆண்டுகளாக தொடர் ஆராய்ச்சியில் ஈடுபட்டு வருகிறோம். கொரோனாவிற்கு எதிரான ஆற்றல்மிக்க மருந்துகளை உருவாக்க மூலிகை தாவரங்களை கொண்டு உயிர் தகவலியல் துறை மற்றும் சுவீடன் ஸ்டாக்ஹோம் ராயல் நிறுவனத்தை சேர்ந்த முனைவர் அருண்முருகனுடன் சேர்ந்து தொடர்ந்து ஆய்வுகள் மேற்கொள்ளப்பட்டு வருகிறது.

பேராசிரியர் ஜெயகாந்தன்.

புட் அண்டு டிரக்ஸ் அட்மினிஸ்ட்ரேசனால் (எப்டிஏ) அங்கீகரிக்கப்பட்ட டெக்ஸா மீத்தாஸோன், அகாலாப்ருட்டினிப், நபாமோஸ்டாட் மருந்துகளை காட்டிலும், ஆயுஷால் பரிந்துரைக்கப்பட்ட கீழா நெல்லி, வெற்றிலை மற்றும் கபசுர குடிநீர் சிறப்பாக செயல்படுகிறது.

இக்குடிநீரில் உள்ள 42 சிறிய மூலக்கூறுகள் சேர்ந்த கலவை, வைரசுக்கு எதிராக ஆன்டி வைரஸாகவும், நோய் எதிர்ப்பாற்றலை அதிகரித்து சிறந்த முறையில் செயல்படுவது கணினி பகுப்பாய்வின் மூலம் ஆராய்ச்சியில் உறுதி செய்யப்பட்டுள்ளது.

இக்கலவை குடிநீரை நோய் எதிர்ப்பு குறைபாடுகளால் பாதிக்கப்பட்டவர்கள் மற்றும் அனைத்து விதமான நோயாளிகளும் பயன்படுத்தலாம். இந்த மூலக்கூறுகளில் உள்ள செபுலாஜிக் ஆசிட், ஜெரானின் மற்றும் ரெபாண்டுசினிக் ஆசிட் ஆகியவை வைரசுக்கு எதிராக சிறப்பாக செயல்படுகிறது.

எப்டிஏ-வால் அங்கீகரிக்கப்பட்ட நடைமுறையில் உள்ள மருந்துகளுடன் ஒப்பிடுகையில் இந்த மருந்து கலவை கொரோனா வைரஸ் தொற்றுக்கு சிறந்த மருந்தாக செயல்படும் என ஆராய்ச்சி மூலம் கண்டறியப்பட்டுள்ளது. இந்த மூலக்கூறுகள் புரத பிணைப்பை பலவீனப்படுத்தி வைரஸ், மனித செல்லினுள் நுழைவதை தடுக்கிறது. கபசுர குடிநீர், கீழாநெல்லி மற்றும் வெற்றிலை ஆகியவற்றின் மருத்துவக் குணங்கள் குறித்து தொடர்ந்து பல்வேறு வகையான ஆராய்ச்சிகள் கணினி மூலம் மேற்கொள்ளப்பட்டு வருகிறது.

இவ்வாறு கூறினார்.

அணைகளின் நீர்மட்டம்

தினகரன் 2/2

அழகப்பா பல்கலைக் கழகத்தில்

உயிர்க்கொல்லி நோய் மருந்து கண்டறிய ஆராய்ச்சி மையம்

துறைத்தலைவர் தகவல்

காரைக்குடி, மே 9: காரைக்குடி அழகப்பா பல்கலைக் கழக உயிரி தகவலியல் துறைக்கு உயிர்க்கொல்லி நோய் மருந்து கண்டறிய ஆராய்ச்சி மையம் துவங்க அனுமதியளிக் கப்பட்டுள்ளது என துறைத்தலைவர் பேராசிரியர் ஜெயகாந்தன் தெரிவித்தார்.

இதுகுறித்து அவர் கூறுகையில், அழகப்பா பல்கலைக்கழக உயிரி தகவலியல் துறையின் சார்பில் பல்வேறு வகையான நோய்களுக்கு மருந்து கண்டுபிடிக்க ஆராய்ச்சி மேற்கொள்ளப்பட்டு வருகிறது. கொசு மூலம் பரவும் டெங்கு, மலேரியா, சிக்குன்குனியா போன்றவைகளால் வரும் காய்ச்சலை குணப்படுத்தும் மருந்து மூலக்கூறுகளை கண்டுபிடிக்கும் ஆராய்ச்சி நடக்கிறது.

தவிர கொரோனா வைரஸின் நோய்த் தொற்று தொடர்பான புரதங்களையும் அதன் உருமாறும் தன்மையையும் கண்டுபிடித்து அதனை அழிக்கும் மருந்துச் சேர்மங்களை கண்டுபிடிக்கும் ஆராயச்சிகள் தொடர்ந்து நடக்கிறது.

இந்நோய்களுக்கான சிறந்த தீர்வுகளை காண்பதற்கு இப்பல்கலைக்கழக உயிரி தகவலியல் துறைக்கு மத்திய அரசின் உயிரி தொழில் நுட்பவியல் துறை உயிர்க்கொல்லி நோய் மருந்து கண்டறியும் ஆராய்ச்சி மையம் நிறுவ அனுமதியளித்துள்ளது. இதற்காக 5 ஆண்டுகளுக்கு 3 கோடியே 50 லட்சம் நிதி வழங்கப்பட்டுள்ளது.

இந்த ஆராய்ச்சிக்கு திட்ட ஒருங்கிணைப்பாளர் மற்றும் முதன்மை ஆய்வாளராக நானும், பேராசிரியர் சஞ்சீவ்குமார் சிங், பேராசிரியர் கார்த்திகேயன் துணை ஆய்வாளர்களாகவும் செயல்பட உள்ளோம்.

தவிர மூன்று ஆராய்ச்சி விஞ்ஞானிகள் மற்றும் ஆராய்ச்சி கூட உதவியாளருடன் இணைந்து புதிய வகை மருந்து மூலக்கூறுகளைக் கண்டறிவதற்கான ஆராய்ச்சிகள் மேற்கொள்ளப்பட உள்ளது.

நோய் தொற்று தொடர்பான புரத இலக்குகளை எளிதில் கண்டறியவும், சமுதாயத்தை அச்சுறுத்தும் நோய்களை குணப்படுத்தும் மருந்து மூலக்கூறுகளை அடையாளம் காண இம்மையம் பயனாக இருக்கும் என்றார்.

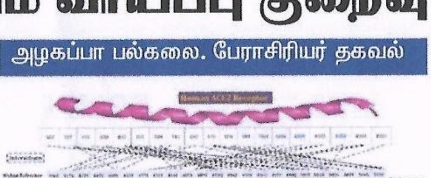
பல்கலைக்கழகத்தில் இம்மையம் அமைந்ததற்கு துணைவேந்தர் பொறுப்புக்குழு தலைவர், உயர்கல்வி செயலாளர் கார்த்திகேயன், துணைவேந்தர் பொறுப்புக்குழு உறுப்பினர்கள் டாக்டர் சுவாமிநாதன், பேராசிரியர் கருப்புச்சாமி, ஆட்சிக்குழு உறுப்பினர்கள் பேராசிரியர்கள் சங்கரநாராயணன், குணசேகரன் ராஜா ஆகியோர் பாராட்டினர்.

DINAKARAN – 21.01.2022

பரவும் தன்மை அதிகமாக இருந்தாலும்

ஒமிக்ரானால் உயிர்ப்பலி ஏற்படும் வாய்ப்பு குறைவு

அழகப்பா பல்கலை. பேராசிரியர் தகவல்



ஸ்பைக் புரத அமைப்பு மற்றும் பிணைப்பு ஏற்படுத்தும் பகுதியை பற்றி கணினி மூலம் கண்டறியப்பட்ட படம்.

காரைக்குடி, ஜன. 21: பரவும் தன்மை அதிகமாக இருந்தாலும் ஒமிக்ரானால் உயிர்ப்பலி ஏற்பட வாய்ப்புகள் குறைவு என அழகப்பா பல்கலைக்கழக உயிரி தகவலியல் துறை தலைவர் தெரிவித்துள்ளார்.

சிவகங்கை மாவட்டம், காரைக்குடி அழகப்பா பல்கலைக்கழக உயிரிதகவலியல் துறை தலைவர் ஜெயகாந்தன் கூறியதாவது :

கொரோனா வைரஸின் ஸ்பைக் புரதத்தில் ஏற்படும் மாற்றங்கள் மற்றும் நோய்த்தொடர்பு புரதங்களை அழிக்கும் மருந்துகள் குறித்து கடந்த 2 ஆண்டுகளாக தொடர் ஆராய்ச்சியில் ஈடுபட்டு வருகிறோம். ஒமிக்ரான் வைரஸ் கடந்த 2021 நவம்பரில் தென் ஆப்ரிக்காவில் கண்டறியப்பட்டது. உலகளவில் பல்வேறு ஆராய்ச்சிகளில் கிடைக்கப்பட்ட தரவுகளின் அடிப்படை மற்றும் உலக சுகாதார அமைப்பின் தரவுகளின் படி, 51 ஸ்பைக்புரதங்களில் ஏற்பட்ட மாற்றங்களை மட்டும் எடுத்துக்கொண்டு ஆராய்ச்சி மேற்கொள்ளப்பட்டது.

நோய் பரவலுக்கு முக்கிய பங்காற்றும் ஸ்பைக் புரதம் 1,273 அமினோ அமிலங்களை கொண்டது. இந்த ஸ்பைக் புரதம் பல்வேறு வகையான மரபணு மாற்றங்களுக்கு உட்படும் தன்மை கொண்டது. இது 13 வகையான ஆல்பா, 10 வகையான பீட்டா, 13 வகையான காமா, 15 வகையான டெல்டா, 32 வகையான ஒமிக்ரான் போன்ற ஸ்பைக்புரத மாற்றங்கள் ஏற்பட்டு இருப்பதாக கண்டறியப்பட்டுள்ளது. துவக்கத்தில் ஸ்பைக் புரத மூலக்கூறும், மனித புரத மூலக்கூறும் பிணைப்பு ஏற்பட்ட போது மைனஸ் 112.2 என இருந்தது. தற்போது அதே ஒமிக்ரான் பிணைப்பு ஏற்படும்போது மைனஸ் 139.8 என்ற நிலையில் உள்ளது. இதனால் ஒமிக்ரான் அதிகமாக பரவி வருகிறது. பரவும் தன்மை அதிகமாக இருந்தாலும் உயிர்ப்பலி ஏற்பட வாய்ப்புகள் குறைவு. நோய்தொற்று தடுப்பு நடவடிக்கையாக அரசின் வழிகாட்டு விதிமுறைகளை கடைபிடிப்பது மற்றும் தடுப்பூசி போட்டுக்கொள்ளுதல் போன்ற முன்னெச்சரிக்கை நடவடிக்கைகளை கடைபிடிப்பதே சிறந்தது. இதன் மூலம் தொற்றிலிருந்து முழுமையாக விடுபட முடியும். இவ்வாறு அவர் கூறினார்.

பேராசிரியர் ஜெயகாந்தன்.

தினகரன் Fri, 21 January 2022
https://epaper.dinakaran.com/c/65730325

Mayiladuthurai recently.

The elocution competition was organised by the State Minorities

Collector addressed the students.

President of the Mayiladuthurai Union Committee Mrs Kamatchi

and students from various colleges attended the function.

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

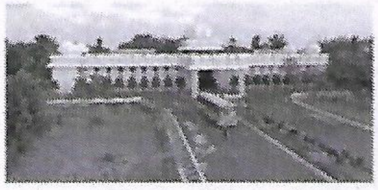
Karaikudi, May 14:

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.

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



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 800 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.Swaminathan, Prof.S.Karuppuchamy, Syndicate Members Prof. K. Sankaranarayanan, Dr K. Gunasekaran, Dr M. L. Raja and the Registrar i/c 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.

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

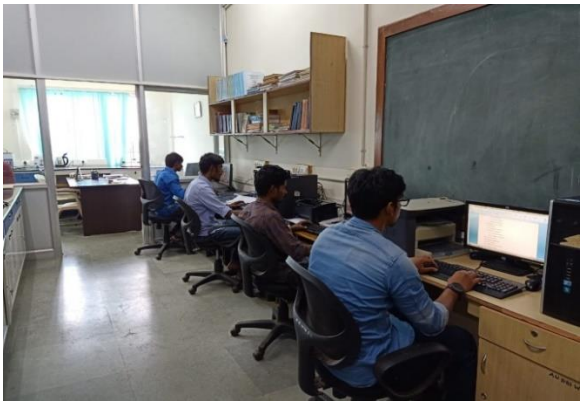
Infrastructure Facilities in the Department

- 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







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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 TANSCHE]**.
- Research scholars also won prizes for Best Presentation of papers at various National and International conferences.

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)

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 (BIDDS) 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.

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3. Registration Fee for Corporate Individuals - INR. 10,000/-
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Bank Name	:	State Bank of India (SBI), Karaikudi
Account name	:	Bioinformatics and Drug Discovery Society
Account number	:	36993002251
IFSC Code	:	SBIN0000855

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CONTACT US

President

Prof. D. Velmurugan , SRMIST, Chennai

Secretary General

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BIDDS

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)

BIDDS 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 BIDDS Life membership for Faculties - INR. 3000/-
  Registration Fee for Student Membership - INR. 500/-
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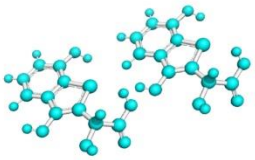

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Account name	:	Bioinformatics and Drug Discovery Society
Account number	:	36993002251
IFSC Code	:	SBIN0000855
CIF	:	89869362836

- **Demand Draft Details:**

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

Contact

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