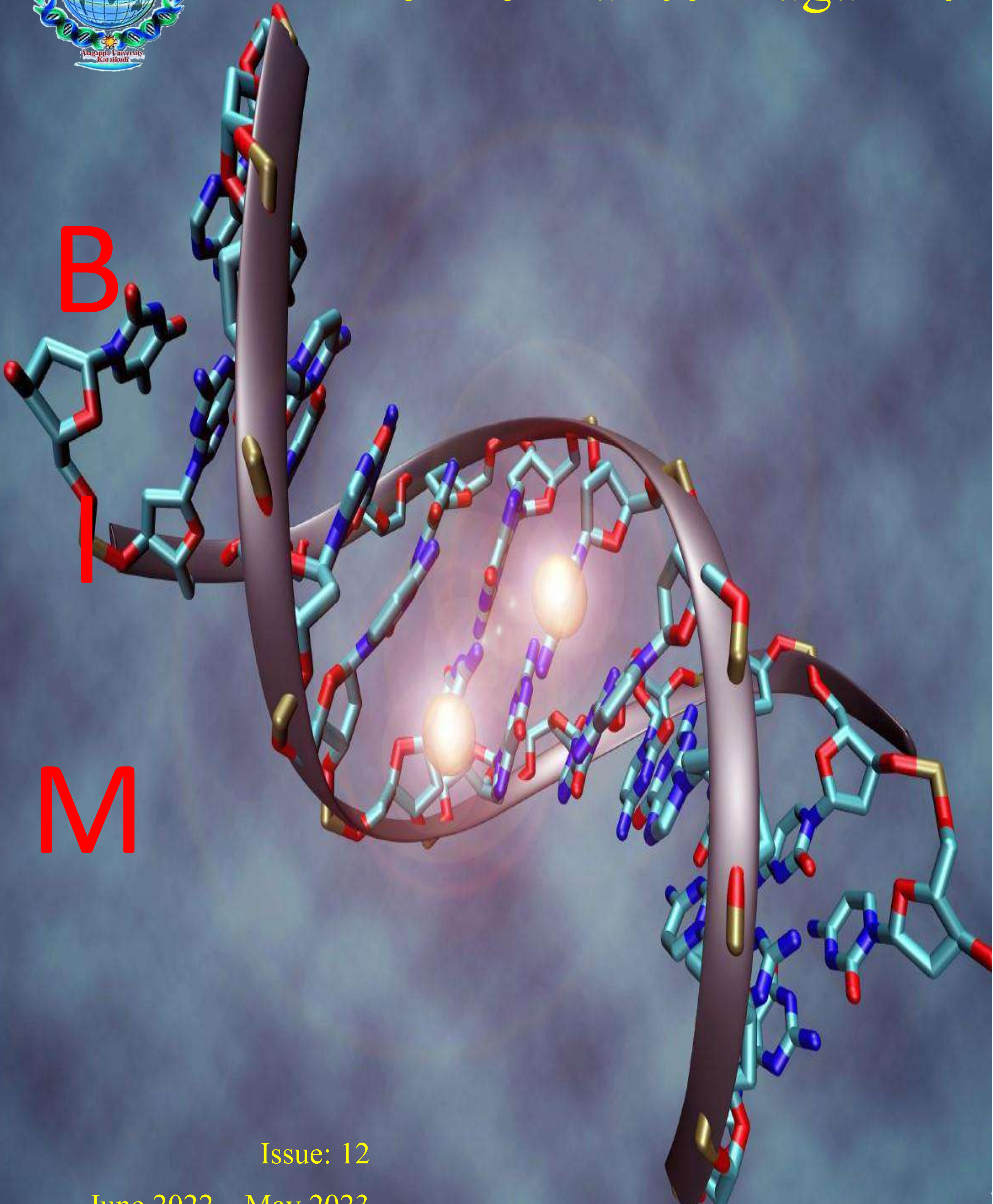
E – Bioinformatics Magazine



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June 2022 – May 2023

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 2022 – May 2023.

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

ADVISORY COMMITTEE

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Dr. P. Boomi
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 2022 to May 2023. It also highlights the International Conference cum Workshop on "Recent trends in Structural Bioinformatics and Computer Aided Drug Design" (ICSBCADD - 2022) and 6th Annual Meeting of Bioinformatics and Drug Discovery Society [BIDDS] was organized by the Department of Bioinformatics, Alagappa University on 21st November 2022 after having conducted for 13 consecutive years on the given theme at National and International level.

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

(Ms. Aarthy. M)

Department Events

(June 2022 to May 2023)

First M.Sc. Bioinformatics 2022-2024 Batch Orientation Programme (05.09.2022)

The Department of Bioinformatics at Alagappa University conducted the Orientation Programme for the First M.Sc. Bioinformatics 2022-2024 Batch on September 5th, 2022. Dr. J. Jeyakanthan, Senior Professor & Head and faculties of the department addressed the newly joined students, welcoming them and introducing the nuances of the Postgraduate programme as well as the department facilities and faculty.

Onam Celebration (08.09.2022)

The Department of Bioinformatics at Alagappa University organized the Onam Celebration on August 09, 2022. The festive event commemorated the annual harvest festival of Kerala with traditional dances, music and feast. Students and faculty members came together to celebrate the harvest festival of Kerala.

SWACHHTA PAKHWADA 2022 (21.09.2022)

The Department of Bioinformatics at Alagappa University organized the Swachhta Pakhwada 2022 from September 21st to October 5th, 2022. This nationwide cleanliness drive focused on spreading awareness about the importance of cleanliness and hygiene. Students and Staffs participated enthusiastically in cleaning activities around the campus and Special talk was given by Dr. A. Arun, Professor & Head, Department of Microbiology on maintaining personal hygiene and a clean environment.

Ayutha Poojai Celebration (30.09.2022)

The Department of Bioinformatics at Alagappa University organized the Ayutha Poojai celebration on September 30th, 2022. This festival honouring tools and instruments was commemorated through traditional rituals and prayers. Students, teachers and non-teaching staff participated in the pooja celebration.

Fresher's Day Celebration (12.10.2022)

The Department of Bioinformatics at Alagappa University organised the Fresher's Day celebration on October 12th, 2022. The event was aimed at welcoming the new batch of M.Sc. students through cultural programs and games. Faculty members and senior students interacted and engaged with the freshers to help them settle in smoothly.

The International Conference cum Workshop on "Recent trends in Structural Bioinformatics and Computer Aided Drug Design" (ICSBCADD - 2022) and 6th Annual Meeting of Bioinformatics and Drug Discovery Society [BIDDS]

The International Conference cum Workshop on "Recent trends in Structural Bioinformatics and Computer Aided Drug Design" (ICSBCADD - 2022) and 6th Annual Meeting of Bioinformatics and Drug Discovery Society [BIDDS] was organized by the Department of Bioinformatics, Alagappa University on 21st November 2022 after having conducted for 13 consecutive years on the given theme at National and International level.

Presiding over the inaugural function, Prof. G. Ravi, Vice-Chancellor, Alagappa University, welcomed the esteemed dignitaries and gathering to the ICSBCADD'2022. He enumerated the feats and milestones achieved by Alagappa University over the years and how the Institution is progressively striving to make its global historic movement on par with global and national Institutes as well as Universities. He further appreciated the department for achieving exemplary growth and progress in a short period by propagating Multidisciplinary Research in the areas of Structural Biology, Computational Molecular Modeling & Drug Design, Pharmacogenomics, Data Mining & Networking, Plant Molecular Biology, Virology & Pathology, Nano Drug Delivery, and Molecular Oncology. The ICSBCADD'2022 was a mammoth event graced by 38 eminent scientists from various countries like the USA, Singapore, Japan, Taiwan, South America and other parts of India and more than 200 participants from various renowned Universities. He also emphasized the department's commitment towards the research on thrust areas like lifestyle diseases like hypertension, Diabetes, Obesity, etc, and life-threatening Viral and Bacterial diseases. Specifically, diseases such as Dengue, Chikungunya, ZIKA, EBOLA, Filariasis, Nocardiosis, and HIV/AIDS infect many people worldwide and claim most of their lives. He also stated World Health Organization (WHO) statistics on Dengue which is rapidly spreading , yet there is no specific treatment so far due to a lack of safe and effective vaccines and appropriate antiviral therapies. He also emphasized the vaccines developed worldwide for the global pandemic coronavirus infection (COVID-19) and also the prominent role played by Bioinformatics during the COVID-19 outbreak. So, he insisted there is a need for human experts to apply their innovative thoughts in scientific information and data science, Computer-aided drug designing, Artificial Intelligence, Next generation sequencing, etc. to discover novel and potential therapeutic drugs to combat these diseases. Finally, he appreciated Prof and Head, Dr. J. Jeyakanthan, and his dedicated team of faculty members and students of Department of Bioinformatics for their streamlined focus on the application of Computational and Experimental techniques against many lifestyle and life-threatening diseases.

Dr. Sekar Vishwanathan, Vice President VIT, in his Inaugural address, rendered his privilege to be a part of the event stating Alagappa University as the temple of Education with the quote " ***எழுத்து அறிவித்தவன் இறைவன்***" from the ancient Tamil scripture to describe the vision of the great Philanthropist Padma Bhushan (Late) Dr.RM. Alagappa Chettiyar for Alagappa University in achieving Excellence in all spheres of Education by affording a Quality-oriented Higher Education to the learners that transformed the intellectually competent human resources that will help in the upliftment of the nation to Educational, Social, Technological, Environmental and Economic Magnificence (ESTEEM). He also appreciated

Alagappa University with its outstanding facilities for quality education and research and also for catering educational needs of rural students. He was also praised that Alagappa University encourages girls' education predominantly and for being an outstanding State University with good NIRF ranking and QS ranking overall. Finally, he provided his insight thoughts on the current perspective of Bioinformatics is the combination of biology and data science, giving machine learning and artificial intelligence methods a real and important purpose with a high focus on personalized medicines.

Prof. T.P. Singh, SERB Distinguished Fellow, All India Institute of Medical Sciences, AIIMS, New Delhi, delivered the thematic address to the gathering. He shared his moments spent with his renowned mentor Late Professor. N. Vijayan and also stated that Bioinformatics will flourish forever and provide progressive growth in various research arenas. He also stressed the point that the demographic balance between the faculties and administration of Institute will aid in paving the better way for new advancements and thought-provoking ideas in research.

Prof. M. Krishnan, Vice-Chancellor, Central University of Tamil Nadu, Thiruvarur in his inaugural address also encouraged and praised the rapid progress of Department of Bioinformatics achieved in these last ten years. He enlightened the gathering on the diverse traditional based knowledge that has been available in our culture for ages together to cure life threatening diseases. And also, he laid emphasis that despite the publications in high standard journals we are still lacking to make our place in the global rankings. He also cited an example about the significance of Tamil tradition, by the brief note on "various types of plough used in agriculture" and also the recent researchers about the variety of food that may change the facial changes of the foetus in the mother's womb and also the significance of pregnant women wearing bangles. Finally, he laid an overview that Tamil Nadu is the only state with full of traditional knowledge and the need to explore. He also enlightened the gathering on the rural knowledge stored in the form of digital laboratory and also, he stressed on the need of the young researchers to identify the area further develop their skills leading to Innovation herby proving beneficial to public by focusing on traditional concepts in India.

Prof. Akio Ebihara, Faculty of Applied Biological Sciences, Gifu University, Japan delivered the Innovative research award. In his speech he stressed on the importance of fundamentals of research networking and building research collaboration. He also said that the senior scientists need to be instrumental and being transparent of sharing the knowledge thereby paving way to the creation of interdisciplinary sciences.

Prof. D. Velmurugan, Honorary Emeritus Professor, Former Head, CAS in Crystallography and Biophysics, University of Madras, Chennai, currently serving as Dean of Research, Marine Biotechnology, AMET University, Chennai, delivered the Felicitation address. In his speech he appreciated the Vice-Chancellor for the rapid progress the University. In his speech he said that most of the biological problems can be solved through Bioinformatics approaches. He also motivated the Head of the Department to keep continuing the pace towards progress and hard work for promoting Bioinformatics on a global level.

Dr. R. Swaminathan, Member of Syndicate, Alagappa University delivered the Felicitation address. He also said that Alagappa University leaves no stone unturned to achieve excellence in all spheres and highlighted on the without discipline, moral values and politics there exists no proper human kind. He also highlighted on the main aim of this grandeur event is to create awareness towards the recent developments in the fields of structural biology, molecular biology, drug discovery, Computational Biology and Chemistry and medicinal research, which have deliberately become an essential for a person pursuing research or profession in modern science which will open up new and powerful insights into treating diseases from cancers to the common cold. Based on the World Health Reports (WHO) majority of the global population will be prone to cancer; diabetes; cardiovascular diseases; Tuberculosis; sexually transmitted diseases through viruses - HIV; Tropical diseases – malaria, filariasis, Zika; and most importantly the ever-pervading Antibiotic-resistant bacteria due to rapid economic development and urbanization.

Prof. and Head, J. Jeyakanthan, Convenor of ICSBCADD-2022 welcomed the gathering and highlighted that the department has conceived another initiative this year to organize a workshop to educate budding researchers. He also stated the crux of this event is to provide the current scenario of interdisciplinary research in the fields of structural biology, molecular biology, drug discovery, Bioinformatics, Computational Chemistry and medicinal research, which have deliberately become essential for a person pursuing research or profession in modern science. Based on the World Health Organization (WHO) report, majority of the global population will be prone to cancer, diabetes, cardiovascular diseases, Tuberculosis, sexually transmitted diseases; Tropical diseases such as malaria, filariasis, dengue, Zika; the ever-pervading Antibiotic-resistant bacteria and most importantly the SARS-COV-2. Henceforth, the research outcomes of our department in the field of Structural Biology and Bioinformatics have streamlined the drug discovery and drug development process that facilitated the identification of novel therapeutics against infectious diseases. Before concluding his address, Professor also highlighted the recent research findings in computational biology for the enhanced drug discovery process. The **University of Illinois** have developed the **first computational human cell** model and simulated it for **15 minutes** to **understand cancer biology**, the **longest time** achieved for any complex biological system. This finding was overtaken by the researchers at the **University of Surrey** where they developed a multi-disciplinary simulation tool called **BioDynaMo** to simulate biological processes with **one billion cells on a single server**, which transformed the current trend in systems biology addressing complex diseases like cancer and neurological disorders (Alzheimer's). Moreover, the **CellTrek tool** developed by researchers at the **University of Texas** helps to **locate individual cell types within a tissue** to provide biological insights into the **cancer microenvironment.** On the other hand, drug discovery has attained another break though at several instances wherein the **university of Cincinnati** has developed a **novel drug AB569** that combats ***Pseudomonas aeruginosa*** at lower concentrations in humanized cells with **least toxicity.** Scientists at **Rockefeller University** have **discovered carboxylic acids on human skin that attracts mosquitoes**. This significant report will aid in **developing novel antimalarials**. Thus, drug discovery Informatics is the field that integrates biology with both Artificial intelligence (AI) and Machine learning (ML) to accelerate the drug development timeline. The significance of this field came to light during the COVID-19 pandemic. Likewise, he also stressed that his department is also focusing on drug discovery research. For instance, in our recent article entitled "Computational investigation on *kabasura kudineer and nilavembu kashayam* phytochemicals to evaluate their potency against SARS-CoV-2 in comparison to known antiviral compounds in drug trials", and have exploited computational tools to predict, antiviral agents and drug cocktails against various protein targets in SARS-CoV-2. Also, expressed that the researchers in his department are developing reliable computational tools to identify novel therapeutics against life-threatening diseases. Furthermore, He also elaborated the progress of the Department in the last 14 years since its inception.

At Inaugural session of the Conference, Honourable Vice-Chancellor, Prof. G. Ravi, Alagappa University, Karaikudi, released the Souvenir and the copy was received by eminent guests of the conference, respected Dr. Sekar Viswanathan, Vice President, VIT, Prof. T.P Singh, SERB Distinguished Fellow, Department of Biophysics, AIIMS, New Delhi, Prof. M. Krishnan, Vice-Chancellor, Central University, Thiruvarur, Prof. Akio Ebihara, Faculty of Applied Biological Sciences, Gifu University, Japan, Prof. D. Velmurugan, Dean Research, AMET University, Dr. R. Swaminathan, Member of Syndicate, Alagappa University.

Followed by this, the 2nd Bioinformatics and Drug Discovery Society (BIDDS) newsletter was released by respected Prof. T.P Singh, SERB Distinguished Fellow, Department of Biophysics, AIIMS, New Delhi and was received by all the above-mentioned eminent guests. It was a pride moment for the department this year in endorsing two awards in memory of our beloved legends in X-ray crystallography and Bioinformatics, the most respected Professors, Dr. M. Vijayan and Dr. N. Srinivasan, whose phenomenal legacy has set a foundation for all research endeavours. In addition, to inspire and encourage the blooming researchers, this year the BIDDS Society presents the “Best Research Student award”, and “Young Scientist award” and commemorates “Lifetime achievement awards”. Finally, vote of thanks was proposed by Prof. Sanjeev Kumar Singh.

Vice Chancellor Visit to Department (09.12.2022)

The Department of Bioinformatics at Alagappa University witnessed the visit of Vice Chancellor Dr. G. Ravi on December 9th, 2022. He interacted with faculty members and students to know about the department's research and academic activities. The Vice Chancellor appreciated their efforts and encouraged the continuous innovations. His visit boosted the student community and reinforced the university's support towards interdisciplinary education and research.

Pongal Celebration (12.01.2023)

The Department of Bioinformatics at Alagappa University organized the Pongal celebration on January 12th, 2023. This popular South Indian harvest festival was commemorated with traditional fervour at the department. Students, faculty and staff members gathered to prepare Pongal. Cultural performances featuring folk arts and community lunch brought everyone together to celebrate the spirit of sharing and thanksgiving during this auspicious occasion.

Untouchability Eradication pledge (30.01.2023)

The Department of Bioinformatics at Alagappa University organized an event to mark the Untouchability Eradication pledge day on 30th January 2023. Students and staff gathered to reaffirm the values of equality, dignity and justice for all. It helped spread awareness about equal rights and social justice.

Bonded Labour Abolition Pledge (09.02.2023)

The Department of Bioinformatics at Alagappa University organized an event to mark the Bonded Labour Abolition pledge day on February 9th, 2023. Students and staff gathered to renew their commitment against all forms of forced labour and human trafficking. An awareness session was held highlighting the provisions in law for abolition and rehabilitation. A pledge was administered to uphold dignity and rights of all people without any discrimination.

AADHAR CAMP 22.02.2023

The Department of Bioinformatics at Alagappa University organized an Aadhaar Camp on February 22nd, 2023. In collaboration with the UIDAI, the camp aimed to help students and staff get enrolled for the 12-digit unique identity number. Over 50 applicants had their photographs and fingerprints captured to apply for Aadhaar cards. The initiative supported the government's goal of having every resident linked to essential services and benefits through this identity platform.

Science Day 28.02.2023

The science day was celebrated by Alagappa University on 28 Feb 2023. 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 08.03.2023

International Women's Day was celebrated in department of Bioinformatics on 8th March 2023 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.

PTAM 2023 29.03.2023

Speaking on the occasion, Dr. J. Jeyakanthan, Senior Professor & Head and Faculty members 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's are holding positions of responsibility in various Government organizations, Private sector and Academic Institutions. He praised the contribution of the Alumni towards the growth and emphasized the need for further strengthening the linkage between the Alumni and current students in the Department of Bioinformatics.

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

Many of the current students also interacted with the passed out seniors and learned from their experiences. Parents gave a 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 was 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.

M.Sc. Farewell 13.04.2023

The Department of Bioinformatics at Alagappa University hosted the M.Sc. Farewell event on April 13th, 2023 to bid adieu to the graduating batch. The event celebrated the achievements and memories of the students. Speeches, cultural programs and award ceremonies marked the occasion. A mood of nostalgia and excitement prevailed as the students geared up for new opportunities and challenges in their careers.

YOGA Session 20.04.2023

The Department of Bioinformatics at Alagappa University organized a Yoga session on April 20th, 2023 to celebrate the International Day of Yoga. Staff and students enthusiastically participated in various asanas and pranayama practices taught by an expert. The session highlighted the importance of integrating physical and mental health through yoga. It aimed to spread awareness about keeping fit and reducing stress through this ancient Indian wellness practice.

Department Annual Day Celebration (20.04.2023)

On 20.04.2023, Department of Bioinformatics conducted **“Department Annual Day Celebration – 2023”**. The Department Head & Senior Professor Dr. J. Jeyakanthan Inaguarted the celebration and addressed the gathering. We successfully conducted the various cultural programs like Dance, Music, Skits etc., were performed by the students. Extracurricular events like Rangoli and Cooking without Fire were organized. The M.Sc. Students who won the prizes in Cultural and Extracurricular events were fellicitated with Trophies and Award Certificates.

Invited Talks/Address

Interactive Session and Technical Presentation on “Application and Salient Features of Q – TOF – LC – MS” Organized by Higher Education Best Practices Cell University Science Instrumentation Centre (USIC) and Department of Bioinformatics, Alagappa University

The Interactive Forum and Lecture entitled “Applications and Salient Features of Q – TOF – LC – MS” was organized by the joint efforts of the Higher Education Best Practices Cell, University Science Instrumentation Centre (USIC) and the Department of Bioinformatics at the Faculty of Science Conference Hall, on 3rd February, 2023. The keynote speaker invited for this event was Dr. Ashish Pargaonkar, Manager, Centre of Excellence, Agilent Technologies India Private Limited, Bangalore. Dr. K. Sankaranarayanan, Professor and Head, Department of Physics and the Director of the University Science Instrumentation Centre, greeted the chief guest with his welcome speech. Dr. Ashish Pargaonkar, a representative on behalf of Agilent Technologies, first gave the audience a brief introduction on the principles and applications of the instrument “Q – TOF – LC – MS”. The abbreviation of “Q – TOF – LC – MS” is “Quadrupole Time of Flight Liquid Chromatography/Mass Spectrometry”.

He outlined the various features of the instrument manufactured by their production company, and the multiple plug – ins and software that will be accompanying the hardware. Furthermore, he mentioned the ways in which the hardware as well as software can be troubleshot, and the assistance that will be provided by the company for the troubleshooting process. Following the technical presentation, an interaction forum was set up to clear any doubts that may have risen during the presentation. During this session, Faculty members, Research scholars and Students asked different questions to the speaker about various aspects of the instrument, and how they can be applied to further progress their research work. Our Guest of Honor answered those questions with patience and the students also gained a lot of understanding and knowledge about the Liquid Chromatography/Mass Spectrometry technique, from this discussion. Finally, the Vote of Thanks was given by Dr. J. Jeyakanthan, Professor and Head, Department of Bioinformatics, Alagappa University who expressed his gratitude to the University Science Instrumentation Centre (USIC), the Higher Education Best Practices Cell and Agilent Technologies for their undying efforts to bring sophisticated technology to the department and improve the research facilities of the lab. With these remarks, the event concluded on a pleasant note.

Eminent Scientist Lecture on “Single Particle Cryo-EM, the Structural Biology Method as a Pipeline for Preclinical Structure-Based Drug Design” Organized by Higher Education Best Practices Cell and Department of Bioinformatics, Alagappa University.

The Higher Education Best Practices Cell and the Department of Bioinformatics, Alagappa University, organized the Eminent Scientist Lecture and Discussion on 20th February 2023. For this Lecture Programme Prof. Ramanathan Natesh of the School of Biology and Centre for High Performance, Institute of Science Education and Research, Thiruvananthapuram, Kerala was invited as an Eminent Scientist to give a detailed lecture on the topic entitled “Single Particle Cryo-EM, the Structural Biology Method as a Pipeline for Preclinical Structure-Based Drug Design” to explore the applications of Electron Microscopy (EM) in which specimens, that are randomly dispersed, unstained biological macromolecules are studied. Dr. J. Jeyakanthan, Professor and Head, Department of Bioinformatics, Alagappa University gave a warm welcome to the esteemed Scientist Dr. Ramanathan Natesh. He is a seasoned researcher in different research areas, specifically in the Single Particle Cryo - Electron Microscopy Techniques and Structure-based Drug Designing. The distinguished resource person focused on the single particle Cryo-EM methods, by providing the audience with an overview of the achievements done by the early pioneers (Jacques Dubochet, Joachim Frank and Richard Henderson) in the single particle cryo electron microscopy field during the 1980s. He further explained how these fundamental discoveries led to the quick progression of improved resolution of protein structure determination using Cryo-EM during the earlier parts of 2012. This method has helped greatly the researchers in Structure-Based Drug Design since the last decade. In addition, he elaborated on how these developments ultimately led the three scientists to receive the Nobel Prize for Chemistry in 2017. The chief guest, an expert in both single particle Cryo-EM and protein crystallography, elegantly presented the strengths and weaknesses of both the methods in Structure – Based Drug Design. As the Founding President of Single Particle Cryo- EM and Three – Dimensional Image Processing (CEM3DIP) Society of India, he concluded his lecture, educating the participants about various research activities that are taking place with the help of Cryo – EM and he referred to its current state in India. At the end of the programme, Dr. P. Boomi, Assistant Professor, Department of Bioinformatics, Alagappa University, expressed his gratitude to the organizers of this event for their meticulous planning that made this event a great success and useful one for the participants.

One Day Seminar on Vision and Ideology of Pandit. Deendayal Upadhyaya- (23.02.2023)

The Department of Bioinformatics at Alagappa University organised a one-day seminar on the vision and ideology of Pandit Deendayal Upadhyaya on 23rd February 2023. Experts spoke about the integral humanism as the cornerstone of a progressive society. The seminar helped students understand Upadhyaya's nationalist ideology and influential contributions in shaping India's development path in a self-reliant manner.

- Dr. J. Jeyakanthan delivered a memorable lecture titled "Explore the Novel Mechanism for Inhibition of Cell wall Biosynthesis -Zeta Toxin as an effective therapeutic target" as an invited speaker at Jamal Mohamed College in Tiruchirappalli during their special lecture series from September 7th to October 8th 2022.

- Dr. J. Jeyakanthan delivered a talk titled "crystal structure of gultaminyl -tRNA synthetase and its complexes from *Thermus thermophilus* HB8" as an invited speaker at AMET University, Chennai during their special lecture series from October 6th to 9th 2022.

- Dr. J. Jeyakanthan delivered a talk titled "High–Throughput Structural Biology & Bio-Computing" as an invited speaker at Dwaraka Doss Goverdhan Doss Vaishnav College, Chennai during their special lecture series from October 19th to 20th 2022.

- Dr. Sanjeev Kumar Singh delivered a talk titled "Designing of Responsive Agent to eradicate HIV: A Computational Drug Discovery Approach" as a resource person at Shree S. K. Patel College of Pharmaceutical Education and Research, Ganpat University, Gujarat during the SERB sponsored workshop on “Hands-On Training on Computer Aided Drug Design and Discovery Tools” from July 11th to 17th 2022.

- Dr. Sanjeev Kumar Singh delivered a presented invited talk on titled "Computer-Aided Drug Design and Structural Bioinformatics (CADDSB-2023)" as a resource person at IIT BHU, Varanasi, U.P during the conference from March 13th to 17th 2023. This

- Dr. M. Karthikeyan delivered an invited talk on titled "SNPs, Mutations & Genomic Instability associated with Dental Diseases and treatment: a Pharmacogenomics perspective view" as an invited speaker at Saveetha Dental College, Saveetha Institute of Medical and Technical Sciences, Chennai on December 3rd 2022.

- Dr. J. Joseph Sahayarayan delivered an invited talk titled "Role of Plant Based Transgenic Products and Drug Discovery" as an invited speaker at the ... Department of Biochemistry, J.J. College of Arts and Science (Autonomous), Pudukkottai, Tamil Nadu on September 16th 2022.

- Dr. J. Joseph Sahayarayan delivered a talk titled "Role of Medicinally Important Plant Products to Develop the Drug for Human Diseases" as an invited speaker at the Department of Microbiology, Arputha College of Arts and Science, Arputha Nagar, Vamban, Alangudi, Pudukkottai, Tamil Nadu on April 12th 2023.

Awards

- Dr. J. Jeyakanthan received the Outstanding Researcher Award – 2022 from Alagappa University, Karaikudi, Tamil Nadu in recognition of his significant research accomplishments and contributions to the university.
- Dr. Sanjeev Kumar Singh received the prestigious INSA Teacher Award-2022 from the Indian National Science Academy, New Delhi for his outstanding contributions to teaching and research.
- Dr. Sanjeev Kumar Sing received the Outstanding Researcher Award – 2022 from Alagappa University, Karaikudi, Tamil Nadu in recognition of his significant research accomplishments and contributions to the university.
- Dr. M. Karthikeyan was conferred with the prestigious C V Raman Prize by the Institute of Researchers, Kerala for his outstanding contributions and research accomplishments in the field of bioinformatics.
- Dr. M. Karthikeyan was conferred with the prestigious Research Excellence Award by the Institute of Researchers, Kerala for his outstanding contributions and research accomplishments in the field of bioinformatics.
- Dr. M. Karthikeyan was conferred with the Promising Researcher Award - 2022 by Alagappa University, Karaikudi for his outstanding research contributions and for being an inspiring young researcher with huge potential in the field of bioinformatics.
- Dr. M. Karthikeyan was honored with the title of Honorary Fellow by the prestigious INTI International University of Malaysia, in recognition of his valuable contributions and expertise in the field of bioinformatics.
- Dr. P. Boomi was conferred the Promising Researcher Award-2022 by Alagappa University, Karaikudi, Tamil Nadu, India for his outstanding early career research and contributions to the department and University.

Key Publications

antibiotics

MDPI

Article

Functional Characterization, Mechanism, and Mode of Action of Putative Streptomycin Adenylyltransferase from *Serratia marcescens*

Dhamodharan Prabhu [1,2,*], Sundararaj Rajamanikandan [1], Mathimaran Amala [2], Poopandi Saritha [2], Jeyaraman Jeyakanthan [2,*] and Palaniappan Ramasamy [1,*]

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Abstract: Nosocomial infections are serious threats to the entire world in healthcare settings. The major causative agents of nosocomial infections are bacterial pathogens, among which *Enterobacteriaceae* family member *Serratia marcescens* plays a crucial role. It is a gram-negative opportunistic pathogen, predominantly affecting patients in intensive-care units. The presence of intrinsic genes in *S. marcescens* led to the development of resistance to antibiotics for survival. Complete scanning of the proteome, including hypothetical and partially annotated proteins, paves the way for a better understanding of potential drug targets. The targeted protein expressed in *E. coli* BL21 (DE3) pLysS cells has shown complete resistance to aminoglycoside antibiotic streptomycin (>256 MCG). The recombinant protein was purified using affinity and size-exclusion chromatography and characterized using SDS-PAGE, western blotting, and MALDI-TOF analysis. Free phosphate bound to malachite green was detected at 620 nm, evident of the conversion of adenosine triphosphate to adenosine monophosphate during the adenylation process. Similarly, in the chromatographic assay, adenylated streptomycin absorbed at 260 nm in AKTA (FPLC), confirming the enzyme-catalyzed adenylation of streptomycin. Further, the adenylated product of streptomycin was confirmed through HPLC and mass spectrometry analysis. In conclusion, our characterization studies identified the partially annotated hypothetical protein as streptomycin adenylyltransferase.

Keywords: functional annotation; antibiotic resistance; streptomycin adenylyltransferase; ANT

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Citation: Prabhu, D.; Rajamanikandan, S.; Amala, M.; Saritha, P.; Jeyakanthan, J.; Ramasamy, P. Functional Characterization, Mechanism, and Mode of Action of Putative Streptomycin Adenylyltransferase from *Serratia marcescens*. *Antibiotics* **2022**, *11*, 1722. https://doi.org/10.3390/antibiotics11121722

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1. Introduction

"Nosocomial" or "Healthcare-Associated Infections (HAI)" are widely used to refer to any class of disease affecting patients while undergoing medical care or even sometimes after treatment procedures. Prolonged stay in hospitals is found to be the root cause of HAI, and its risk factors range from simple to critical health infections, leading up to fatalities [1]. A recent study reported that these HAIs are rigorously intensifying in primary infections, even leading to deaths, with developing countries bearing 75% of the burden of infection-associated mortality, especially in neonates [2]. HAIs have become unavoidable complications in medical procedures due to (i) aging, (ii) prolonged stay of immune compromised patients in hospitals, (iii) rapid advancements in invasive devices-assisted diagnosis, and (iv) inappropriate usage of antimicrobial agents [3]. The causative agents of HAIs are microbes viz. bacteria, protozoa, fungi, viruses, and mycobacteria, but 90% of these infections are caused by bacteria [4]. *Staphylococcus aureus*, *Acinetobacter* spp., *Pseudomonas aeruginosa*, *Streptococcus* spp., and *Enterobacteriaceae* family members including *Klebsiella pneumoniae*, *Proteus mirablis*, *Escherichia coli*, and *Serratia marcescens* are widely reported to be the bacterial species causing HAIs [1].

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Computational identification of potential lead molecules targeting rho receptor of *Neisseria gonorrhoeae*

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ABSTRACT

Gonorrhea, one of the sexually transmitted disease caused by a gram negative diplococcus bacteria *Neisseria gonorrhoeae*. Rho protein is indispensable for bacterial viability due to its versatile functions in physiology apart from RNA dependent transcription termination. Based on conserved function and wider role in several cellular processes, inhibitors specifically targeting Rho proteins are largely in use these days to treat various bacterial infections. In this study, three dimensional structure of Rho protein was modeled using the template protein from *E. coli* and further the optimized model was simulated for 100 ns to understand the structural stability and compactness. Owing to the therapeutic potential of Rho, traditional structure-based virtual screening was applied to identify potential inhibitors for the selected target. Based on empirical glide scoring functions two potent lead molecules (ChemBridge_6121956 and ChemBridge_5232688) were selected from ChemBridge database. The pharmacokinetic properties of these lead molecules are within the permissible range. DFT descriptor revealed that the lead molecules are more reactive, which also supports the molecular docking studies. The stability of Rho and Rho-inhibitor complexes was studied using molecular dynamics simulation. Parameters include binding free energy calculation, RMSD, RMSF and hydrogen bond analysis depicts the stability of Rho and Rho-inhibitors throughout the simulation. Altogether, the identified lead molecules require further optimization towards the design and development of new antibiotics against *N. gonorrhoeae*.

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KEYWORDS
Neisseria gonorrhoeae; Rho; structure-based virtual screening; DFT and molecular dynamics simulation

1. Introduction

Neisseria gonorrhoeae an opportunistic human pathogen affects both male and female reproductive tracts, and a major etiological agent of sexually transmitted infection (STI) (Hill et al., 2016; Humbert & Christodoulides, 2019; Quillin & Seifert, 2018). Based on WHO report, 4 Sexually Transmitted Infections (STIs) such as syphilis, gonorrhea, chlamydia and trichomoniasis cause annually 376 million infections and it is the second notable disease in the United States (Rowley et al., 2019; Kidd & Workowski, 2015). CDC reports 63% increase in cases of gonorrhea since 2014 [CDC, 2019]. However, the Indian scenario is even more alarming as STIs accounts for 6% of the adult population in the country (Patel & Mazumdar, 2019). The serious sequeleae of gonorrhea increases the risk of HIV infection transmission (Galvin & Cohen, 2004). Asymptomatic or unnoticed infections in the reproductive tract including the fallopian tubes, cervic, uterus and the urethra in women can lead to long term consequences (LenZ & Dillard, 2018). Without proper treatment, the infection spreads and cause pelvic inflammatory disease (PID) in women and urethritis, epididymo-orchitis in men and also increases the risk of ectopic pregnancy in women which leads to tubal-factor infertility (Patil, 2012; Piszczek et al., 2015).

Since no vaccine is available, antibiotics are the only source to treat gonorrhea. Dual antimicrobial therapy Ceftriaxone 250 mg intramuscular (IM) single dose plus 1 g oral dose of azithromycin is a preferred option for treating gonorrhea infections (Kidd & Workowski, 2015; Unemo, 2015). The emergence of multi drug-resistance among all strains of *N. gonorrhoeae* has complicated the treatment of gonorrhea infections (Alirol et al., 2017). However, still there is no effective treatment available to treat gonorrhea emphasizes the pressing need for new antibiotics to combat drug resistant *N. gonorrhoeae*.

Recent development suggests, targeting bacterial Rho protein with small molecule inhibitors are the platform for the successful development of new antibiotics. Bacterial cell viability relies on accurate termination apart from initiation and elongation transcription process (Botella et al., 2017). In general, two modes of transcriptional termination process are commonly reported in prokaryotes. One terminates the transcription process based on the specific sequences at the end of coding region and another mode relies on the RNA dependent ATPase referred as Rho protein (Peters et al.,

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OPEN

Triphenylphosphonium conjugated gold nanotriangles impact Pi3K/AKT pathway in breast cancer cells: a photodynamic therapy approach

Nadar Manimaran Vinita[1], Umapathy Devan[2], Sabapathi Durgadevi[1], Selvaraj Anitha[1], Dhamodharan Prabhu[3], Sundarraj Rajamanikandan[3,4], Muthusamy Govarthanan[5,6], Ananthanarayanan Yuvaraj[7], Muniyandi Biruntha[1], Arockiam Antony Joseph Velanganni[2], Jeyaraman Jeyakanthan[8], Pitchan Arul Prakash[9], Mohamed Sultan Mohamed Jaabir[9] & Ponnuchamy Kumar[1]✉

Although gold nanoparticles based photodynamic therapy (PDT) were reported to improve efficacy and specificity, the impact of surface charge in targeting cancer is still a challenge. Herein, we report gold nanotriangles (AuNTs) tuned with anionic and cationic surface charge conjugating triphenylphosphonium (TPP) targeting breast cancer cells with 5-aminoleuvinic acid (5-ALA) based PDT, in vitro. Optimized surface charge of AuNTs with and without TPP kill breast cancer cells. By combining, 5-ALA and PDT, the surface charge augmented AuNTs deliver improved cellular toxicity as revealed by MTT, fluorescent probes and flow cytometry. Further, the 5-ALA and PDT treatment in the presence of AuNTs impairs cell survival Pi3K/AKT signaling pathway causing mitochondrial dependent apoptosis. The cumulative findings demonstrate that, cationic AuNTs with TPP excel selective targeting of breast cancer cells in the presence of 5-ALA and PDT.

Despite significant lab and clinical research, the prevalence of breast cancer continues to rise, inflicting misery on women[1,2]. As a result, low- and middle-income countries face several obstacles in cancer detection, diagnosis, and their related therapies[3–5]. Hence, providing patients with effective drugs that minimize harmful effects is the need of the hour. To combat this issue, nanotechnology has emerged as a superior platform for the simultaneous delivery of drugs[6–9].

In this journey, therapeutic nanoparticles selectively target tumors, enhance anticancer effectiveness and circumventing drug resistance[10–12]. For instance, gold nanoparticles are among the most promising agents for cancer treatment due to these reasons; (i) small and capable of selectively penetrating cancer cells through the enhanced permeability and retention (EPR) effect[13,14] (ii) their ability to bind proteins and drugs in targeting cancer cells that possess cell surface receptors[15,16] (iii) can absorb light radiations and provide better contrast images than conventional agents[17,18].

Over the last few decades, gold nanoparticles have been conjugated with various functionalizing moieties, including ligands, therapeutic agents, DNA, amino acids, proteins, peptides, oligonucleotides, etc[19–22]. Recently, a research study demonstrated the utilization of PEG ligands with gold nanoparticles to functionalize doxorubicin

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Protocol Article

Promoter–motif extraction from co-regulated genes and their relevance to co-expression using *E. coli* as a model

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Abstract

Gene expression varies due to the intrinsic stochasticity of transcription or as a reaction to external perturbations that generate cellular mutations. Co-regulation, co-expression and functional similarity of substances have been employed for indoctrinating the process of the transcriptional paradigm. The difficult process of analysing complicated proteomes and biological switches has been made easier by technical improvements, and microarray technology has flourished as a viable platform. Therefore, this research enables Microarray to cluster genes that are co-expressed and co-regulated into specific segments. Copious search algorithms have been employed to ascertain diacritic motifs or a combination of motifs that are performing regular expression, and their relevant information corresponding to the gene patterns is also documented. The associated genes co-expression and relevant cis-elements are further explored by engaging *Escherichia coli* as a model organism. Various clustering algorithms have also been used to generate classes of genes with similar expression profiles. A promoter database 'EcoPromDB' has been developed by referring RegulonDB database; this promoter database is freely available at www.ecopromdb.eminentbio.com and is divided into two sub-groups, depending upon the results of co-expression and co-regulation analyses.

Keywords: Gene regulation; Co-expression; Motif discovery; Microarray data analysis; E.coli; E.coli promoter database; EcopromDB

Introduction

The articulate expression of the genetic information residing in the whole genome is governed by a subset of genes that works in a complex manner, giving rise to the Genomic Regulatory Machinery [1]. Promoters located upstream of the gene are recognized by significant elementary proteins or transcription factors (TFs), aiding the assembly of complex switches [2, 3]. Promoter search and identification have been termed the most enigmatic step in transcription initiation. This is achieved with the help of

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Anuraj Nayarisseri is the Principal Scientist and the Director of Eminent Biosciences, Indore, India. His research area is translational bioinformatics approaches for the implementation of precision medicine in the clinical setting. He led multiple projects to find genetic variants driving complex diseases, clinical traits and phenome-wide associations and has designed, developed and implemented clinical workflows to include genomic data in electronic medical records, thus rapidly reducing the time for translating biological, genetics or genomics discovery to improve healthcare delivery.

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ORIGINAL ARTICLE

Structure-Based Virtual Screening, Molecular Docking, Molecular Dynamics Simulation of EGFR for the Clinical Treatment of Glioblastoma

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Abstract

Glioblastoma (GBM) is a WHO Grade IV tumor with poor visibility, a high risk of comorbidity, and exhibit limited treatment options. Resurfacing from second-rate glioma was originally classified as either mandatory or optional. Recent interest in personalized medicine has motivated research toward biomarker stratification-based individualized illness therapy. GBM biomarkers have been investigated for their potential utility in prognostic stratification, driving the development of targeted therapy and customizing therapeutic treatment. Due to the availability of a specific EGFRvIII mutational variation with a clear function in glioma-genesis, recent research suggests that EGFR has the potential to be a prognostic factor in GBM, while others have shown no clinical link between EGFR and survival. The pre-existing pharmaceutical lapatinib (PubChem ID: 208,908) with a higher affinity score is used for virtual screening. As a result, the current study revealed a newly screened chemical (PubChem CID: 59,671,768) with a higher affinity than the previously known molecule. When the two compounds are compared, the former has the lowest re-rank score. The time-resolved features of a virtually screened chemical and an established compound were investigated using molecular dynamics simulation. Both compounds are equivalent, according to the ADMET study. This report implies that the virtual screened chemical could be a promising Glioblastoma therapy.

Keywords EGFR · Glioblastoma · Virtual screening · Molecular docking · MD simulation · R programming · ADMET · Boiled egg plot

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sustainability

Article

Expressing *OsiSAP8*, a Zinc-Finger Associated Protein Gene, Mitigates Stress Dynamics in Existing Elite Rice Varieties of the 'Green Revolution'

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Abstract: Key message: Overexpression of *OsiSAP8* driven by *Port Ubi2.3* from *Porteresia coarctata* imparts drought and salinity stress tolerance in transgenic rice. Stress associated proteins (SAPs) possess the zinc-finger domains that are wildly evolving functional and conserved regions/factors in plants to combat abiotic stresses. In this study, the promoter region of *OsiSAP8*, an intron-less, multiple stress inducible gene, was compared in silico with a strong constitutive promoter, *Port Ubi2.3*. This resulted in developing rice, resistant to drought and salinity expressing *OsiSAP8* promoted by *Port Ubi2.3*. (*Porteresia coarctata*), through *Agrobacterium*-mediated transformation in the popular rice varieties, IR36 and IR64. Southern blot hybridization confirmed the integration of *OsiSAP8*, and the T0 transgenic lines of IR36 and IR64 were evaluated for their drought and salinity tolerance. The IR36-T1 progenies showed an enhanced tolerance to water withhold stress compared to wild type and IR64-T1 progenies. Physiological parameters, such as the panicle weight, number of panicles, leaf wilting, and TBARS assay, showed the transgenic IR36 to be superior. The transgenic lines performed better with higher 80–95% relative leaf water content when subjected to drought for 14 days. Gene expression analysis of *OsiSAP8* in IR36 T1 showed a 1.5-fold upregulation under mannitol stress. However, IR64 T1 showed a two-fold upregulation in NaCl stress. An enhanced drought and salinity stress tolerance in the transgenic IR36 cultivar through overexpression of *OsiSAP8* was observed as it had a native copy of *OsiSAP8*. This is perhaps the first study using a novel ubiquitin promoter (*Port Ubi2.3*) to generate drought and salinity stress-tolerant transgenic rice. Thus, we report the overexpression of a rice gene (*OsiSAP8*) by a rice promoter (*Port Ubi2.3*) in rice (IR36) to resist drought and salinity.

Keywords: abiotic stress; IR36; *OsiSAP8*; *Port Ubi2.3*; promoter; zinc-finger protein

1. Introduction

Rice (*Oryza sativa* L.), being the most popular and domesticated *kharif* crop, is the staple source of carbohydrate to nearly half of the world's population [1–4]. The sessile and

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An *in silico* analysis of the impact *of POLE* mutations on cladribine docking

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Abstract. – OBJECTIVE: Polymerase ε exonuclease (POLE) is an enzyme involved in DNA replication and may be an attractive therapeutic target in various cancers. Here we sought to model the impact of specific *POLE* mutations on protein function. Due to the lack of a crystal structure, the tertiary structures of the wild type and four common mutants were modeled using I-Tasser server.

MATERIALS AND METHODS: Molecular docking and dynamic simulation studies were performed, and the structure and function of the mutants analyzed through residue conservation analysis and protein folding energy changes.

RESULTS: All mutants of *POLE* gene had favorable binding affinities compared with their wild type of counterpart. The P286R variant, but not the other variants, disrupted cladribine binding to the protein. Similarly, dynamics studies revealed instability of the P286R mutant, while V411L, L424V, and L424F appeared to favor cladribine binding.

CONCLUSIONS: Since P286R is a hotspot mutation in endometrioid carcinomas, patients with this variant may not respond to cladribine. Population-based pharmacogenomics studies will be required to validate our results.

Key Words:

Molecular docking, Molecular dynamics, Residue conservation, Mutation, POLE, SNP, Gynecology cancer.

Introduction

DNA polymerase epsilon (POLE) is a B-family DNA polymerase that plays an important role in leading strand synthesis in nuclear DNA replication[1]. The enzyme has four subunits: p261 (POLE), p59 (POLE2), p17 (POLE3), and p12 (POLE4). p261, encoded by the polymerase ε exonuclease (*POLE*) gene, has a conserved polymerase exonuclease domain (ED), a proofreading domain responsible for detecting and removing mis-incorporated nucleotides[2]. Defects in the proofreading function of the POLE enzyme contribute to genomic instability in different cancers[3]. All reported somatic and germline *POLE* mutations are heterozygous and no loss of heterozygosity has been reported[3]. Although they exist in heterozygous form, the pathogenicity of these mutations remains unclear and the role of these mutations on tumor development is not explained[4]. It has been recently shown[5] that different *POLE* mutant alleles differentially influence and drive tumor mutation burden, thereby dividing patients into distinct subgroups. Interestingly, all *POLE* mutations reported in patients with ultramutated tumors are located in the proofreading ED. *POLE* is frequently mutated in different solid cancers and leukemias[6], with 92 *POLE* ED mutations reported in different cancers according to the cBioPortal database (available at: https://www.cbioportal.org/, accessed in November, 2021)[7,8].

Cladribine (2-chlorodeoxyadenosine; 2-CdA) is a nucleoside analogue developed nearly 50 years ago and is now commonly used to treat variety of tumors[9] and individuals with multiple sclerosis due to its immunosuppressive activity[10].

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RESEARCH ARTICLE

HTNpedia: A Knowledge Base for Hypertension Research

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Abstract: ***Background***: Hypertension is notably a serious public health concern due to its high prevalence and strong association with cardiovascular disease and renal failure. It is reported to be the fourth leading disease that leads to death worldwide.

Objective: Currently, there is no active operational knowledge base or database for hypertension or cardiovascular illness.

Method: The primary data source was retrieved from the research outputs obtained from our laboratory team working on hypertension research. We have presented a preliminary dataset and external links to the public repository for detailed analysis to readers.

Result: As a result, HTNpedia was created to provide information regarding hypertension-related proteins and genes.

Conclusion: The complete webpage is accessible *via* www.mkarthikeyan.bioinfoau.org/HTNpedia.

Keywords: Hypertension, knowledge base, SNP, proteins, genes, drug molecules.

1. INTRODUCTION

It is widely known that the interaction between biological proteins is highly intricate. Furthermore, they are closely associated with biological, chemical and metabolic signalling pathway(s). Proteins are presumed to be the best molecular targets in drug discovery for many disorders. However, no definitive link between the proteins and the disease has been established [1, 2]. On the contrary, genomic data analysis revealed that proteins and genes are involved in a specific pathway. Alternative splicing and post-translational alterations contribute to this complexity [3, 4]. As a result, a comprehensive understanding of hypertension aetiology is expected to overcome barriers in hypertension management strategies [5].

A lot of evidence is available in public domains and open-source databases, which has a significant impact on the development of pathway-based drugs using *in silico* techniques. Evidence on signalling and metabolic pathway(s) provides a basic understanding of the role of cellular proteins in the development of hypertension, allowing for the identification of potential treatment targets [6]. In the event that the target protein does not respond to treatment, an alternate target from a disease-related biochemical pathway(s) may be used to address the issue [7]. The dispersed nature of information important to biochemical pathways and linked proteins in literature and online biological databases makes mining the necessary data extremely difficult [8, 9]. Even when a researcher obtains relevant data for a specific target protein from multiple sources, it is done separately, which takes time to establish a perfect link.

2. MATERIALS AND METHODS

2.1. Data Acquisition

The hypertension related-data, including research articles and information related to genes, proteins, and drugs, *etc*., were manually collected from several resources available from primary databases, such as SwissProt [10], UniProtKB [11], and Ensembl genome browser [12]. For research articles, we used the Google Scholar search engine to find the most relevant articles matching our keywords. Further reviews and articles were filtered using a combination of keywords, including hypertension, RAAS pathway, protein, drug discovery, drug molecules, and anti-hypertensive treatment [13]. Finally, curated articles and information were obtained by excluding articles lacking relevant information and articles other than in the english language.

Open-source biological databases are critical for assisting life science researchers in gaining access to the most recent information derived from numerous distributed literature and databases in a concise and easily accessible manner. Changes in gene expression and its products (proteins) are universally acknowledged to cause dysfunction in biochemical pathways related to blood pressure regulation, drug metabolism, and homeostasis, among other factors, resulting in hypertension [14].

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PLANT TISSUE CULTURE

Meta-topolin enhances regeneration and *Agrobacterium*-mediated genetic transformation in radish (*Raphanus sativus* L.)

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Abstract

Meta-topolin (*m*T) is a novel aromatic cytokinin that stimulates morphogenesis and is an alternative source of cytokinins frequently employed in regeneration systems. Hence, the present research explored the prospect of *m*T for improving regeneration and genetic transformation efficiency. Cotyledonary node explants were cultured on optimum plant growth regulator medium incorporated with *m*T for enhanced shoot induction (93.6%, 2.0 mg l^{-1} BA and 0.9 mg l^{-1} *m*T), elongation (89.3%, 2.0 mg l^{-1} GA$_3$ and 0.9 mg l^{-1} *m*T), and rooting (90.3%, 0.9 mg l^{-1} IBA and 0.9 mg l^{-1} *m*T) respectively. The plant transformation study was carried out through *Agrobacterium*-mediated transformation using the pCAMBIA1301 vector containing the LB4404 strain for standardizing transformation strategies. Transformed shoots and rooting were determined in two stages using 10 and 6 mg l^{-1} hygromycin B for exterminating chimeric explants. After co-cultivation, explants were cultured at the optimal concentration of 0.9 mg l^{-1} *m*T, 2.0 mg l^{-1} BA, 2.0 mg l^{-1} GA$_3$, and 0.9 mg l^{-1} IBA for enhanced transformation efficiency (27.3%), corresponding to transformed regeneration without *m*T (18.6%) occurring with less efficiency. The existence of transgenes in the radish genome was ascertained by the GUS assay, PCR, RT-PCR, and qRT-PCR. Overall, our investigation demonstrated that including *m*T increases regeneration and enhances transformation efficiency in radish. Therefore, diverse radish varieties could use a designed transformation strategy to acquire essential traits.

Keywords *Raphanus sativus* · Cotyledonary node · *Meta*-topolin · pCAMBIA1301 · *Agrobacterium tumefaciens* · Hygromycin B

Introduction

Radish (*Raphanus sativus* L., $2n = 18$), associated with the Brassicaceae family (Gómez-Campo 1980), is an annual or biennial, commonly significant vegetable crop cultivated in tropical and temperate regions. It has been developed globally on 70,773 ha, predominantly cultivated in Japan, China, and Korea (Kurina *et al.* 2021). Each year, Japan produces 3.7 million tons of radish daikon and imports another 0.9 million tons from various countries. In contrast, China produced 1.2 million ha and occupied 6% of the cultivated area for vegetable crops (Kurina *et al.* 2021). It contains high levels of vitamin C (18%), potassium (5%), calcium (3%), iron (3%), and protein (1%) (USDA 2020). The significant edible portion of the juicy taproot in radish includes high nutritional content and health benefits (Yu *et al.* 2016; Pervitasari *et al.* 2022). Aside from the roots, the leaves and sprouts also have nutritious and therapeutic values (Takaya *et al.* 2003; Manivannan *et al.* 2019). Both round and extended radishes are consumed raw or pickled, preserved later, or boiled in various oriental cuisines (Park *et al.* 2005). It has a good source of antioxidants, including pyrogallol, vanillic acid, coumaric acid, catechin, and other phenolic compounds, which assist in preventing diabetes, neurological disorders, cancer, Parkinson's, and cardiovascular diseases (Manivannan *et al.* 2019).

Conventional breeding is vital for designing superior radish varieties. Nevertheless, breeding success rates are hindered by sexual incompatibility and difficulty finding viable progenies (Elayaraja *et al.* 2019). Furthermore,

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microorganisms

MDPI

Review

Microbial Volatile Organic Compounds: An Alternative for Chemical Fertilizers in Sustainable Agriculture Development

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Abstract: Microorganisms are exceptional at producing several volatile substances called microbial volatile organic compounds (mVOCs). The mVOCs allow the microorganism to communicate with other organisms via both inter and intracellular signaling pathways. Recent investigation has revealed that mVOCs are chemically very diverse and play vital roles in plant interactions and microbial communication. The mVOCs can also modify the plant's physiological and hormonal pathways to augment plant growth and production. Moreover, mVOCs have been affirmed for effective alleviation of stresses, and also act as an elicitor of plant immunity. Thus, mVOCs act as an effective alternative to various chemical fertilizers and pesticides. The present review summarizes the recent findings about mVOCs and their roles in inter and intra-kingdoms interactions. Prospects for improving soil fertility, food safety, and security are affirmed for mVOCs application for sustainable agriculture.

Keywords: food security; induced systemic resistance; microbial volatile organic compounds; soil fertility; sustainable agriculture

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1. Introduction

Microbial volatile organic compounds (mVOCs) are a type of volatile organic compound produced by microorganisms, especially bacteria and fungi, during their metabolism [1,2]. The mVOCs are designated as lipophilic compounds with a low boiling point, low molecular mass (an average of 300 Da), and high vapor pressure (0.01 kPa) [3,4]. These characteristics facilitate the evaporation and diffusion of mVOCs and their roles in plant growth and protection via pores in soil and rhizosphere environments. In addition, mVOCs act as an ideal signal/messenger molecule for mediating interactions at both short and long distances in microbes and plants [1–6]. The richness of mVOCs has been cataloged in the mVOCs 2.0 and 3.0 database [7,8]. Based on a literature survey, in 2014, the mVOCs 2.0 database comprised ~1000 volatiles emitted by 69 fungi and 349 bacteria [7], whereas, in 2018, the mVOCs 3.0 database contained 1860 unique mVOCs emitted from 604 bacterial and 340 fungal species [8]. Recent studies have also been strengthened based on their importance in food production, food safety, and eco-friendly, cost-effective, and sustainable approaches to help modern agriculture [1–9]. The mVOCs possess broad-spectrum bioactivities such as plant growth promotion [10], abiotic stress resistance [11–13], plant defense [14], insect-pest resistance [15], etc. There are various kinds of microbial interactions taking place belowground/aboveground such as bacteria–plant, fungi–plant, bacteria–bacteria, fungi–fungi, fungi–bacteria, bacteria–protists, and bacteria–fungi–plant interactions. Among microorganisms, *Bacillus subtilis* remain the principal microorganism in mVOCs production and characterization [16]. Other microorganisms include *Bacillus amyloliquefaciens* [13], *Pseudomonas fluorescens* [17], *Pseudomonas putida* [18,19], *Pseudomonas donghuensis* [20], *Streptomyces fimicarius* [21], *Trichoderma* sp. [11], etc. Thus, the mVOCs possess the potential efficacies for the replacement of chemical fertilizers and pesticides not only in field

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IN SILICO INVESTIGATION OF NATURAL PHYTOCONSTITUENTS OF *TERMINALIA CHEBULA* AGAINST COVID-19

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Abstract

Coronavirus Disease-2019 (COVID-19) caused by the SARS-CoV-2 type of virus has scrambled the entire world with its mortality rate. Since it is a global pandemic, US-FDA endorsed the use of broad-spectrum antiviral medicationremdesivir from Gilead Sciences for its treatment. Recently, Molnupiravir tablets from Merck company got approval from the Britain has attracted the scientific community to find newer agents for the treatment of COVID-19. One of the important validated targets for designing and developing a new drug against COVID-19 is the main protease of SARS-CoV-2. In parallel, the knowledge of traditional medicines has been re-evaluated and can be considered to identify novel and effective approaches for the treatment of COVID-19. In our study,

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ORIGINAL RESEARCH

Quercetin-induced apoptosis in HepG2 cells and identification of quercetin derivatives as potent inhibitors for Caspase-3 through computational methods

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Abstract

Quercetin is a bioflavonoid which possesses immune-enhancing activity, anti-inflammatory, antioxidant properties and considered effective against various cancers. In the present study, quercetin has been extracted from *Ocimum basilicum* and was used to evaluate its anticancer activity against human liver cancer cell lines (HepG2) by assessing cell viability (MTT) and variations in nuclear morphology (AO/EtBr dual staining) during apoptosis. Since Caspase-3 enables the activation of cascade which is responsible for apoptosis, their effects were also investigated using computational approaches like molecular docking, molecular dynamics, covalent docking, ADME prediction, DFT approaches, and pharmacophore modeling besides identifying the binding affinity, stability, drug likeliness properties of top-ranked compounds. Amount of quercetin extracted from *O. basilicum* leaves was found to be 0.82 mg with the retention time of 2.827 min. Quercetin showed dose-dependent anticancer activity against HepG2 cells with IC_{50} value 50 μg/mL due to apoptosis that could have been mediated by Caspase-3 activity. Computational analysis of quercetin inhibiting Caspase-3 showed better binding affinity of compounds ChEMBL_38464, ChEMBL_501025, and ChEMBL_525002 and no violations were observed in the Lipinski Rule of 5. The molecular dynamics simulation evidenced the presence of water molecule in the catalytic site stabilizes the complex. The DFT analysis also explored that the identified compounds have the least HOMO–LUMO gap. The identified compounds also exhibit the pharmacophoric features such as hydrogen bond acceptor, hydrogen bond donor, aromatic ring, and hydrophobic features. Moreover, the study indicates the importance of water molecule in the catalytic site which may suppress the growth of tumor cells which could assist in the selection of potential leads for further analysis against liver cancer.

Keywords Apoptosis · Caspase-3 · Quercetin · HepG2 cells · Molecular docking · Molecular dynamics · DFT analysis · Pharmacophore analysis · LigandScout

Introduction

The uncontrolled growth and rapid dissemination of the abnormal or atypical cells are referred as cancer. According to WHO statistics, cancer is the leading cause for death globally. The comprehensive understanding of the molecular pathways will assist in investigating novel cancer chemotherapeutic targets which in turn would offer new opportunities for the discovery and development of new potential drugs [1, 2]. Liver cancer is leading among various cancers, which registers approximately 8,00,000 cases per year globally and turned out as the second leading cause of cancer-related deaths [3, 4]. The liver cancer frequently affects people suffering from liver diseases such as chronic hepatitis B and hepatitis C [5]. With the aid of recent developments, surgery,

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Press Release

அழகப்பா பல்கலையில் நவ.,21 ல் பன்னாட்டு கருத்தரங்கு

காரைக்குடி, நவ.18– மருந்து வடிவமைப்பில் உயிரி தகவலியல், கம்ப்யூட்டர் உதவியின் சமீபத்திய போக்குகள் குறித்த தேசிய கருத்தரங்கு காரைக்குடி அழகப்பா பல்கலையில் நவ., 21 அன்று துவங்குகிறது. பல்கலை துணைவேந்தர் ஜி.ரவி தலைமை வகிக்கிறார்.

வேலுார் இன்ஸ்டிடியூட் ஆப் டெக்னாலஜி துணை தலைவர் சேகர் விஸ்வநாதன் துவக்க உரை ஆற்றுகிறார். டில்லி எய்ம்ஸ் மருத்துவமனை பேராசிரியர் டி.பி., சிங், திருவாரூர் மத்திய பல்கலை துணைவேந்தர் எம்.கிருஷ்ணன், திருச்சி பாரதிதாசன் பல்கலை முன்னாள் துணைவேந்தர் பி.மணிசங்கர், ஜப்பான் பல்கலை அப்ளைடு பயாலஜிகல் சயின்ஸ்' துறை தலைவர்அகியோஎபிஹரா பங்கேற்கின்றனர். கன்வீனர் ஜெயகாந்தன் கருத்தரங்கு ஏற்பாடுகளை செய்து வருகின்றார். நவ., 25 வரை தொடர்ந்து 5 நாட்கள் இக்கருத்தரங்கு நடைபெறும்.

தினகரன் 7/12

தாவர நோய்களை தடுத்தால் மனித நோய்களை தவிர்க்கலாம்

சர்வதேச கருத்தரங்கில் ஆராய்ச்சியாளர்கள் தகவல்

▸ காரைக்குடி அழகப்பா பல்கலைக்கழக உயிரி தகவலியல் துறை சார்பில் நடந்த சர்வதேச கருத்தரங்கில் துறைத்தலைவர் பேராசிரியர் ஜெயகாந்தன் பேசினார்.

காரைக்குடி, நவ. 29: தாவரங்களுக்கு வரும் நோய்களை தடுத்தால் மனிதர்களுக்கு வரும் பெரும்பாலான நோய்களை தடுக்க முடியும் என, காரைக்குடி அழகப்பா பல்கலைக்கழகத்தில் நடந்த சர்வதேச கருத்தரங்கில் தெரிவிக்கப்பட்டது.

சிவகங்கை மாவட்டம், காரைக்குடி அழகப்பா பல்கலைக்கழக உயிரி தகவலியல் துறை சார்பில் உயிரி தகவலியல் கட்டமைப்பு மற்றும் கணினி சார்பு மருந்து கண்டறிதலின் நவீன உத்திகள், வளர்ச்சிகள் குறித்த சர்வதேச கருத்தரங்கம் நேற்று நடந்தது. ஒருங்கிணைப்பாளர் பேராசிரியர் சஞ்சீவ்குமார் வரவேற்றார். துணைவேந்தர் பேராசிரியர் ஜி.ரவி தலைமை வகித்து துவக்கி வைத்தார்.

கருத்தரங்கு குறித்து உயிரி தகவலியல் துறை தலைவரும், கருத்தரங்கின் அமைப்பாளருமான பேராசிரியர் ஜெயகாந்தன் கூறியதாவது: இப்பல்கலைக்கழக உயிரி தகவலியல் துறை, சர்வதேச மற்றும் தேசிய அளவில் ஆய்வறிக்கைகளை சமர்ப்பித்து ரூ.16 கோடிக்கும் அதிகமான நிதி உதவிகளை பெற்றுள்ளது. சர்வதேச ஆராய்ச்சி கண்டுபிடிப்புகளை முன்னிலைப்படுத்தி இப்பல்கலைக்கழக உயிரி தகவலியல் துறை மருந்து கண்டுபிடிப்பு ஆராய்ச்சி மேற்கொண்டு வருகிறோம். இதில் உயிர்க்கொல்லியான கோவிட்க்கு எதிரான மருந்து கலவையை தாவர மருந்து சேர்மங்களில் இருந்து கண்டறிந்துள்ளோம். தவிர உயிருக்கு ஆபத்தான நோய்களுக்கு எதிரான புதிய சிகிச்சை முறைகளை அடையாளம் காண நம்பகமான கணக்கீட்டு கருவிகளை உருவாக்கி வருகிறோம்.

இக்கருத்தரங்கில் புதிய டிரக் மாடல் கண்டுபிடிப்புகள் குறித்து விவாதிக்கப்பட்டது. செயற்கை உரங்களை பயிர்களுக்கு அளவுக்கு அதிகமாக பயன்படுத்தும்போது, அவை தேவையான உரங்களை மட்டும் எடுத்துக் கொள்ளும். மீதம் உள்ள தேவையற்ற உரம் மண்ணில் தங்கிவிடும். இதனால் மண் கெட்டுப்போவதோடு மனித உடலுக்கும் பாதிப்பை ஏற்படுத்தும். எனவே எவ்வளவு தேவையோ அந்த அளவு மட்டுமே உரத்தை பயன்படுத்த வேண்டும். மனிதர்களுக்கு வரும் அனைத்து பாதிப்புகளும் தாவரங்களுக்கு வரும். தாவரங்களை தாக்கும் பாக்டீரியா, வைரஸ் வேர் மற்றும் இலைகளை தாக்கும். இதன் மூலம் மனிதர்களுக்கு பரவும். தாவரங்களுக்கு வரும் நோய்களை தடுத்தால் மனிதர்களுக்கு வரும் பெரும்பாலான நோய்களை தடுக்க முடியும் என ஆராய்ச்சியாளர்கள் கருத்தரங்கில் தெரிவித்துள்ளனர்.

இவ்வாறு கூறினார்.

அழகப்பா பல்கலையில்

சிறந்த ஆராய்ச்சியாளர்களுக்கு விருது

காரைக்குடி அழகப்பா பல்கலையில் சிறந்த ஆராய்ச்சியாளர்களுக்கு துணைவேந்தர் ஜி.ரவி விருதினை வழங்கினார்.

காரைக்குடி, டிச.4: காரைக்குடி அழகப்பா பல்கலைக்கழகத்தின் உயிரித் தகவலியல் துறையில் சமீபத்திய ஆய்வுகளை பயன்படுத்தி மருந்து கண்டுபிடிக்க உயிரி தகவலியல் துறை மற்றும் மருந்து கண்டுபிடிப்பு அமைப்பு (பிட்ஸ்) உருவாக்கப்பட்டது. இவ் அமைப்பு சார்பில் உலகம் முழுவதிலும் உள்ள சிறந்த ஆராய்ச்சியாளர்களுக்கு விருது வழங்கப்பட்டு வருகிறது. உயிரி தகவலியல் துறைத் தலைசர் மற்றும் பிட்ஸ் அமைப்பின் தலைவர் பேராசிரியர் ஜெயகாந்தன், செயலாளர் பேராசிரியர் சஞ்சீவ்குமார் சிங் ஆகியோர் இந்த ஆண்டுக்கான விருது வழங்கும் விழாவை நடத்தினர்.

இதில் பேராசிரியர் விஜயன் நினைவு விருதினை உத்திரபிரதேசம் அலிகார் பல்கலைக்கழக உயிரிதொழில் நுட்பவியல் துறை டாக்டர் ரிஸ்வான் ஹசனுக்கு அழகப்பா பல்கலைக்கழக துணைவேந்தர் பேராசிரியர் ஜி.ரவி வழங்கினார். வாழ்நாள் சாதனையாளர் விருதினை புதுடெல்லி எய்ம்ஸ் உயிரி இயற்பியல் துறை டாக்டர் புனித் கவுருக்கு விஐடி பல்கலைக்கழக துணைத் தலைவர் டாக்டர் சேகர் விஸ்வநாதன் வழங்கினார். பேராசிரியர் சீனிவாசன் நினைவு விருதினை ஆராய்ச்சியாளர் டாக்டர் கிருபாதேஷ்முக், குஜராத் பல்கலைக்கழக வேதியியல் துறை பேராசிரியர் ஹிதேஷ் டி பட்டேல் ஆகியோருக்கு மத்திய பல்கலைக்கழக துணைவேந்தர் கிருஷ்ணன் வழங்கினார். இளம் விஞ்ஞானி விருதினை வாரணாசி ஐஐடி உயிரி வேதியியல் துறை சார்ந்த டாக்டர் ஆதித்யகுமார் பதிக்கு, ஜப்பான் பல்கலைக்கழக பேராசிரியர் அகியோ எபிஹாரா வழங்கினார். சிறந்த ஆராய்ச்சி மாணவர் விருதினை புதுடெல்லி ஜமியா மில்லா இஸ்லாமிய பல்கலைக்கழக அடிப்படை அறிவியல் மையத்தை சேர்ந்த டாக்டர் தாஜ் முகமதுக்கு இந்திய மருத்துவ அறிவியல் நிறுவன பேராசிரியர் டி.பி.சிங் வழங்கினார். ஆட்சிக்குழு உறுப்பினர் டாக்டர் சுவாமிநாதன் உள்பட பலர் கலந்து கொண்டனர்.

அழகப்பா பல்கலை.யில் சர்வதேசக் கருத்தரங்கு

அழகப்பா பல்கலைக்கழகத்தில் உயிரி தகவலியல் துறை சார்பில் திங்கள்கிழமை நடைபெற்ற சர்வதேசக் கருத்தரங்கு தொடக்க விழாவில் விழா மலரை வெளியிட்ட துணைவேந்தர் க. ரவி.

காரைக்குடி, நவ.21: காரைக்குடி அழகப்பா பல்கலைக்கழகத்தில் உயிரி தகவலியல் கட்டமைப்பு, கணினி சார்பு மருந்து கண்டறிதலின் நவீன உத்திகள், வளர்ச்சிகள் குறித்த கருத்தரங்கம் திங்கள்கிழமை தொடங்கியது.

நவ. 25 வரை நடைபெறும் இக் கருத்தரங்கில், துணைவேந்தர் க. ரவி தலைமை வகித்துப் பேசினார். வேலூர் தொழில்நுட்ப நிறுவனத்தின்(விஐடி) துணைத்தலைவர் சேகர் விஸ்வநாதன் கருத்தரங்கை தொடக்கி வைத்தார்.

புதுதில்லி அனைத்து இந்திய மருத்துவ அறிவியல் நிறுவன பேராசிரியர் டி.பி. சிங், திருவாரூர் மத்தியப் பல்கலைக் கழக துணைவேந்தர் ஆ. கிருஷ்ணன், ஜப்பான் பல்கலைக்கழக பேராசிரியர் அகியோ எபிஹாரா, சென்னைப் பல்கலைக் கழக ஆராய்ச்சி முதன்மையர் டி. வேல்முருகன், அழகப்பா பல்கலைக் கழக ஆட்சிகுழு உறுப்பினர் ஆர். சுவாமிநாதன் ஆகியோர் பேசினர்.

முன்னதாக உயிரித்தகவலியல் துறைத் தலைவர் ஜெ. ஜெயகாந்தன் வரவேற்றுப் பேசியதாவது:

அழகப்பா பல்கலைக்கழக உயிரித் தகவலியல் துறை சர்வதேச அளவிலும், தேசிய அளவிலும் ஆய்வறிக்கைகளை சமர்ப்பித்து ரூ. 16 கோடிக்கும் அதிகமான நிதி உதவிகளை பெற்றுள்ளது. மேலும் 650-க்கும் மேற்பட்ட ஆய்வறிக்கைகளை வெளியிட்டு சர்வதேச கல்வி நிறுவனங்களுக்கு நிகராக விளங்குகிறது. இங்குள்ள உயிரி தகவலியல் துறை மருந்து கண்டுபிடிப்பில் தொடர்ந்து ஆராய்ச்சிகளை மேற்கொண்டுள்ளது.

உயிர்க் கொல்லிகளுக்கு (சார்ஸ் கோவிட்-2) எதிரான மருந்துக் கலவையை தாவர மருந்து சேர்மங்களிலிருந்து கண்டறியப்பட்டுள்ளது. மேலும், இத்துறையின் ஆராய்ச்சியாளர்கள் உயிருக்கு ஆபத்தான நோய்களுக்கு எதிரான புதிய சிகிச்சை முறைகளை அடையாளம் காண நம்பகமான கணக்கீட்டு கருவிகளை உருவாக்கி வருகின்றனர் என்றார். கருத்தரங்கின் ஒருங்கிணைப்பாளர் சஞ்சீவ்குமார் சிங் நன்றி கூறினார்.

தினகரன்

அறிவை, ஆராய்ச்சி உத்திகளை மேம்படுத்த

இளம் ஆராய்ச்சியாளர்கள் எதிர்கால ஆராய்ச்சிகள் குறித்து அறிய வேண்டும்

காரைக்குடி அழகப்பா பல்கலைக்கழக உயிரிதகவலியல் துறை சார்பில் நடந்த சர்வதேச கருத்தரங்கில் விழா மலரை துணைவேந்தர் ஜி.ரவி வெளியிட்டார்.

துணைவேந்தர் ஜி.ரவி பேச்சு

காரைக்குடி, நவ. 22: அறிவையும், ஆராய்ச்சி உத்திகளையும் மேம்படுத்த இளம் ஆராய்ச்சியாளர்கள் எதிர்கால ஆராய்ச்சிகள் குறித்து தெரிந்து கொள்ள வேண்டும் என துணைவேந்தர் ஜி.ரவி தெரிவித்துள்ளார்.

சிவகங்கை மாவட்டம், காரைக்குடி அழகப்பா பல்கலைக்கழக உயிரி தகவலியல் துறை சார்பில் கணினி சார்பு மருந்து கண்டறிதலின் நவீன உத்திகள், வளர்ச்சிகள், உயிரி தகவலியல் கட்டமைப்பு குறித்த 5 நாட்கள் சர்வதேச கருத்தரங்கின் துவக்கவிழா நடந்தது.

விழாவில் துணைவேந்தர் பேராசிரியர் ஜி.ரவி தலைமை வகித்து பேசியதாவது :

இப்பல்கலைக்கழகம் உலக அளவில் வியந்தகு வளர்ச்சியையும், சிறந்த அங்கீகாரத்தையும் பெற்றுள்ளது. இக் கருத்தரங்கில் சர்வதேச அளவில் 38 ஆராய்ச்சியாளர்கள், பேராசிரியர்கள் மற்றும் 200க்கும் மேற்பட்ட ஆராய்ச்சி மாணவர்கள் கலந்து கொண்டுள்ளனர். தகவலியல் துறை முதன்மை துறையாக விளங்குவதுடன், உள் கட்டமைப்பு, கற்பித்தல் மற்றும் ஆராய்ச்சி நிதியாக ரூ.3 கோடியே 50 லட்சம் உயிரி தொழில்நுட்பவியல், உயிரி தகவலியல் கணினி உயிரியல் துறையிடம் இருந்து பெற்றுள்ளது. இளம் ஆராய்ச்சியாளர்கள் அறிவையும், ஆராய்ச்சி உத்திகளையும் மற்றும் மேம்படுத்தப்பட்ட எதிர்கால ஆராய்ச்சி குறித்து தெரிந்து கொள்வது அவசியம். அதற்கு இதுபோன்ற கருத்தரங்குகள் நல்ல வாய்ப்பாக அமையும்.

இவ்வாறு பேசினார்.

மேலும் இந்த விழாவில் புதுடெல்லி அனைத்து இந்திய மருத்துவ அறிவியல் நிறுவன பேராசிரியர் டி.பிசிங், ஜப்பான் பல்கலைக்கழக பேராசிரியர் எபிஹாரா, சென்னை ஏஎம்இடி பல்கலைக்கழக ஆராய்ச்சி முதன்மையர் பேராசிரியர் வேல்முருகன், அழகப்பா பல்கலைக்கழக ஆட்சிக்குழு உறுப்பினர் முனைவர் சுவாமிநாதன் உள்பட பலர் கலந்து கொண்டனர்.

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., D.Sc.	Structural Biology and Bio-Computing
Dr. Sanjeev Kumar Singh Professor	M.Sc., Ph.D., D.Sc.	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

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	DBT-BIC	UGC	DST	CSIR	AURF	TNSCST	TANSCHEE	ICMR	DAE- BRNS	UGC-Innovative Program[#]	DST INDO-TAIWAN	MHRD-RUSA 2.0	DST-FIST Level-I	DST-PURSE Phase-II
296.90	183.8	96.11	160.75	36.16	08.08	01.89	49.965	54.59	30.33	54.00	73.72	173.35	62.00	09.40
										Total		1291.045		

[#] 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	
Orbito Asia Diagnostics, Coimbatore	2022-27
ICAR- National Research Centre for Banana	2022-*
N. Rama Varier Ayurveda Foundation (NRAF), Madurai	2019-*
Bishop Heber College (Autonomous), 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
Orbito Asia Diagnostics, Coimbatore	2022-27
ICAR-National Research Centre for Banana	2022-27

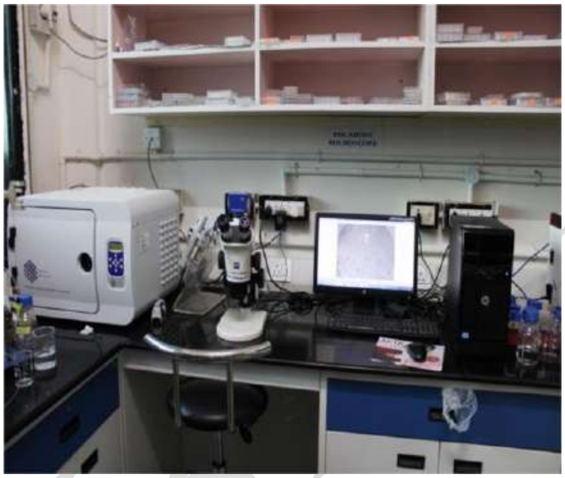
International	
National Synchrotron Radiation Research Center, Taiwan	2022-27
University of Manchester, Manchester, United Kingdom	2016-21
National Institute of Health, United States of America	2016-21
Institute of Experimental Medicine, Czech Republic	2016-21
School of Science, Osaka University, Japan	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
- DBT-BIC Centre
- DST-FIST Facilities
- UGC Innovative Facilities

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

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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)

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.

JOIN US

Web link : http://www.bidds.org/
Google form link: https://rb.gy/bxwed

1. Registration Fee for BIDDS Life membership for Faculties/PDF/ - INR. 3000/-.
2. Registration Fee for BIDDS 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.bidds@gmail.com
Ph: +91-4565-223342

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BIDDS REGISTRATION

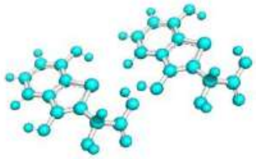
Membership Details

- **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/-
  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 1st 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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