E – Bioinformatics Magazine

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Issue: 9 June 2019 – May 2020

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 2019 – May 2020.

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

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Message From the Chief Editor



Dear all,

It is with immense delight that I write this editorial for the current issue of "e-Bioinformatics Magazine" (e-BIM). Our department was found in 2008, since then it has achieved exponential growth and stardom among the other departments of Alagappa University, Karaikudi as well as other institutions. The tireless efforts by the faculty members in research and teaching in various fields have paved way to attain greater heights. Our department is funded by several funding agencies like DST, DBT, CSIR, ICMR, UGC and TNSCST. It is also sponsored by UGC Innovative programme, DST-FIST and DST-PURSE. Our faculty members believe that teaching and research are like two eyes that look far into wider horizons with a view to broadening the frontiers of knowledge. Besides this, extension activities have become imperative today and the department cannot isolate themselves from this responsibility. It is these extension activities that carry the fruits of research and knowledge to the society at large. Research scholars and students have always been noteworthy in their contributions for our department e-BIM highlights various Departmental events, Invited talks by Eminent Scientists, Student activities, Publications, Achievements, Recognitions, Contributions, Conference related activities, etc., during academic year June 2019 – May 2020. It also highlights the yearly event of Three-Day International Conference on "Recent Trends in Structural Bioinformatics and Computer Aided Drug Design" (ICSBCADD - 2019) and the 3rd Annual Meeting of Bioinformatics and Drug Discovery Society [BIDDS] were inaugurated on 11th to 13th December 2019.

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. R. Santhosh)

DBI e-Magazine

Department Events

(June 2019 to May 2020)

MoU signed between Department of Bioinformatics, Alagappa University and N. Rama Varier Ayurveda Foundation, Madurai

Dr. Sanjeev Kumar Singh, Professor, Department of Bioinformatics has signed a MoU with N. Rama Varier Ayurveda Foundation (NRAF), Madurai on 24th June, 2019 in the presence of Prof. N. Rajendran, Vice- Chancellor, Alagappa University, Karaikudi, Tamil Nadu.



Memorandum of Understanding signed between Prof. Sanjeev Kumar Singh, Department of Bioinformatics and Ramesh R. Varrier, MD, N. Rama Varier Ayurveda Foundation (NRAF) in the presence of Vice Chancellor, Alagappa University, Karaikudi on 24th June, 2019.

International Conference

INTERNATIONAL CONFERENCE ON STRUCTURAL BIOINFORMATICS AND COMPUTER AIDED DRUG DESIGN - (ICSBCADD2019)

A Three-Day International Conference on "Recent Trends in Structural Bioinformatics and Computer Aided Drug Design" (ICSBCADD - 2019) and the 3rd Annual Meeting of Bioinformatics and Drug Discovery Society [BIDDS] were inaugurated on 11th December 2019 under the aegis of the Department of Bioinformatics, Alagappa University, Karaikudi. After conducting the National-level Symposium-cum-Workshop on SDCADD for 11 successive years, this is the first international conference to be organized by the Department. Presiding over the inaugural function, Prof. N. Rajendran, Vice-Chancellor, Alagappa University, enumerated the feats and milestones achieved by Alagappa University over the years and the current efforts of the University to take it to global standards. He referred to the achievements of university that raised its status to one among the top 10 State Universities in India. As a sequel Alagappa University was sanctioned a grant of Rs.100 crore by MHRD-RUSA for expansive infrastructure development and enhancing quality of teaching and research activities. He further stated that University h-index has risen to 74 owing to quality contribution of the Faculty and Research Scholars of Alagappa University. He stated that the MHRD-RUSA fund has enabled this University to create a conducive atmosphere for improving research and to sustain the research status already obtained. He said that ICSBCADD'2019 is a mega event with financial support from RUSA where 11 international and 22 Indian scholars of eminence in this field have gathered to give 33 plenary lectures. He also enlightened the gathering on the importance of cross and inter-disciplinary research and hoped that Bioinformatics and other disciplines together can fulfil this aspect that has been stressed in the New National Education Policy-2019.

Vice-Chancellor, Prof. N. Rajendran released the ICSBCADD'2019 Souvenir and delegates Prof. M. Krishnan, Prof. T. P. Singh, Dr. Gulshan Wadhwa, Prof. Gerhard Grüber, Prof. Chun-Jung Chen, Prof. Balázs Zoltán Gulyás, Prof. Seiki Kuramitsu, Prof. D. Velmurugan, Dr. R. Swaminathan and Prof. Narayanan Ramasubbu received the copies of the Souvenir. Dr. Gulshan Wadhwa, Director, DBT presented the first copy of the book titled "Current Trends in Bioinformatics: An insight" authored by him to Vice-Chancellor Prof. N. Rajendran.

Prof. M. Krishnan, Vice-Chancellor, Madurai Kamaraj University, Madurai, in his inaugural address, praised the rapid progress that the Department of Bioinformatics has achieved the last ten years. He enlightened the participants on the traditional knowledge that has been available in our culture for ages to cure life threatening diseases. He said that despite the publications in high standard journals we are still lacking to make our place at the global level. Quoting a simple example, he said that neem leaves can be used to kill the mosquito larvae thereby preventing the onset and progression of diseases associated with it. Also, he referred to vitellogenin a female specific protein which is responsible for receptor mediated endocytosis and this protein is often transferred from human to pest and hence a drug molecule has been identified in his lab that will suppress the interaction without affecting beneficial organisms and minimizing the environmental problems. He also suggested to identify the medicine from the source. Secondly, he made a reference to the prevalence of Cancer in India and to ensure specificity of anticancer drug delivering nanoparticles in therapeutic regimen to attain the full potential of drugs. Finally, he gave an overview of the ancient and traditional medicines available in Karaikudi where a small herb and medicinal plant can be used to control the disease. "Ayurvedic Informatics" introduced by the DBT and DST is the latest source helping young researchers. Also, he stressed the need for industry-academia collaboration for fruitful results. He also enlightened the crowd that the present research scenario requires young researchers to identify the fields and develop their skills for innovative findings that are beneficial to public.

Prof. T.P. Singh, SERB Distinguished Fellow, All India Institute of Medical Sciences, New Delhi, in his thematic address, stressed on the phase of incubation, creation of knowledge and the realization of speedy Drug Discovery Process. He also said that the future of Scientific Research belongs to modern era of Bioinformatics and the roles are changing where so much of data produced from the experimental sciences can be managed with the help of Bioinformatics tools and techniques to acquire maximum knowledge. He lauded Alagappa University for concentrating on science research and added that "great science happens in small Universities".

Dr. Glushan Wadhwa, Director, Department of Biotechnology, New Delhi delivered a speech on Innovative Research. He cited few examples to show how some innovations that were existing in ancient India had been modernized by the Westerners claiming them as their findings. He also said that Tamil Nadu is the only State with deep traditional knowledge and it needs to be explored. He also enlightened the gathering on the availability of the rural knowledge stored in the form of digital laboratory by the DST. He also mentioned about the spray discovered by DBT and patented by BCIL that will eat away mosquito larvae. He also motivated the faculty to keep the current continuing pace towards promoting Bioinformatics to the global level with innovative research.

Prof. Gerhard Grüber, Deputy Head, Division of Structural and Computational Biology, Nanyang Technological University, Singapore, delivered the keynote address. He stressed the importance of research networking and building research collaboration. Referring to the recent disease scenario in South-East Asian countries diseases like malaria, TB and dengue account for 46% and out of which 25% is reported in India. He also lauded the efforts of India to make this nation TB free by 2025. He also said that the senior scientists need to be transparent in sharing their knowledge thereby paving the way for creation of interdisciplinary research; and he welcomed the collaborative efforts of Alagappa University with NTU, Singapore and other universities.

Prof. Chun-Jung Chen, Deputy Director at National Synchrotron Radiation Research Centre, Taiwan, in his special address, highlighted the need for proper environment to carry out high level research and appreciated the development of the Department of Bioinformatics which has progressed to a great extent in short period of time. He also mentioned about the MoU existing between NSRRC and Alagappa University and at present three students from Prof. J. Jeyakanthan's lab are pursuing their research work in the area of Structural Biology and Protein Crystallography in combating malarial parasites. He also said that this International Conference will definitely pave the way for sharing of knowledge to the mutual advantage of the participants.

Prof. Balazs Zoltan Gulyas, Director, Centre for Neuroimaging Research, Nanyang Technological University, Singapore, in his speech said, truth and morality should be part and parcel of good science research and all such qualities need to be embedded in research institutes and this conference will provide the right platform to learn of new trends.

Prof. Seiki Kuramitsu, Honorary Emeritus Professor, Osaka University, Japan, while delivering the felicitation address, said that most of the biological problems can be solved through serious Bioinformatics approaches.

Prof. D. Velmurugan, Honorary Emeritus Professor, Former Head, CAS in Crystallography and Biophysics, University of Madras, Chennai and Dr. R. Swaminathan, Member of the Syndicate, Alagappa University, delivered felicitation address.

Thirty-two scientists from various prestigious institutions of international repute would be delivering lectures about the methodologies that play a major role in developing drugs, the importance of Bioinformatics tools in Health. 300 participants from across the country, are attending this three-day event.

Dr. J. Jeyakanthan, Professor and Head, Department of Bioinformatics while welcoming the gathering, referred to several issues confronting India and the immediate need to find solutions using computational sources. He emphasized on the various research findings where Researchers in Liverpool School of Tropical Medicine has recently identified that three genes (Cyp6m2, Cyp6p3 and Gste2) as markers for insecticide resistance in malaria-carrying mosquitoes. Another complication caused by Plasmodium falciparum called Cerebral malaria has been diagnosed by scientists. P. falciparum erythrocyte membrane protein 1 is produced by this bacterium on its surface which can bind to host cells lining the blood vessels in many organs, including the brain leading to cerebral malaria. According to a new study, Dengue virus replication was found to be due to the interaction between non-structural protein 1 (NS1) in virus and a novel uncharacterized viral protein NS4A-2K-NS4B. Characterizing this uncharacterized viral protein will help to suppress viral replication and severe disease manifestations. Dengue virus exists as smooth spherical surface particles while growing at the mosquito's physiological temperature (29°C). It then changes to bumpy surfaced particles at human physiological temperature (37°C). This ability to change their morphology helps the virus to attack the human immune system. Therefore, understanding this change in morphological characteristic of virus is important for drug and vaccine development. In another study, using the gene-editing tool CRISPR-Cas9, researchers identified the key molecule Mxra8 that facilitate the entry of chikungunya virus into host cells. Also, the persistent knee and joint pain or chronic arthritis after chikungunya viral infection in the acute and chronic stages of disease is due to the presence of persistent chikungunya virus RNA in infected host. These findings, along with future studies could help for better understanding the mode of infection of these microbes and in the development of drugs to treat diseases.

He also said that the global small molecule drug discovery market was valued at 29,363.85 million USD in 2018 and is estimated to be at 46,882.22 million USD in 2024, with a CAGR of 8.11%. The lead optimization is found to have largest market size and is expected to witness a Compound Annual Growth Rate (CAGR) of 7.93%. Based on the above considerations, the Department is mainly focusing on the applications of computing power to streamline drug discovery and drug development process that will facilitate to the discovery of novel leads against life-threatening diseases such as Cancer, Filariasis, Chikungunya, Malaria, Dengue, Diabetes, HIV, Zika, Cardiovascular disease etc.

Finally, a vote of thanks was delivered by Prof. Sanjeev Kumar Singh of the Department of Bioinformatics.



ICSBCADD 2019 – DELIGATES

ICSBCADD 2019 – PARTICIPANTS

Dr. RM. Vidhyavathi - Participation in International Conference on Engineering Medicine Science and Technology ESTIC 2019, Malaysia

Dr. RM. Vidhyavathi participated and presented her research findings in international conference on Engineering, Medicine, Science and Technology ESTIC 2019 organized by Faculty of Engineering & Information Technology, Mahsa University in Kuala Lumpur, Malaysia during 14th & 15th October 2019.



INTERNATIONAL PARTICIPANTS IN ESTIC 2019



The Department of Bioinformatics organized a seven-day **E-Learning Program on "BIOINFORMATICS AS CARTOGRAPHIC TOOL IN DRUG DISCOVERY - 2020"** between 19th to 30th May 2020 through Alagappa University Online Programme (ALUOP) portal which is hosted by Alagappa University to carry out online programmes. All the faculties of the Department delivered the lectures related to Drug Discovery Applications and about 851 participants all over India registered for the E-Learning Program.

Dr. J. Jeyakanthan, Professor and Head, convened this program and delivered the lecture on (i) "Accelerating Drug Discovery Using Integrative Structural Biology" followed by faculty members delivered their respective lectures which is as follows with (ii) Dr. Sanjeev Kumar Singh, Professor, enlightening on (ii) "Advancement in computational drug Discovery". (iii) Dr. M. Karthikeyan, Assistant Professor, emphasized his talk in (iii) "Computational Investigation on Cross-talking Cancer Signalling of Tankyrase, Ring Finger146 and Axin Complex". (iv) Dr. RM. Vidhyavathi, Assistant Professor, mainly focused her lecture on "Applications and Effects of Machine Learning in Drug Discovery". (v) & (vi) Dr. J. Joseph Sahayarayan, and Dr. P. Boomi, Assistant Professor(s), provided the audience with various dimensions of other disciplines in Drug Discovery in their lectures as mentioned "Role of Plant-based Medicinal Products in Drug Discovery" and "In silico Identification and Development of Novel Nano Drugs against Human Diseases" and finally the programme was concluded with (vii) Dr. V. K. Langeswaran delivering his lecture on "Computational Prediction and Identification of potent Drugs for Cancer". E-certificates are given to all the participants at the end of the E-learning program who actively participated in all the seven days programme.

Invited Talks/Address

Prof. Singh has given invited lecture on "Designing of Responsive agents using *In silico* Strategies: The way to Eradicate HIV Infections" in International conference on New Horizons in Biotechnology at Trivandrum, Kerala organized by The Biotech Research Society on 20th-24th November, 2019.



Dr. J. Jeyakanthan - Participation in 16th Conference of the Asian Crystallographic Association (AsCA 2019) held in National University of Singapore, Singapore

Dr. J. Jeyakanthan, Prof. & Head participated and presented his research findings on the topic "Structural studies on Aminoimidazole Ribonucleotide Synthase (AIRS) from *Pyrococcus horikoshii* OT3 (SG-ASCA1483)" on 19th December 2019 in 16th Conference of the Asian Crystallographic Association (AsCA 2019) organized by Department of Chemistry National University of Singapore, Singapore during 17th - 20th December 2019.



 Dr. P. Boomi, Assistant Professor, Department of Bioinformatics, Alagappa University, delivered an invited talk on 25.10.2019 at Zhengzhou International Convention & Exhibition Centre, Zhengzhou, Henan Provinces, China. He explained about the importance of Biomedical Applications using Nano bioinformatics. He has received the Young Visiting Researchers Award with cash price Rs. 25000/-, School of Biological Science and Food Engineering, Anyang Institute of Technology, China.



Dr. P. Boomi - Young Visiting Researchers Award with cash price Rs. 25000/-

- Dr. J. Jeyakanthan, Professor & Head, Department of Bioinformatics, Alagappa University, delivered an invited lecture on "Structural and Functional Characterization of Streptomycin adenyl transferases from *Serratia marcescens* FGI94" in the Webinar series organized by Science & Humanities, M. Kumarasamy College of Engineering, Thalavapalayam, Karur, Tamil Nadu on 15th May, 2020.
- Consecutively, Dr. J. Jeyakanthan, Professor & Head, Department of Bioinformatics, Alagappa University, delivered an invited lecture on "Accelerating Drug Discovery using Integrative Structural Biology" in the Webinar series organized by Department of Biotechnology, Karunya Institute of Technology and Sciences, Coimbatore on 29th May, 2020.

Editor in Journals

Dr. J. Jeyakanthan, Professor and Head, Department of Bioinformatics has been selected as the Editorial Board member in Current Bioinformatics Journal under Bentham Science Publishers and Academic Editor in PLOS ONE.

Key Publications

JOURNAL OF Article JOURNAL OF CHEMICAL INFORMATION AND MODELING Cite This: J. Chem. Inf. Model. 2020, 60, 175–191 pubs.acs.org/jcim

Insights into Exogenous Tryptophan-Mediated Allosteric Communication and Helical Transition of TRP Protein for Transcription Regulation

Richard Mariadasse, Sanjay Kumar Choubey, and Jeyaraman Jeyakanthan*®

Structural Biology and Bio-Computing Lab, Department of Bioinformatics, Science Block, Alagappa University, Karaikudi, 630 004 Tamil Nadu, India

Supporting Information

ABSTRACT: In this study, the binding recognition and allosteric mechanism of tryptophan-responsive regulatory protein (TRP)–DNA and bound exogenous tryptophan (Trp) amino acid complexes for transcriptional regulation were explained through the molecular docking, molecular dynamics (MD), free-energy landscape (FEL), binding free energy (molecular mechanics Poisson–Boltzmann surface area, MMPBSA), and protein structural network (PSN) analyses. The domain transition of helix–turn–helix (HTH) and effector binding domain (EBD) of TRP protein is the vital process for allosteric network communication, DNA recognition, and transcription. TRP protein consists of four putative active site pockets (Act1, Act2, Act3, and Act4) with the



binding specificity of exogenous Trp amino acid, which modulates the binding energy of TRP–DNA complexes by conferring the specific residual network and internal helical orientation of DNA-binding domain (DBD) for regulatory mechanism. In the TRP–DNA complex, interaction of Arg28 (helix-1) and Arg36 (helix-2) with the DNA molecule plays a vital role in DNA recognition. As a consequence, allosteric induction of exogenous Trp in the Act3 binding site retains the structural integrity and is quite comfortable with DNA major groove; therefore, it produces less binding energy for complex formation and may involve in oligomeric association for transcription regulation. Meanwhile, Trp in the Act1 binding site induces high helical orientation and fluctuations, leading to dissociation of DNA from the TRP protein. The remaining two complexes of Trp with Act2 and Act4 are predicted to partially affect the transcription mechanism. The present study aims to unravel the role of exogenous Trp amino acid in TRP protein for transcriptional regulatory mechanism.

■ INTRODUCTION

Archaea is unique in three different domains of life, and the archaeal transcriptional regulation significantly differs from the bacterial transcriptional regulation. The archaeal proteins are structurally homologous with human proteins that provide the basis for understanding the transcriptional regulatory mechanism in human. Feast/famine regulatory proteins (FFRP) are global family of the leucine-responsive regulatory (Lrp) protein, widely distributed in the two domains of life (Archaea and Bacteria), and it plays a major role in amino acid biosynthesis, transport, and metabolism by controlling more than 75 operons in *Escherichia coli*.^{1–5} Transcription regulation of FFRP proteins depends on the availability of exogenous amino acids present in the medium. The high level of exogenous amino acids in the medium binds with protein and modulates the geometry of DNA, thereby regulating the transcriptional mechanism. E. coli Lrp, a well-characterized family member of FFRP, which alters the metabolism from famine to feast in the presence of leucine amino acid-rich nutrient, is referred to as a feast/famine regulatory protein that controls 10% of gene expression.⁶⁻⁸ Subsequently, several exogenous amino acids bind with protein that regulates, either activate or repress, the transcription mechanism.⁵ The Lrs and Ptr2 proteins of the FFRP family may help to understand the molecular mechanism of transcriptional activation/repression.⁵ LrpA from *Pyrococcus furiosus* prevents the recruitment of RNA polymerase by blocking the transcriptional initiation site, whereas Lrs14 from *Saccharolobus soljataricus* inhibits the binding of TATA box binding protein (TBP) and transcription factor B (TFB) in the promoter to suppress DNA transcription.^{5,10,11} During transcriptional activation, Ptr2 from *Methanocaldococcus jannaschii* protein binds with TATA box of rubredoxin 2 gene, which consecutively recruits TBP to TATA box to enhance the transcriptional activity.^{5,12} Moreover, the typical monomer of Lrp proteins comprises two domains, namely, N-terminal heltx-turn-helix (HTH) domain and C-terminal α/β AsnC effector binding domain (EBD).^{5,15,16,11} domain the heliose connected by the loop that binds to the major groove of DNA molecule, and AsnC is an

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These authors contributed equally to the work.

Keywords: missing regions; polypeptides; X-ray diffraction; molecular replacement; electron density.



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MRPC (Missing Regions in Polypeptide Chains): a knowledgebase

Rajendran Santhosh,^{a,b} Namrata Bankoti,^b‡ Adgonda Malgonnavar Padmashri,^b‡ Daliah Michael,^b Jeyaraman Jeyakanthan^a* and Kanagaraj Sekar^b*

*Structural Biology and Bio-computing Laboratory, Department of Bioinformatics, Alagappa University, Karaikudi 630 004, India, and *Department of Computational and Data Sciences, Indian Institute of Science, Bangalore 560 012, India. *Correspondence e-mail: jjkanthan@gmail.com, sekar@iisc.ac.in

Missing regions in protein crystal structures are those regions that cannot be resolved, mainly owing to poor electron density (if the three-dimensional structure was solved using X-ray crystallography). These missing regions are known to have high B factors and could represent loops with a possibility of being part of an active site of the protein molecule. Thus, they are likely to provide valuable information and play a crucial role in the design of inhibitors and drugs and in protein structure analysis. In view of this, an online database, Missing Regions in Polypeptide Chains (MRPC), has been developed which provides information about the missing regions in protein structures available in the Protein Data Bank. In addition, the new database has an option for users to obtain the above data for non-homologous protein structures (25 and 90%). A user-friendly graphical interface with various options has been incorporated, with a provision to view the three-dimensional structure of the protein along with the missing regions using JSmol. The MRPC database is updated regularly (currently once every three months) and can be accessed freely at the URL http://cluster.physics.iisc.ac.in/mrpc.

1. Introduction

In the past few decades, as a result of advances in datacollection technology and various ambitious structural genomics initiatives, numerous macromolecular crystal structures have been X-ray analysed and deposited in the Protein Data Bank (PDB) (Berman et al., 2000; Balamurugan et al., 2007). The sequence and three-dimensional structure of a protein molecule contains crucial information defining its structure and function (Samaya Mohan et al., 2005; Balamurugan et al., 2005, 2006; Gopalakrishnan et al., 2007; Ravella et al., 2012). The primary sequence of a protein is determined by various known sequencing techniques and the three-dimensional structure is resolved by biophysical techniques such as X-ray crystallography, NMR etc. (Bernstein et al., 1977; Berman et al., 2000; Gopalakrishnan et al., 2008). X-ray crystallography has for many years been the paramount technique for determining the three-dimensional structure of proteins (Praveen et al., 2008; Berman et al., 2014). In X-ray crystallographic experiments, and thus in many of the three-dimensional structures deposited in the PDB, the loops and ends of the polypeptide chains and certain residues in the middle portion of the chain are not observed owing to poor electron density (Sumathi et al., 2006; Saravanan et al., 2010; Djinovic Carugo & Carugo, 2015; Gurusaran et al., 2016). Thus, these regions will not be available in the atomic coordinates file submitted to the PDB and they are referred to as 'missing regions'

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Constitutive Inflammatory Cytokine Storm: A Major Threat to Human Health

Krishna Kant Gupta,¹ Mohd. Aqueel Khan,² and Sanjeev Kumar Singh²

Immune cells secrete small protein molecules that aim for cell–cell communications. These small molecules are called cytokines. Targeting cancer cells with administration of bispecific antibodies and natural extracts results in elevated circulating levels of inflammatory cytokines, including interferon- γ and interleukin (IL)-6, which lead to cell toxicity. Sustained release of cytokines due to immunotherapy or hormonal issues causes various diseases. Novel T cell-engaging therapies and monoclonal antibodies cause cytokine release syndrome. Efforts are being carried out to maximize the chance for therapeutic benefit from immunotherapy while minimizing the risk for life-threatening complications of sustained cytokines. The phenomenon is called cytokine storm. Cytokines can act antagonistically or synergistically. Constitutive expression of proinflammatory cytokines such as IL-3 and IL-6 causes organ damage and unbearable pain. In this review, we will discuss the regulators of cytokine release, its types, its implications on human health, and treatment.

Keywords: antibodies, B-cell, T-cell, cytokines, neurodegeneration, cardiac, toxicity

Introduction

MMUNOTHERAPY FOR CANCER is a landmark treatment, but sustained inflammatory cytokine release after treatment causes adverse effects on patient health. The massive release of inflammatory cytokines due to immune cell hyperactivation leads to multiple organ dysfunction syndrome (Fig. 1). The adrenaline hormone was found to fuel the expression of inflammatory cytokines. Inhibition of tyrosine hydroxylase (an enzyme important for production of adrenaline) with metvrosine reduced inflammation (Riddel 2018). Atrial natriuretic peptide was reported to reduce cytokinemediated inflammation (Staedtke and others 2018). Protein (antibody) (Pihusch and others 2002) and nonprotein-based cancer drugs (Tonini and others 2002) caused the release of inflammatory cytokines. Viral infections such as influenza lead to massive stimulation of T cells that result in the cytokine storm (Tisoncik and others 2012).

There are so many symptoms (from mild to severe) that signify the massive cytokine release: fever, fatigue, headache, rash, arthralgia, and myalgia. Severe cases have elevated creatinine, disturbed coagulation, changed expression level of liver enzymes, circulatory shock, vascular leakage, disseminated intravascular coagulation, and multiorgan system failure (Shimabukuro-Vornhagen and others 2018). This review will focus on the inflammatory cytokine storm and its implications on human health.

Cytokines

Cytokines are small protein molecules (<60kDa) that mediate messages among cells, especially immune cells. Cytokines are produced by many cell populations. The helper T cells (Th) and macrophages are the predominant ones. Cytokines are of different types: lymphokines (cytokines produced by lymphocytes), monokines (cytokines produced by monocytes), chemokines (cytokines with chemotactic activities), and interleukins (ILs) (cytokines that are made by one leukocyte, but act on different leukocytes). These cytokines have very high affinity for their receptors (Ramesh and others 2013). Therefore, they produce a biological effect at picomolar concentrations. Cytokines have a pleiotropic effect, that is, the same cytokine acts on different cell types. On the other hand, different cell types secrete the same cytokines. Similar functions are exhibited by different cytokines. Cytokines act synergistically or antagonistically (Coondoo 2011). The summary of important cytokine functions is presented in Table 1.

¹School of Chemical and Biotechnology, Sastra University, Thanjavur, India.
²Department of Bioinformatics, Alagappa University, Karaikudi, India.





Article

Bacillus subtilis CBR05 for Tomato (*Solanum lycopersicum***) Fruits in South Korea as a Novel Plant Probiotic Bacterium (PPB): Implications from Total Phenolics, Flavonoids, and Carotenoids Content for Fruit Quality**

Murugesan Chandrasekaran ¹⁽⁰⁾, Se Chul Chun ²⁽⁰⁾, Jae Wook Oh ^{3,*}⁽⁰⁾, Maniyannan Paramasiyan ⁴, Ramesh Kumar Saini ⁵⁽⁰⁾ and Jesudoss Joseph Sahayarayan ⁶

- Department of Food Science and Biotechnology, Sejong University, Gwangjin-gu, Seoul 05006, Korea; chandrubdubio@gmail.com
- ² Department of Environmental Health Science, Konkuk University, Gwangjin-gu, Seoul 05029, Korea; scchun@konkuk.ac.kr
- ³ Department of Stem Cell and Regenerative Biotechnology, Konkuk University, Gwangjin-gu, Seoul 05029, Korea
- ⁴ Department of Microbiology, Bharathidasan University, Tiruchirappalli 620024, India; manivannan3065@gmail.com
- ⁵ Department of Crop Science, Konkuk University, Gwangjin-gu, Seoul 05029, Korea; saini_1997@yahoo.com
 ⁶ Department of Bioinformatics, Alagappa University, Karaikudi 630 003, India;
- jjsrbioinformatics2016@gmail.com
- * Correspondence: ohjw@konkuk.ac.kr

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MDPI

Abstract: Plant growth-promoting rhizobacteria (PGPR) are naturally occurring soil biota which benefit plants by improving plant productivity and immunity. The aim of the present work was to evaluate the effect of the inoculation of PGPR strain, *Bacillus subtilis* CBR05 on the quality of tomato fruits produced under greenhouse conditions. Results were compared with mock-inoculated control and market sample. We found a significant increase in total phenol and flavonoid contents of tomato fruits in PGPR strain *B. subtilis* CBR05 inoculated plants compared to those of mock-inoculated control and market sample. Moreover, *B. subtilis* CBR05 inoculation stimulated antioxidant activities and levels of carotenoid (β carotene and lycopene) content in plants. In addition, the inoculation of the strain *B. subtilis* CBR05 produced the highest content of lycopene (21.08 µg/g FW) in tomato fruits as compared to mock-inoculated plants. Our results show that the PGPR strain *B. subtilis* CBR05 is a versatile soil bacterium that enhances tomato production by elevating antioxidant activities and carotenoid (β carotene and lycopene) levels in fruit.

Keywords: Bacillus subtilis; tomato; antioxidant activity; carotenoids; probiotics; PGPR

1. Introduction

Tomato (*Solanum lycopersicum*) is regarded as the second most vegetable crop next to potato in the agricultural implications of human consumption. According to agricultural statistics, tomatoes along with sweet corn and snap beans constitute 93% of crop production and processing strategies (Agricultural Statistics, United States Department of Agriculture (USDA), 2016). The positive benefits of tomato consumption have been rigorously proved against a variety of diseases like chronic degenerative diseases, owing to the escalated content of significant phytochemicals with potent health benefits,

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www.mdpi.com/journal/agronomy

ORIGINAL PAPER



A Novel Design and Fabrication of Ascorbic Acid Sensitive Biosensor Based on Combination of HAP/rGO/AuNPs Composite and Ascorbate Oxidase

Chenyu Zhao¹ • Junfeng Jiao² • Wencui Zhou¹ • Yong Zhang¹ • Han Liu¹ • Xiaogang Yang¹ • Boomi Pandi³ • Yurong Cai¹

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Abstract

In this study, a new HAP/rGO/AuNPs-AO modified carbon electrode (GCE) was fabricated for amperometric detection of ascorbic acid. The HAP/rGO/AuNPs composite was prepared by one-step hydrothermal method. The large specific surface area, strong adsorption and excellent biocompatibility of HAP nanowires enabled fast, stable and accurate detection of ascorbic acid. As array of quantum dot, AuNPs had strong electrocatalytic activity in addition to good adsorption to enzymes, which could provide high sensitivity and low limit of detection for biosensor. Then rGO ensured that current signal could be quickly transferred from the composite to electrode. Under the optimum conditions, the prepared biosensor demonstrated a wide linear range from 0.39 to 36 mM ($R^2 = 0.99845$), a low limit of detection (3.39 μ M, S/N = 3) and a high sensitivity (15.949 mA moL⁻¹) with good selectivity, stability (10.8%) and repeatability (3.9%), which might providing a reasonable and reliable way for ascorbic acid detection.

Keywords Ascorbic acid · Hydroxyapatite · Reduced graphene-oxide · Gold nanoparticle

Introduction

The ascorbic acid, also known as vitamin C, which produced by the normal metabolism of organisms and exists in most lives [1]. The concentration of ascorbic acid is kept within an appropriate concentration range in the human

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Yurong Cai caiyr@zstu.edu.cn

- ¹ The Key Laboratory of Advanced Textile Materials and Manufacturing Technology of Ministry of Education, National Engineering Lab for Textile Fiber Materials and Processing Technology, School of Materials Science and Engineering, Zhejiang Sci-Tech University, Hangzhou 310018, China
- ² College of Foreign Languages, Zhejiang Sci-Tech University, Hangzhou 310018, China
- ³ Department of Bioinformatics, Alagappa University, Karaikudi, Tamilnadu 630003, India

body [2]. If the ascorbic acid concentration is not within the normal range, it will lead to the development of some human diseases [3, 4], and the most common disease is the scurvy caused by the deficiency of ascorbic acid [5].

At present, the frequently used methods for ascorbic acid detection include colorimetry [6], chemiluminescence [7, 8] and high-performance liquid chromatography (HPLC) [9–11], etc., but there are still some deficiencies in these methods, such as spectrophotometry is susceptible to external interference, and chromatography equipment is expensive with complicated operation. With the development of sensor technology, enzyme-based biosensor has been a satisfactory method due to its simple operation, rapid analysis, high sensitivity and great specificity [12]. Nevertheless, up to now, the key problem still remains how to achieve stable immobilization of enzymes.

As of now, a great variety of methods are used for the immobilization of enzymes, including covalent crosslinking [13, 14], adsorption [15, 16], embedding [17], etc., among these, adsorption has become one of the research hot spots due to its simple operation and negligible effect on the activity of enzymes [18]. As we all know, hydroxyapatite (HAP) is the main inorganic component of natural

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Students Page

Mr. D. Prabhu, Research Scholar participated and presented his research findings in the 16th Conference of Asian Crystallographic Association (AsCA-2019) organized by Department of Chemistry, National University of Singapore, Singapore during 17th - 20th December 2019.



D. Prabhu - 16th Conference of the Asian Crystallographic Association (AsCA 2019) held in National University of Singapore, Singapore

Visit to NSRCC, Taiwan under DST-INDO-TAIWAN Research Collaboration

Three Research Scholars Mr. R. Guru Raj Rao, Ms. M. Amala and Ms. P. Saritha are pursuing Ph.D under the guidance of Prof. J. Jeyakanthan, in the Department of Bioinformatics and the opportunity is given to carry out their research work for a term of one year (01.08.2019 to 28.08.2020) through student exchange program at National Synchrotron Radiation Research Centre (NSRRC), Taiwan under the direction of Prof. C.J. Chen, Deputy Director, NSRRC and Joint Professor, Institute of Biotechnology, National Cheng Kung University, on the basis of Memorandum-of-Understanding (MoU) between Alagappa University, Karaikudi, India and National Synchrotron Radiation Research Centre, Taiwan. During their stay at NSRRC, they have performed various experiments in the field of Protein Crystallography including, Expression, Purification, Crystallization of proteins with clinical significance. Also, they have been trained to handle the Synchrotron beamlines for structure determination of the proteins that plays crucial role in controlling filariasis disease and enzymes involved in cancer pathways which could be useful to design drug against those vital targets.

GLIMPSES OF NSRRC, TAIWAN ALONG WITH PROF. C.J. CHEN & HIS TEAM







Press Release

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DINAKARAN - 17.03.2020

கொரோனா தாக்காமல் இருக்க

வரையறுக்கப்பட்ட உணவுகளை மட்டுமே உண்ணவேண்டும் அழகப்பா பல்கலை உயிரி தகவல் தோழில்நட்பலியல் துறை தலைவர் தகவல்

தப்படைய செட ஸ்.பா இக்கப்பட் ரிட மிரைக

வில்லை. இதன் ர சுகா தார தடை முறை களை தோம்ம பின்பற்றுவதன் மூலமும், இருமும் நின்ம பொதும், துல்மும் போதும்ம ரத்துவ என்றார்

DINAMALAR - 06.06.2020



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)

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

Faculty Members

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), N	Madurai	2019-*			
Bishop Heber College (Autonomous), Tiruchirap	opalli	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	2017-20				
University of Manchester, Manchester, United K	2016-21				
National Institute of Health, United States of Am	2016-21				
Institute of Experimental Medicine, Czech Repu	2016-21				
School of Science, Osaka University, Japan	2010-15				
RIKEN, Kanagawa, Japan	2010-15				
Institute of Protein Research, Osaka University,	2010-15				
Bio-Metal Science Lab, RIKEN, Harima Institut	2010-15				
National Collaboration					
Anna University, Tiruchirappalli					
Bharathidasan University, Tiruchirappalli	versity, Kanpur				
CSIR - Central Drug Research Institute,	hemical Research				
Lucknow					

CSIR - Centre for Cellular and Molecular	CSIR-National Chemical Laboratory Pune
Biology, Hyderabad	Contentational Chemical Laboratory, 1 une
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 TM 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 •











Contact Us Dr. J. JEYAKANTHAN Professor and Head Department of Bioinformatics 4th Floor, Science Campus, Alagappa University, Karaikudi - 630 004 Phone : +91 - 4565-230725 Fax : +91 - 4565-225202 Email : bioinfoau@gmail.com Web : www.alagappauniversity.ac.in, www.bioinfoau.org

ALAGAPPA UNIVERSITY PLACEMENT CELL

Alagappa University, Karaikudi 630 003

1.1 Details required the preparation of department profile for the Academic Year 2019-20

CORE COMPETENCY

Department of Bioinformatics focuses 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 development of novel and potent therapeutics. The generated data are compiled, stored and maintained in the form of user-friendly databases to make it resourceful and easily accessible for global Scientific Community. Moreover, Department of Bioinformatics will shortly be blooming as pioneered and Established Department since DBT-BIC and NNP will be incepted in the department to cater the needs of students, Researchers, Scientific Community and Society (NATION WIDE) in the field of Modern Biology. The Department will provide an extensive support to the intra and inter-institutional students (especially with rural background) and faculties to utilize the computational facility for updating themselves with recent innovations in Bioinformatics and Computational Biology. Moreover, the industry-academia collaboration brought about in the Centre will certainly enhance the training opportunities for the students, research scholars and faculty members. Apart from the training, the Centre will also refine and hone the identified leads to next phase of clinical evaluations leading to product-oriented outcomes in the form of Patents and application-oriented outcome resonating Research publications in esteemed journals.

HALLMARKS

- ★ 69 Research articles are published in scientific journals of high repute.
- \star Faculties are members in the editorial boards of several national and international journals.
- ★ 2 Book Chapters are accepted by the international publishers namely Bentham Science and Springer Nature.
- ★ Two of the faculties have provided invited lectures and hands-on-training to various universities.
- ★ Ongoing Projects include DAE-BRNS (during 2018-2021), DST INDO-TAIWAN (2018-2022), MHRD-SPARC IIT-Mandi (2019-2021) and ICMR (2019-2022).
- ★ Four of the Faculties have participated and presented their research in international conferences at Singapore, Dubai and Malaysia.
- \star The department is supported by the
 - 1. University Grants Commission (UGC) under the scheme of Innovative Programme - Teaching & Research in Interdisciplinary and Emerging Areas
 - 2. the Department of Science & Technology (DST)
 - 3. Fund for Improvement of S&T Infrastructure in Higher Educational Institutions (FIST) and Promotion of University Research And Scientific Excellence

Collaborative research work with the following leading Institutions:

- > DST INDO-TAIWAN collaborative research project, Taiwan.
- > DAE-BRNS, MHRD-SPARC, ICMR.
- > Nanyang Technological University, Singapore
- University of Manchester, U.K National Institute of Health, USA and Institute of Experimental Medicine, Czech Republic
- IISc Bangalore, University of Madras, Chhatrapati Shivaji Maharaj University, Kanpur, CSIR-NCL, Pune, CSIR-CDRI, Lucknow, CSIR-CECRI, Karaikudi.
- > IIT Madras, Guwahati, Delhi and Mandi.
 - DEEDS & DEVELOPMENTS
- Organized a Three-Day First International Conference on "Recent Trends in Structural Bioinformatics and Computer Aided Drug Design" (ICSBCADD - 2019) to provide a global platform for thought-provoking deliberations with renowned experts in various fields.
- Conducted 3rd Annual Meet of Bioinformatics and Drug Discovery Society [BIDDS]
- 300 delegates have participated in ICSBCADD'2019 that served as one umbrella displaying recent break throughs and significant developments.
- E-Learning Program on "BIOINFORMATICS AS CARTOGRAPHIC TOOL IN DRUG DISCOVERY - 2020" was organized from 19th to 30th May 2020 through Alagappa University Online Programme (ALUOP) portal.
- Faculties delivered the lectures related to Drug Discovery Applications and about 851 participants across the country have registered for the E-Learning Program.

AWARDS & ACHIEVEMENTS

Faculty achievements/awards:

- MoU was signed between Department of Bioinformatics, Alagappa University and N. Rama Varier Ayurveda Foundation, Madurai.
- A Faculty have received Young Visiting Research Award from School of
 Biological and Food Engineering, Anyang Institute of Technology, Henan province, China.

Students/Research scholar:

- **4** Alumni students were placed in reputed universities (**SPDF**, **NPDF**, **PDF**, **Research Associate**)
- + Three research scholars were selected for student Exchange Program at National
- **4** Synchrotron Radiation Research Centre (NSRRC), Taiwan.
- Research Scholar participated and presented his research findings in the 16th Conference of Asian Crystallographic Association (AsCA-2019) organized by Department of Chemistry, National University of Singapore.
- **4** Research Scholars have won best Poster Presentation Award in various International Conferences.
- About 09 Research Scholars have received meritorious fellowship from Govt. of .India and renowned funding agencies including International Travel grant.





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

📩 WHO WE SERVE

Students

• Academicians • Scientists • Research Scholars • Industrialists



- Conference's
- Symposium & Workshop
- Awards



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 : <u>http://www.bidds.org/</u>

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
Accountname	: Bioinformatics and Drug Discovery Society
Account number	[:] 36993002251
IFSC Code	: 58IN0000855
	Scan & Register

President

Prof. D. Velmurugan, SRMIST, Chennai

Secretary General Prof. Sanjeev Kumar Singh

Email: secretary.bidds@qmail.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 1 st Street, Sekkalai Karaikudi-630002, Tamil Nadu
Account name	:	Bioinformatics and Drug Discovery Society
Account number	:	36993002251
IFSC Code	:	SBIN0000855
CIF	:	89869362836





• Demand Draft Details:

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



Contact Prof. Sanjeev Kumar Singh Secretary General - BIDDS Department of Bioinformatics Science Campus, Alagappa University Karaikudi - 630004 Tamil Nadu, India. Phone: +91-04565-223342 Email: secretary.bidds@gmail.com Web link: http://www.bidds.org