



E – Bioinformatics Magazine

B

I

M



Issue: 8

June 2018 – May 2019

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 the Academic Year June, 2018 to May, 2019.

This magazine is free of charge to all alumni of DBI, as well as to faculty members, staffs, research scholars and students.

The contents of this magazine © June 2018 to May 2019 by the Department of Bioinformatics, Alagappa University.

DBI – BIM

EDITOR IN CHIEF

Mr. D. Prabhu

EDITORS

Mr. R. Santhosh

Mr. Guru Raj Rao

Mr. M. Richard

EDITORIAL BOARD

Ms. Jayashree Biswal
Mr. Vijaya Prabhu
Mr. Lakshmanan K
Mr. Umesh Panwar
Ms. Prajisha. J
Mr. John Marshal. J
Ms. Aarthi. M
Mr. Ishwar Chandra
Ms. Chirasmitha Nayak
Mr. Raghu. R

Mr. Anuraj N. S
Mr. Veerapandiyan. M
Mohamed Aqueel Khan
Ms. Chirasmitha Nayak
Mr. Raghu. R
Ms. Saritha P
Ms. Amala M

TECHNICAL SUPPORT

Ms. Abhirami R	Ms. Sangavi P
Ms. Indhumathi T	Ms. Soundarya S
Ms. Kavya K	Ms. Swathi M
Ms. Kohila G	
Ms. Komatha Malarvizhi	
Ms. Muthumanickam S	
Ms. Muthuselvi S	
Ms. Rathidevi M	

ADVISORY COMMITTEE

Dr. J. Jeyakanthan
Professor & Head



Dr. Sanjeev Kumar Singh
Professor



Dr. M. Karthikeyan
Assistant Professor



Dr. RM. Vidhyavathi
Assistant Professor



Dr. J. Joseph Sahayarayan
Assistant Professor



Dr. P. Boomi
Assistant Professor



Dr. V. K. Langeswaran
Assistant Professor



Content	Pg. No.
Message From the Chief Editor	6
Department Events	7
Achievements, Awards and Recognition	15
Research Projects, Grants, Fellowships	16
Invited Talks/Address/Seminars/Conference	21
Recent and Key Publications	25
Students Page	29
Press Release	34
Department Profile	35
Placement	40
BIDDS Brochure	44

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 2018 to May 2019. It also highlights the yearly event of **11th National Symposium cum Workshop on “Recent Trends in Structural Bioinformatics and Computer Aided Drug Design” (SBCADD’2019) and 2nd Annual Meeting of Bioinformatics and Drug Discovery Society [BIDDS]**, which was held during 12th to 14th February, 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. D. Prabhu)

Department Events

(June 2018 to May 2019)

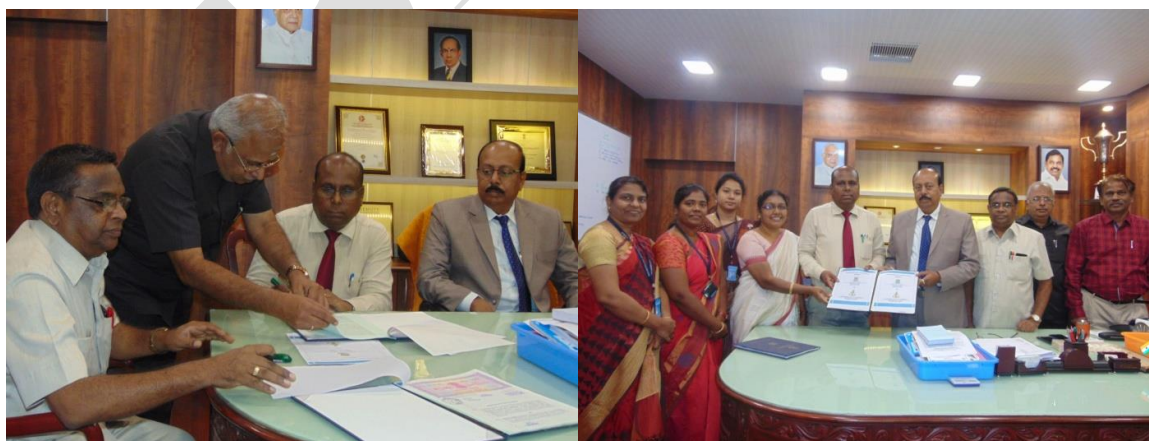
Nomination as the Finance Committee Member

Dr. J. Jeyakanthan, Professor and Head, Department of Bioinformatics has been nominated as the Finance Committee Member of Alagappa University on 03rd August, 2018.

MoU between Alagappa University and Bishop Heber College (Autonomous), Tiruchirappalli

Alagappa University (ALU) has signed the Memorandum of Understanding (MoU) with Bishop Heber College (Autonomous), Tiruchirappalli (BHC) for the term of five years. The MoU fosters to propagate Joint Research & Development, Project work/Internship/Summer Project, Joint Symposia/Conferences/Workshops/Short-term Refresher courses, short and long-term developmental programs, Faculty exchange for guest lectures and extending access to other facilities.

Alagappa University signed the MoU with Dr. D. Paul Dhayabaran, Principal, Bishop Heber College, Tiruchirappalli. The MoU will be effective for five years from 29th August, 2018. Through this MoU, the framework for a mutually beneficial collaboration between BHC and ALU will be facilitated to learn and enhance their professional expertise in Bioinformatics and Biotechnology based Research.



Dr. D. Paul Dhayabaran, Principal, Bishop Heber College, Tiruchirappalli, **Prof. N. Rajendran**, Hon'ble Vice-Chancellor of Alagappa University, **Prof. H. Gurumallesh Prabu**, Registrar, **Prof. V. Balachandran**, Special Officer (Planning and Development) and **Dr. J.**

Jeyakanthan, Professor and Head, Department of Bioinformatics during the MoU signing between ALU and BHC on 29th August, 2018.

Teacher's Day Celebration

The students and scholars of the Department of Bioinformatics organized the Teacher's Day Celebration for the faculty members. The faculty members were appreciated and the students expressed their gratitude for making the person they are today. The day was loaded with flashes of laughter and joyous moments.



Faculty members and Teaching Assistants on the occasion of Teacher's Day Celebration at the Department of Bioinformatics on 05th September, 2018.



**Swachh Bharat organized at Ariyakudi during 15th, September to 02nd October, 2018.
(Rally-25th Sep. 2018)**

Pooja Celebrations at the Department of Bioinformatics on 17th October, 2018.





Pongal Celebrations on 14th January, 2019

National Symposium

Title: National Symposium “11th National Symposium cum Workshop on “Recent Trends in Structural Bioinformatics and Computer Aided Drug Design” (SBCADD’2019) and 2nd Annual Meeting of Bioinformatics and Drug Discovery Society [BIDDS] (12th -14th February, 2019)”



SBCADD’2019 Souvenir Release by the Hon’ble Vice-Chancellor and Esteemed Scientists



Participants at the SBCADD’2019

The 11th National Symposium cum Workshop on “Recent Trends in Structural Bioinformatics and Computer Aided Drug Design” (SBCADD’2019) and 2nd Annual Meeting of Bioinformatics and Drug Discovery Society [BIDDS] was organized by the Department of Bioinformatics, Alagappa University on 12th February 2018 for the eleventh consecutive time.

Presiding over the inaugural function, Prof. N. Rajendran, Vice-Chancellor, Alagappa University, welcomed the esteemed dignitaries and participants to the SBCADD'2019. Emphasizing on the important aspects of exemplary growth, the University has achieved over the years and its unfathomable recognition at the global level. Furthermore, the University has been linked in the form of collaborations with the top most ranking global Universities. Furthermore, he lauded the Department of Bioinformatics faculty members for their immeasurable contributions towards universities achievements such as NAAC "A+" Accreditation, NIRF Ranking and in the grant of Rs.100 crore by MHRD-RUSA 2.0. In addition, he quoted the importance of Biosciences towards transforming lives towards finding immediate therapeutics from nature breakthroughs. Concluding his speech, he welcomed the delegates abroad and wishing them a proverbial Karaikudi hospitality.

Prof. T.P Singh, INSA- Senior Scientist, All India Institute of Medical Sciences, New Delhi in his inaugural address appreciated the former Vice-Chancellors who were inspirational in the creation of visionary "Department of Bioinformatics". Furthermore, he exclaimed the background behind the materialization of vision of BIDDs focusing to promote and encourage Bioinformatics and Drug Discovery from the bottom-up approach which will have its headquarters at Karaikudi that will serve the purpose of familiarizing the place among the scientific community. He also added that India has been an enriched source of human resource and technologies. Finally, he concluded his speech by praising the Organizing Secretary and others. In addition, he appreciated the Vice-Chancellor for his efforts, hard work and never-ending attitude for bringing the University to zenith heights.

Prof. Pinakpani Chakrabarti, Bose Institute Kolkata in his keynote address enlightened the gathering about the Origin of Bioinformatics way back at 1952 where the theoretical prediction of biological molecules was predominant among the scientists which fetched them the coveted Nobel prizes for instance Watson & Crick for the structure determination of DNA, Venkatraman Ramakrishnan for the studies and function of ribosome and most important it's the crystallographers who get away with the Nobel prize. Furthermore, with the aid of Computational Chemistry and Drug Discovery efforts to identify and discover potent drugs against influenza and HIV has been feasible through computational and subsequent validation which is crucial to realize the hypothesis made by the theoretical scientists. Furthermore, he laid emphasis on three words of wisdom that reflect the complete Bioinformatics profile "PROPOSE, HYPOTHEZIZE AND VALIDATE". Finally, he concluded his speech by asking the participants to make use of the opportunity of diverse experts gathered for the deliberations in Structural Biology and Computer Aided Drug Design.

Prof. G.P.S. Raghava, Indraprastha, Institute of Information Technology, New Delhi in his thematic address highlighted the strength of Indian Scientists excelling in Structural Biology and the high number of contributions made towards the prediction of protein structures deposited in the protein repository data bank (PDB). He also mentioned the need to develop a best benchmarking method that will utilize the open-source tools to solve the scientific problems and also promote them among the Bioinformatics community. Furthermore, he concluded his address by bringing into forefront of the qualities that need to be enriched and propagated among the fellow scientists that will in turn be beneficial in nurturing our society.

Prof. D. Velmurugan, UGC-BSR Faculty, CAS in Crystallography and Biophysics, University of Madras, Chennai delivered the Felicitation address. In his speech he appreciated

the Vice-Chancellor for the rapid progress, the University has made and congratulated the Convenor and Organizing Secretary for having organize the National Symposium cum Workshop for eleventh consecutive time and materializing the Bioinformatics and Drug Discovery Society [BIDDS]. 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.

Nineteen Eminent Scientists from various prestigious institutions would be delivering lectures in how the Computation methods could play a major role in developing drugs for the human kind, the importance of Bioinformatics tools in Human Health care and over 150 participants across the country, including Faculty members and Research Scholars attending this four-day event.

Dr. Sanjeev Kumar Singh, Professor Department of Bioinformatics, Organizing Secretary of SBCADD'2019 welcomed the gathering and highlighted several issues confronting India and the immediate need to find solution using computational sources. He enumerated on the proceedings of the conference and the delegates gathered from various parts of India. In addition, he also briefly mentioned the progress and achievements made by the Department of Bioinformatics in receiving the grants from UGC under the Innovative Scheme, DST-FIST Level-I, DST-PURSE Phase-II and MHRD-RUSA 2.0. Finally, the vote of thanks was proposed by Dr. M. Karthikeyan.

Parents Teachers Alumni Association meet

Parents Teachers Alumni Association Meet-2019, April 8th (PTAM-2019), held at Department of Bioinformatics, Conference Hall, Fourth Floor, Science Campus Alagappa University.





International Expert Visit to Department

International Expert Dr. Anthony Hay, USA visit to Alagappa University for the Broad-Based Board of Studies Meeting during 20th -22nd May, 2019 in the Department of Bioinformatics, Alagappa University, Karaikudi

Dr. Anthony Hay has visited the Department of Bioinformatics; he congratulated Prof. J. Jeyakanthan and the faculty members for their efforts in bringing the excellent infrastructure and research facilities developed on par with global standards. He further added that the students and scholars have the flexibility and feasibility to carry out any work related to Bioinformatics discipline.



In the BBOS Meeting, the experts were very impressed with the diversity, depth and the magnitude of the course work that is being taught to M.Sc and M.Phil Bioinformatics students at the Alagappa University, Karaikudi. They compared the curriculum of M.Sc and

M.Phil Bioinformatics with other graduate programs in USA and Indian premier institutes. Bioinformatics, a multidisciplinary area requires sufficient programming proficiency to develop a tool, supporting appropriate back-end scripts for solving real time biological problems or creating feasible information repositories up-to date relevant to the scientific community. They suggested that there are a few areas and few modules/classes that can be added to the existing program to further improve its standard on par with the international programs.



Achievements, Awards and Recognition

- Prof. Sanjeev Kumar Singh has been awarded with the **Biotech Research Society, India (BRSI) Fellow Award - 2018** from the **Biotech Research Society, India** for his outstanding contributions in the area of Structural Bioinformatics and Computer Aided Drug Design. The awards were presented during the inaugural function of International Conference on “Biotechnological Research and Innovation for Sustainable Development” (BioSD-2018) held at Indian Institute of Chemical Technology (IICT), Hyderabad on November 22nd -25th, 2018.
- Dr. M. Karthikeyan has been invited and appointed as a **Distinguished Adjunct Faculty** at Saveetha Dental College and Hospitals, Chennai from 10th January 2019.
- Prof. J. Jeyakanthan was selected for the **Leadership for Academicians Programme (LEAP)** sponsored by the Ministry of Human Resource Development (MHRD) and jointly hosted by the National Institute of Technology – Tiruchirappalli (NIT-T), the Indian Institute of Information Technology (IIIT), Sri City (Andhra Pradesh) and Nanyang Technological University (NTU)-Singapore during 04th -23rd February, 2019.



Prof. J. Jeyakanthan receiving the meritorious certification on successful completion of the MHRD-LEAP programme from the respective directors of the organizing institutes.



Prof. C. Sekar (Left) and Prof. J. Jeyakanthan (Right) along with Hon'ble Vice-Chancellor Prof. N. Rajendran congratulated the awardees on successful completion of the MHRD-LEAP.

Research Projects, Grants, Fellowships

Research Project Grant Release by DST

Third year grant release of Rs.12 lakhs has been sanctioned on 13th August, 2018 by the DST for the Research project entitled “Identification of Potential Anti-Filarial drug targeted enzymes Wbm0441, Wbm0042 from Wolbachia endosymbiont *Brugia malayi*” to Dr. J. Jeyakanthan, Professor and Head, Department of Bioinformatics, Alagappa University.

Fellowship Awarded

Mr. Umesh Panwar, Full-time Ph.D. Scholar has been awarded the Senior Research Fellowship with Rs. 28,000/- per month by the Indian Council of Medicinal Research (ICMR), New Delhi, for his work on the identification of novel inhibitors to diminish HIV infection.

INDO-TAIWAN Research Project Approved

Research project proposal in collaboration with Prof. C.J. Chen, NSRRC, Taiwan under the INDO-TAIWAN scheme was accepted and granted Rs. 227.29 lakhs in December, 2018 for the period of three years to Dr. J. Jeyakanthan, Professor and Head, Department of Bioinformatics, Alagappa University.

University Delegations visit to Taiwan

The delegation comprising Mr. Mangat Ram Sharma, Principal Secretary, Higher Education Department, Government of Tamil Nadu, Professor N. Rajendran, Vice-Chancellor, Alagappa University, Prof. C. Sekar, Director, Centre for International Relations and Dean-Research, Prof. J. Jeyakanthan, Member-Syndicate and Head of the Department of Bioinformatics reached Tangshan on the late afternoon of 7th April 2019. The team was very well received by Mr. Liu Shaohui, Director of Tangshan Education Bureau, Dr. Zhang Jianjun, President of TPC, Prof. Tian Xiuping, former President of TPC and Prof. Ma Liangjun, Vice President of TPC. As one of the top officials from the Department of Higher Education, Mr. Liu Shaohui extended a warm welcome and assured total support for the cooperation and exchanges between TPC and ALU. A high-level meeting was held at TPC and both sides discussed the various aspects of cooperation and signed a cooperation agreement. The two sides agreed to cooperate in both academic and research. A newly constructed Alagappa University-TPC Research and Development Center was formally inaugurated in the TPC campus on 8th

April 2019 by the VC of ALU and President of TPC. There was no financial commitment from our university side in any aspect. It was agreed to make use of the existing resources for scientific and technological development, to carry out new research projects and to apply and transform the results into useful products. It was also decided to start a new Center/Department of Ceramics and Art Design to offer specialized programmes leading to Diploma/PG Diploma and an undergraduate degree in the School of Skill Development at ALU. The TPC will depute experts in ceramics and art design for training teaching staffs and students in ALU. It was also decided that the students of TPC shall visit to Alagappa University to continue their studies. The two sides shall jointly organize international conferences, symposiums and forums to promote academic exchanges; Exchange of teachers between two sides will be strengthened in order to promote scientific research and development.

During the stay in Tangshan, we had visited the history museum of TPC, the industrial robot technology training centre, the EMU technical training area, the Hebei provincial excellent academician workstation (rapid manufacturing center), and the preschool education department teaching area. Facilities and equipment of TPC are very impressive. We also visited Tangshan Asia Times Ceramics Co., Ltd. and Art Porcelain Factory of TPC to further understand the production process of ceramics and the development of Tangshan Ceramics.

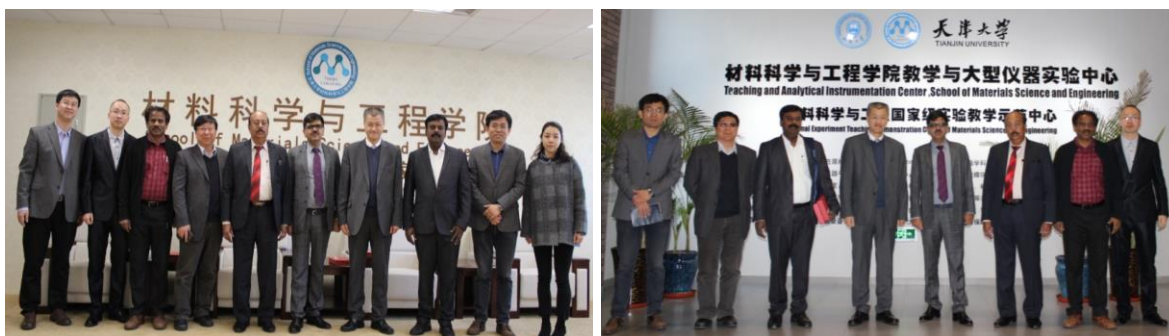
As an outcome of earlier visits, 3 faculty of TPC are currently pursuing doctoral degree in Alagappa University, which laid the foundation for the signing of the present agreement and the establishment of the R&D center in TPC.





Mr. Mangat Ram Sharma, Principal Secretary, Higher Education Department, Government of Tamil Nadu, Professor N. Rajendran, Vice-Chancellor, Alagappa University, Prof. C. Sekar, Director, Centre for International Relations and Dean-Research, Prof. J. Jeyakanthan, Member of Syndicate and Head of the Department of Bioinformatics, at Tangshan Polytechnic College (TPC) on 08th April, 2019.

The team visited another partnering Institute by name Tianjin University on 10th April 2019. TU is one of the oldest and National Key Universities of China with QS world ranking of 443. Vice-President of the TU Prof. Songsan Xiao, Director of School of Materials Science and Engineering Prof. Yahoo Geng, Head of Chemical Engineering Department Prof, Shuqian, Director of International Office Dr. Yuesheng Li and Dr. Kunyu Zhang and Prof. Pan Li of Tianjin University welcomed the delegates and a formal meeting meeting was arranged at 9.30 am on 10.04.2019. After detailed deliberations, a memorandum of understanding was signed for collaboration between the two institutions. Ministry of Human Resource Development (MHRD)-Government of India has already funded a joint proposal under the Scheme for Promotion of Academic and Research Collaboration (SPARC) for faculty and student exchange between Tianjin University and Alagappa University. During the visit, the modalities of the work and sharing of the facilities, exchange of students and faculty and possibility of extending cooperation in other areas like materials, chemistry and social sciences were discussed and agreed upon.



Mr. Mangat Ram Sharma, Principal Secretary, Higher Education Department, Government of Tamil Nadu, Professor N. Rajendran, Vice-Chancellor, Alagappa University, Prof. C. Sekar, Director, Centre for International Relations and Dean-Research, Prof. J. Jeyakanthan, Member of Syndicate and Head of the Department of Bioinformatics, at Tianjin University on 10th April, 2019

While returning from China, the delegates visited Nanyang Technological University (NTU)-Singapore and held discussion with the Director of Lee Kong Chian School of Medicine Prof. Balazs Gulyas for possible collaboration with NTU. The NTU-Singapore is one of the leading universities with the credentials of being No. 1 and 13 respectively in the QS Asian and World Rankings 2018. Earlier, two of our senior faculty members Professors C. Sekar and J. Jeyakanthan had visited NTU recently under the Leadership for Academicians Programme (LEAP) sponsored by MHRD and established contacts with LKC School of Medicine. Upon arrival at NTU on 12th April 2019, Mr. Daryl Gomes received the team and introduced the campus model and functioning. Later Prof. Time White, Senior Vice-President of NTU and his team held discussion and exchanged details about the possible areas of cooperation. It has been decided to have formal research cooperation in the area of biological sciences particularly with the Departments of Bioelectronics and Biosensors, Biotechnology, Bioinformatics, Biomedical Science and Microbiology. The cooperation will be extended to the other areas including management and social sciences. Prof. B.V.R. Chowdari, Senior Executive Director, President's Office at Nanyang Technological University arranged the meetings and agreed to support cooperation between Alagappa University and NTU.



Mr. Mangat Ram Sharma, Principal Secretary, Higher Education Department, Government of Tamil Nadu, Professor N. Rajendran, Vice-Chancellor, Alagappa University, Prof. C. Sekar, Director, Centre for International Relations and Dean-Research, Prof. J. Jeyakanthan, Member of Syndicate and Head of the Department of Bioinformatics, at Nanyang Technological University (NTU), Singapore on 12th April, 2019.

Invited Talks/Address/Seminars/Conference

- **Dr. J. Jeyakanthan**, Professor and Head, Department of Bioinformatics, Alagappa University delivered Special talk on “Protein Structure Determination and its importance in Drug Discovery” on the occasion of Helix Association Inaugural function organized by the Department of Biotechnology & Bioinformatics, Bishop Heber College (Autonomous), Tiruchirappalli on 25th July, 2018.
- **Dr. M. Karthikeyan** delivered a special lecture on "Bioinformatics Applications in Forensic Science" in the “Workshop on Forensic Bioinformatics” organized by NCoE (MHRD), Thiagarajar College, Madurai on 08.09.2018.
- **Dr. J. Jeyakanthan**, Professor and Head, Department of Bioinformatics, Alagappa University delivered a talk on “Structural and functional analysis of Asparaginyl-tRNA synthetase (*TtAsnRS*) from *Thermus thermophilus* HB8 and its complexes” in the International Conference on “Extremophilic Microbes for Sustainable Development in Agriculture, Environment and Health (EMAEH-2018) organized by the Department of Microbiology, Periyar University, Salem on 21st December, 2018.
- **Dr. M. Karthikeyan**, Assistant Professor, Department of Bioinformatics, Alagappa University delivered an invited lecture on “Workshop on Pharmacoinformatics” organized by NCoE (MHRD), Thiagarajar College, Madurai on 02nd December, 2018.
- **Dr. Sanjeev Kumar Singh**, Professor, Department of Bioinformatics, Alagappa University delivered an invited lecture on “Computational Drug Discovery Approaches” at Bishop Heber College, Trichy (23rd January, 2019)
- **Dr. J. Joseph Sahayarayan**, Assistant Professor, Department of Bioinformatics, Alagappa University participated as a Keynote Speaker and presented his research finding entitled as “Enhancement of Acibenzolar-S-methylon on the expression of Phenylpropanoid Biosynthetic Genes and the collection of Phenylpropanoids in *Mentha* species” in the International Conference on New Frontiers in Engineering, Science, Law, Management, Humanities and Social Science 2019 (INFES 2019) at Gauhati University. (23rd -24th February, 2019)
- **Dr. J. Jeyakanthan**, Professor and Head, Department of Bioinformatics, Alagappa University was invited as a Resource Person and delivered a talk on” Protein Structure Prediction and its importance in Drug Discovery” in A Special Interdisciplinary UGC Sponsored Workshop on the Bioinformatics and Chemoinformatics tools for Molecular Analysis (BCTMA’2019) organized by the PG and Research, Department of Physics, National College, Tiruchirappalli on 08th March, 2019
- **Dr. Sanjeev Kumar Singh**, Professor, Department of Bioinformatics, Alagappa University delivered an invited lecture on “Drug Discovery and other Computational studies to identify potential antivirals” at Centre for Bioinformatics, Pondicherry University, Puducherry on 12th April, 2019.
- **Dr. P. Boomi**, Assistant Professor, Department of Bioinformatics, Alagappa University presented his research findings in the 03rd Asian Conference on Science Technology & Medicine (ACSTM-2019) and also participated at the 06th Annual Conference of the

ACSE (Asian Council of Science Editors) held at Carlton Palace Hotel, Diera Dubai. (12th -14th February, 2019).



Dr. P. Boomi presenting his research findings in the 03rd Asian Conference on Science Technology & Medicine (ACSTM-2019) held at Carlton Palace Hotel, Diera Dubai. (12th -14th February, 2019).

- **Dr. J. Jeyakanthan**, invited as a resource person in A Special Interdisciplinary UGC Sponsored Workshop on the Bioinformatics and Chemoinformatics tools for Molecular Analysis (BCTMA'2019) organized by the PG and Research, Department of Physics, National College, Tiruchirappalli on 08th March, 2019.



- **Dr. Sanjeev Kumar Singh**, Professor, Department of Bioinformatics, Alagappa University organized the special lecture in theme of "Distinguished lecture series" presented by Mr. Suresh K Goel, a veteran IFS officer and an Ambassador of India in Lao PDR on 22nd April, 2019 at Alagappa University, Karaikudi.
- **Dr. Sankar Prasath Kannuajia** IIT, Guwahati, delivered special lecture on 07th May, 2019 at Department of Bioinformatics, Alagappa University, Karaikudi.



- Dr. Anthony Hay delivered a special lecture entitled “**You’re smarter than the machines: Biological inferences from Bioinformatics**” on 22nd May, 2019 where he enlightened on how Bioinformatics represent a key to understand and decipher the complexity of genetic data as well as facilitate discovery of new therapeutics/diagnostics to the gathering from various disciplines. He also briefly enumerated on the opportunities and programs at the graduate as well as post-doctoral levels in USA for Bioinformatics based studies.





Dr. Anthony Hay, USA delivering special lecture to the diverse gathering comprising of faculty members, students and research scholars from various disciplines on 22nd May, 2019.



JOURNAL OF
APPLIED
CRYSTALLOGRAPHY

ISSN 1600-5767

computer program



PlaneFinder: a methodology to find the best plane for a set of atoms involved in the metal coordination in protein structures

J. Janu Sahana,^{a,†} S. Sriraghav,^{a,†} T. A. Vijeth,^{a,†} T. Nagarushyanth,^{a,†} R. Santhosh,^b D. Michael,^a Z. Sameer Ahmed,^a K. P. R. Nisha,^a J. Jeyakanthan^b and K. Sekar^{a,*}

Received 16 January 2018
Accepted 4 June 2018

^aDepartment of Computational and Data Sciences, Indian Institute of Science, Bangalore 560 012, India, and
^bDepartment of Bioinformatics, Alagappa University, Karaikudi 630 004, India. *Correspondence e-mail: sekar@iisc.ac.in

Edited by F. Meilleur, Oak Ridge National Laboratory, USA, and North Carolina State University, USA

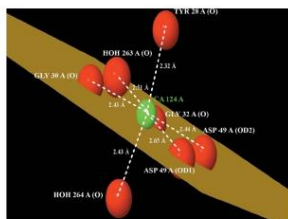
† These authors contributed equally to this work.

Keywords: *PlaneFinder*; metal planes; metal geometry; metalloproteins; metal complexes.

Metal ions play a considerable role in protein structure and function. The roles of most metals and their importance are determined by the arrangements of the interacting atoms in the three-dimensional protein structure. This information is essential in predicting the geometry of the atoms involved in metal coordination. The deviation of the other atoms from the best plane is another crucial factor. The proposed web server, *PlaneFinder*, provides a fast and efficient method to calculate the best-fit plane for a set of atoms involved in the metal coordination. It provides in addition other possible planes by considering the maximum number of interacting atoms as well as user-selected atoms. The deviations of the selected atoms and other atoms from the best-fit plane are also displayed. *PlaneFinder* is freely available and can be accessed at <http://bioserver1.physics.iisc.ac.in/plane/>.

1. Introduction

Bound metal atoms play an essential role in the structure and function of protein molecules (Harding, 1999). Understanding the geometry of the metal coordination is of paramount importance in the analysis of the structure and function of proteins (Andreini *et al.*, 2012; Harding, 2004; Thomson & Gray, 1998; Zheng *et al.*, 2008; Harding *et al.*, 2010). Along with the massive increase in the number of three-dimensional protein structures in the Protein Data Bank (PDB), their analysis has become increasingly crucial (Berman *et al.*, 2000) and there is a growing need for the in-depth analysis of existing metal-bound protein structures (Zheng *et al.*, 2008). One of the most intuitive ways of studying the structure of the protein complex is to visualize the contained metal(s) with the corresponding coordinating atoms (protein atoms and water molecules) (Harding, 2001; Harding *et al.*, 2018). The foremost purpose of this methodology is to allow the user to explore the geometry of metal coordination in proteins. *GEOMCALC* is a program in the *CCP4* (Winn *et al.*, 2011) suite, in which the output generated is in text format (*e.g.* equation of the plane). The *FindGeo* (Andreini *et al.*, 2012) tool also generates coordinate text files, which requires the user to additionally employ and run a visualization tool to view the generated coordinates. Neither of these tools provide visualization of the generated plane. The proposed tool, *PlaneFinder*, not only computes the best-fit plane but also provides visualization of the plane. There are no additional dependencies required, as the visualization tool is incorporated in the package. If the client machine does not have the java plug-in *Jmol*, we have equipped the tool with *JSmol* as well, which runs in the





Hydroxychloroquine Inhibits Zika Virus NS2B-NS3 Protease

Ankur Kumar,[†] Brooke Liang,^{‡,§} Murali Aarthy,[‡] Sanjeev Kumar Singh,[‡] Neha Garg,^{†,¶} Indira U. Mysorekar,^{‡,§,||} and Rajanish Giri^{*,†,¶,||}

[†]Indian Institute of Technology Mandi, Mandi 175005, Himachal Pradesh, India

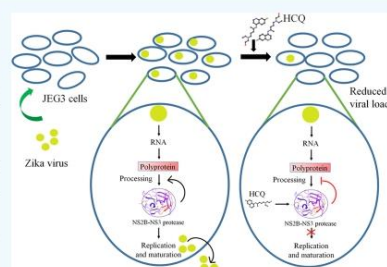
[‡]Department of Obstetrics and Gynecology, [§]Center for Reproductive Health Sciences, and ^{||}Department of Pathology and Immunology, Washington University School of Medicine, 660 South Euclid Avenue, St. Louis, Missouri 63110, United States

[‡]Department of Bioinformatics, Computer Aided Drug Design and Molecular Modeling Laboratory, Alagappa University, Science Block, Karaikudi 630003, Tamil Nadu, India

[¶]BioX Center, Indian Institute of Technology Mandi, Mandi 175005, Himachal Pradesh, India

Supporting Information

ABSTRACT: Zika virus is a mosquito-transmitted flavivirus that causes devastating fetal outcomes in the context of maternal infection during pregnancy. An important target for drugs combatting Zika virus pathogenicity is NS2B-NS3 protease, which plays an essential role in hydrolysis and maturation of the flavivirus polyprotein. We identify hydroxychloroquine, a drug that already has approved uses in pregnancy, as a possible inhibitor of NS2B-NS3 protease by using a Food and Drug Administration-approved drug library, molecular docking, and molecular dynamics simulations. Further, to gain insight into its inhibitory potential toward NS2B-NS3 protease, we performed enzyme kinetic studies, which revealed that hydroxychloroquine inhibits protease activity with an inhibition constant (K_i) of $92.34 \pm 11.91 \mu\text{M}$. Additionally, hydroxychloroquine significantly decreases Zika virus infection in placental cells.



INTRODUCTION

Zika virus (ZIKV) belongs to the *Flavivirus* genus and is a member of the *Flaviviridae* family. Recent research has revealed that ZIKV is associated with microcephaly in fetuses^{1,2} and neurological disorders such as Guillain-Barré syndrome in adults.^{3–5} The rapid spread of this virus, affecting over a million people⁶ across multiple continents, has spurred researchers to search for effective therapeutic intervention. A broad-spectrum antiviral agent against shared flavivirus proteins would be especially attractive, given the preponderance of related flavivirus infections (such as dengue and West Nile viruses) in areas where ZIKV has been most prevalent.

Zika virus is an enveloped virus like other flaviviruses, encapsulating a single-stranded, positive-sense, RNA genome encoding a single polyprotein precursor.⁸ It is hydrolyzed into three structural proteins (E, prM/M, and C) and seven nonstructural proteins (NS1, NS2A, NS2B, NS3, NS4A, NS4B, and NS5)^{8–10} by the host and viral proteases.¹⁰ Among these viral and host elements, the viral NS2B-NS3 protease is an attractive drug target due to its essential role in the virus life cycle. The crystal structure of NS2B-NS3 protease reveals that NS2B (only the hydrophilic part was taken in the construct for crystallographic studies, approximately residues 49–95 of the full-length NS2B protein constituting ~130 residues) can be found in two conformations. In the presence of inhibitor/substrate, NS2B forms a β -hairpin and lies near the substrate

binding site of NS3 protease, adopting a closed conformation, but in the absence of inhibitor/substrate, it adopts an open conformation.^{11–14} The NS2B-NS3 protease structure with PDB ID: SLC0¹³ (hydrophilic part, residues 49–95 of NS2B fused via a Gly4–Ser–Gly4 linker to the N-terminal of the NS3 protease) shows NS2B wrapping around NS3 in such a way that the C-terminal residues of NS2B form a β -hairpin that contributes to the S2 pocket of the NS3 protease.^{13–15} As reported NS2B protein has a high abundance of disorder promoting residues containing a 37-residue disordered region (62–98).^{16,17} The NS2B interaction with NS3 protease facilitates NS3-mediated cleavage of polyprotein thus, it acts as an important cofactor for the activity of NS3 protease.¹⁸ Generally, disordered proteins lead to functionality only upon interaction with its binding partner such as transactivation domain of cMyb, in which cMyb becomes functional only upon binding its ordered counterpart, KIX.^{19–22} Together, NS2B and NS3 form the NS2B-NS3 protease complex that hydrolyzes the ZIKV polyprotein into functional proteins used for viral propagation and maturation.¹¹

Viral proteases are considered excellent targets for the identification of potential drug candidates, as protease plays an

Received: May 15, 2018

Accepted: December 5, 2018

Published: December 24, 2018



In Vitro and In Silico Studies of Chitin and Chitosan Based Nanocarriers for Curcumin and Insulin Delivery

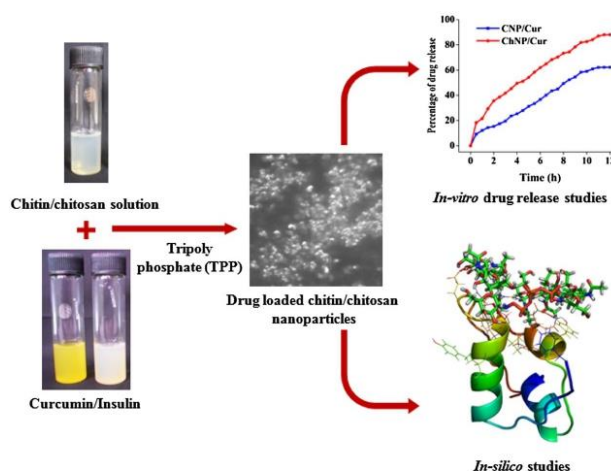
Solairaj Dhanasekaran¹ · Palanivel Rameshthangam² · Suryanarayanan Venkatesan³ · Sanjeev Kumar Singh³ · Sri Ramkumar Vijayan⁴

Published online: 23 July 2018
© Springer Science+Business Media, LLC, part of Springer Nature 2018

Abstract

The evaluation of drug delivery potential, molecular interactions of the polymeric nanoparticles with the drug molecule and release kinetics encounters more time consumption and also cost. In this study, we have adopted the combination of in vitro and in silico approaches to evaluate the drug delivery property of the polymeric nanoparticles viz. chitin and chitosan. Herein, two different therapeutic agents such as curcumin (a hydrophobic drug) and insulin (a therapeutic protein) were used to study the delivery potential of chitin and chitosan nanoparticles. The drug loaded chitin and chitosan nanoparticles were prepared and characterized using Fourier transform infra red spectroscopy, X-ray diffraction, dynamic light scattering and scanning electron microscopy analysis. In the in vitro drug delivery experiments, chitosan nanoparticles exhibited better encapsulation efficiency, drug loading capacity and prolonged release of the drug molecules than that of the chitin nanoparticles to both curcumin and insulin. Meanwhile the in silico experiments such as molecular docking and molecular dynamics predicted the molecular interactions and binding energy involved between the nanoparticles and the drug molecules. From this study, we suggest that the chitosan nanoparticles could be used as a carrier molecule for both curcumin and insulin.

Graphical Abstract



Keywords Chitin · Chitosan · Curcumin · Drug delivery · Insulin · Molecular dynamics

Extended author information available on the last page of the article

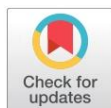
RESEARCH ARTICLE

A theoretical insight to understand the molecular mechanism of dual target ligand CTA-018 in the chronic kidney disease pathogenesis

Selvaraman Nagamani, Karthikeyan Muthusamy*

Department of Bioinformatics, Alagappa University, Karaikudi, India

* mkbioinformatics@gmail.com



OPEN ACCESS

Citation: Nagamani S, Muthusamy K (2018) A theoretical insight to understand the molecular mechanism of dual target ligand CTA-018 in the chronic kidney disease pathogenesis. PLoS ONE 13(10): e0203194. <https://doi.org/10.1371/journal.pone.0203194>

Editor: Utpal Sen, University of Louisville, UNITED STATES

Received: November 15, 2017

Accepted: August 16, 2018

Published: October 4, 2018

Copyright: © 2018 Nagamani, Muthusamy. This is an open access article distributed under the terms of the [Creative Commons Attribution License](https://creativecommons.org/licenses/by/4.0/), which permits unrestricted use, distribution, and reproduction in any medium, provided the original author and source are credited.

Data Availability Statement: All relevant data are within the paper and its Supporting Information files.

Funding: Authors gratefully acknowledge financial support provided by Indian Council of Medical Research (ICMR), Govt. of India Senior Research Fellowship to S. Nagamani (F. No.: BIC/11(09)/14).

Competing interests: The authors have declared that no competing interests exist.

Abstract

The level of the vitamin D in the bloodstream is regulated by cytochrome P450 enzyme 24-hydroxylase A1 (CYP24A1). Over expression of CYP24A1 enzyme is correlated with vitamin D deficiency and resistance to vitamin D therapy. Chronic kidney disease (CKD) patients are commonly reported with the above said expression variations. This deregulation could be solved by ligands that act as a vitamin D receptor (VDR) agonists and CYP24A1 antagonists. Posner et al., (2010) first time reported two new vitamin D analogues namely CTA-091 and CTA-018 to inhibit CYP24A1. The CTA-018 inhibited CYP24A1 with an IC_{50} 27 ± 6 nM (10 times more potent than the ketoconazole (253 ± 20 nM)). CTA-018 induced VDR expression (15-fold lower than $1\alpha,25(OH)_2D_3$) and is under phase II clinical trial, whereas CTA-091 was not able to efficiently induce the VDR expression (>2000 nM). To explore the molecular mechanism, binding specificity of these two vitamin D analogues along with native ligand was extensively studied through *in silico* approaches. Through molecular dynamics simulations studies, we shown that the sulfonic group ($O = S = O$) in the side chain of CTA-018 plays an important role in the regulation of VDR agonistic activity. The electron lone pairs of the sulfonic group that interacted with His393 lead to be a factor for agonistic mechanism of VDR activity. Compared to azol-based compounds, CTA-018 binds the different sites in the CYP24A1 binding cavity and thus it could be a potent antagonist for CYP24A1 enzyme.

Introduction

Worldwide, Chronic kidney disease (CKD) is a major public health problem; it is one of the high-risk factors for hypertension and diabetes [1] patients. Progressive reduction of circulating $1\alpha,25$ -dihydroxy vitamin D_3 ($1\alpha,25(OH)_2D_3$) and 25-hydroxyvitamin D_3 ($25(OH)_2D_3$) are common expression variation observed in CKD patients [2]. Several vitamin D analogues like $1\alpha,25(OH)_2D_3$ (i.e., calcitriol) and $25(OH)_2D_3$ (i.e., cholecalciferol) were used for the treatment of secondary hyperparathyroidism (sHPT) among CKD patients but their efficacy is

Students Page

Conferences Attended

- Ms. Jayashree Biswal and Ms. J. Prajisha, Research Scholars under the guidance of Prof. J. Jeyakanthan attended and presented the posters in the International Conference cum Workshop on Informatics Tools in Drug Discovery and Drug Delivery (iT-DDD 2018) organized by the Association of Pharmaceutical Teachers of India (APTI) Punjab & Department of Pharmaceutical Sciences and Drug Research, Punjabi University, Patiala (01st-04th November, 2018). They received the Best poster prize presentations (3rd and Consolation) respectively.



Receiving the Best Poster Presentation (3rd and Consolation prize) at iT-DDD'2018 (01st-04th November, 2018)

- Ms. N. Madhana Priya, Research Scholar under the guidance of Prof. J. Jeyakanthan attended and presented the poster in the International Conference on Recent trends in Zoology, Genetics, Environmental Science and Biodiversity (ICBUB-2018) Department of Zoology, Bangalore University, Bangalore (04th- 05th December, 2018).
- Mr. M. Nachiappan, Ms. M. Amala and Ms. P. Saritha, Research Scholars under the guidance of Prof. J. Jeyakanthan attended and presented their research work in the International Conference on Advanced Chemical and Structural Biology (ICACSB-2019) organized by the Prist University, Chennai on 19th -21st February, 2019.
- Lakshmanan Loganathan, Research Scholar under the guidance of Dr. M. Karthikeyan presented poster on the title “Computational study on Cross-talking of Colorectal Cancer Signalling mechanism between TNKS, Axin and RNF146 Complexes” in International Conference on Cancer Inferno and Its Prevention Strategies-ICCIPS-2019 on 22nd February 2019 at Periyar EVR College, Trichy and won best Poster Presentation Award.



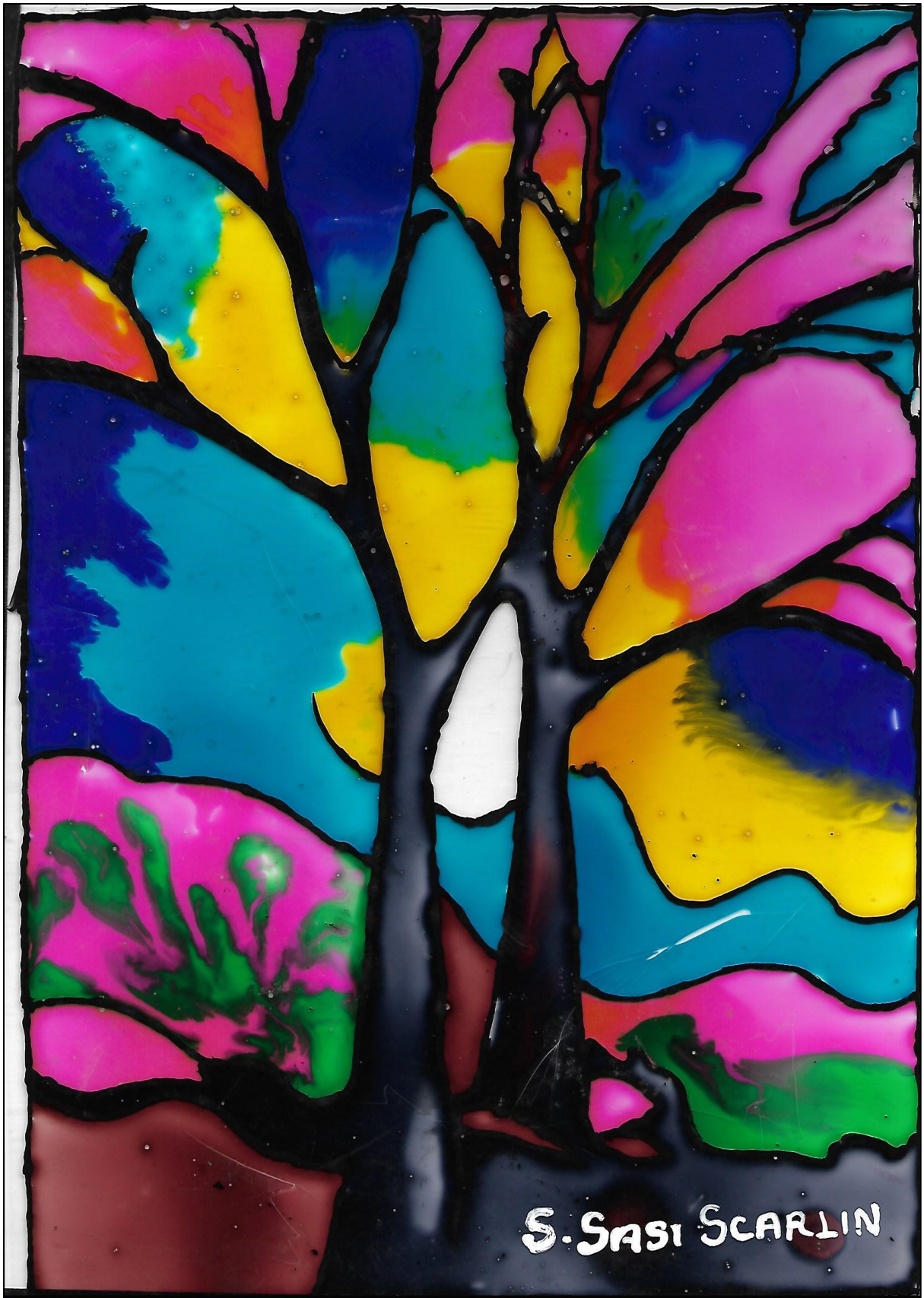
Lakshmanan Loganathan receiving the Best Poster Presentation Certificate at the International Conference on Cancer Inferno and Its Prevention Strategies-ICCIPS-2019 on 22nd February 2019.

Students Artworks:





S. SASI SCARLIN





Art by
Rajeshwar

DBI-Y



தினமலர்

மதுரை | புதன் | 13.2.2019

உணவு பழக்க வழக்கத்தால் மரபு வழி ஜீன்களில் மாற்றம்

உயிரி தகவலியல் பேராசிரியர் தகவல்

காரைக்குடி, பிப். 13-

“உணவு பழக்க வழக்கம், தனி மனித ஒழுக்கம், சுற்றுச்சூழல் மாக ஆகியவற்றால் மரபு வழி ஜீன்களில் மாற்றம் ஏற்படுவதாக” சென்னை பல்கலை பேராசிரியர் வேல்முருகன் கூறினார்.

காரைக்குடி அழகப்பா பல்கலை உயிரி தகவலியல் துறை சார்பில் “மருந்து மூலக்கூறுகளின் சம்பந்திய கண்டுபிடிப்புகள் மற்றும் ஆராய்ச்சி தொடர்பான தேசிய கருத் தரங்கம் துணைவேந்தர் ராஜேந்திரன் தலைமையில் தொடங்கியது.

ஒருங்கிணைப்பாளர் சஞ்ஜய் குமார் சிங் வா வேற்றார், இந்திய அறிவியல் தொழில் நுட்ப அழகத்தின் உயிரி தகவலியல் துறை பேராசிரியர் டி.பி. சிங் தொடங்கி வைத்தார். சென்னை பல்கலை பேராசிரியர் வேல்முருகன் : மூலக்கூறுகளில் 10 சதவீத மருத்துவ குணங்கள் உள்ளது.

அதனால் தான் விலங்கு தன் தாவரங்களை உண்டு தங்கள் தோயை போக்கி கொள்கிறது.

மனித உடலில் 30 ஆயிரம்

மரபு வழி ஜீன், 20 ஆயிரம் புது மூலக்கூறு உள்ளது.

ஒவ்வொரு புரதத்துக்கும் ஒரு செயல் உண்டு. உணவு பழக்க வழக்கம், சுற்றுச்சூழல் மாக ஆகியவற்றால் மரபு வழி ஜீன்கள் மற்றும் புரதங்களில் மாற்றம் ஏற்படுகிறது.

வைரஸ் தாக்கம் ஏற்படும் போது புரதங்களில் உள்ள அமினோ அமிலங்கள் கட்டமைப்பு மாறுகின்றன. இதனால், முன்பு வடிவமைக்கப்பட்ட மருந்துகள் உட்கொள்ளும்

போது அமினோ அமிலங்களில் பிணைப்பு சரியாக ஏற்படாமல் மருந்துகள் செயல் இழக்கிறது.

எனவே, அனைத்து புரதங்களின் கட்டமைப்பை கண்டறிந்து அதற்குரிய மருந்துகளை கண்டறிதல் அவசியம், என்றார்.

நிகழ்ச்சியில் டில்லி இத்தா பிரஸ்தா தகவல் தொழில் நுட்ப பேராசிரியர் சாகவா, கொல்கத்தா போஸ் இன்ஸ்டிடியூட் பேராசிரியர் பினக்பான் சக்பாபாதி உள்ளிட்ட பலர் பங்கேற்றனர்.

Department Profile

DEPARTMENT PROFILE

Objectives

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

Special Features

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

Programs Offered

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

Faculty Members

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

Research Focus on

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

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

Funding Agencies

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

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

Award/ Recognition

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

Research Collaborating Organizations/ Institutes

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

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

Infrastructure Facilities in the Department

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

Resources

- AKTA 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
- Ice Flakers
- In-house protein database
- Kinetics Spectrophotometer
- Microscope
- Milli-Q Integral Water Purification System
- Multiplate Reader
- Nano Spectrophotometer
- Orbital Shaker
- Power backup (20, 10 and 5 KVA UPSs)

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



DBI



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 2018-19

CORE COMPETENCY
Department of Bioinformatics was incepted in the year 2008, to facilitate the teaching and research in the interdisciplinary areas of Small and Macro Molecule X-ray Crystallography, Structural Biology, Structural Bioinformatics, Molecular Modelling, Computer-Aided Drug Design, Pharmacoinformatics, Chemoinformatics, Molecular Cell Biology, Genetic Engineering, Genomics, Proteomics, Bio-computing, Quantum Chemistry and development of Database or Software. The Department is funded by • University Grants Commission (UGC) under the scheme of Innovative Programme for Teaching & Research in Interdisciplinary and Emerging Areas • Department of Science & Technology (DST) for Improvement of S & T Infrastructure in Higher Educational Institutions (FIST) • Promotion of University Research and Scientific Excellence (PURSE), • Indian Council of Medical Research (ICMR), • Tamil Nadu State Council for Science & Technology (TNSCST) and • Rashtriya Uchchatar Shiksha Abhiyan (RUSA) 2.0. Our research focuses on Computational/Experimental analysis of interaction between predicted lead molecules or drugs with proteins or nucleic acids besides analysing their biochemical mechanism of action to enhance discovery of novel therapeutics for various diseases and disorders in human. The infrastructure, research facility and internship programs ensure every student as an all-rounder with academic excellence, research skills and industrial exposure. The Department is offering M.Sc., M.Phil., Ph.D. & PG programmes in Bioinformatics with extensive research publications in aforesaid research areas.
HALLMARKS
★ About 432 research articles Published in Top journals with high Impact Factor, Books, Chapters and Monographs. ★ Execution of Research projects including DAE-BRNS (2018-2021). DST INDO-TAIWAN (2018-2022), MHRD-SPARC IIT-Mandi (2019-2021) and ICMR (2019-2022). ★ Developed and maintained Local server containing utilities such as E-library Database, In-house Protein Databank and Knowledgebase (DAPD, DAMPD, NIMS, MIPS and PDB goodies). ★ Installed Innovative Smart Classrooms and 24x7 laboratory with internet facilities. ★ Organized Hands-on Training (Workshop) for students and other participants to update themselves with the recent innovations in Computer Aided Drug Design. ★ Organized Industrial visits at reputed institutes to promote knowledge sharing with eminent scientists.

Collaborative Research with the following leading Institutions:

- **DST INDO-TAIWAN** collaborative research project, Taiwan
- Nanyang Technological University (**NTU**), Singapore
- University of Manchester, U.K National Institute of Health, **USA** and Institute of Experimental Medicine, **Czech Republic**
- **IISC** Bangalore, University of Madras, Chhatrapati Shahuji Maharaj University, Kanpur, **CSIR-NCL**, Pune, **CSIR- CDRI**, Lucknow, **CSIR-CECRI**, Karaikudi
- **IIT** –Madras, Guwahati, Delhi and Mandi

DEEDS & DEVELOPMENTS

- ❖ The 11th National Symposium cum Workshop on **Recent Trends in Structural Bioinformatics and Computer Aided Drug Design [SBCADD'2019]**
- ❖ **SBCADD'2019** Conference with plenary lectures from renowned experts in various disciplines
- ❖ **Eminent scientists** from various prestigious institutions delivered lectures on applications of Computational Biology in developing therapeutics.
- ❖ Over **150 participants** including Faculty members and Research Scholars across the country participated in the four-days' workshop cum workshop.
- ❖ Organized Broad Based Board of Studies (**BBOS**) Meeting with International Expert **Dr. Anthony Hay**, Cornell University, **USA**

AWARDS & ACHIEVEMENTS

Faculty achievements/awards:

- ✚ A Faculty was selected in MHRD-LEAP programme (NIT Trichy, IIIT Sri City, Andhra Pradesh, and NUT Singapore).
- ✚ **Memorandum of Understanding** was signed with Department of Chemical Engineering, Konkuk University, Seoul, South Korea. ALU and BHC (Bishop Heber College) Trichy.
- ✚ Acquired Research project under **INDO-TAIWAN scheme** in collaboration with Prof. C.J. Chen, NSRRC, Taiwan.
- ✚ Received Bio -Tech Research Society, India (**BRSI**) Fellow Award for the year 2018.
- ✚ **Head of the Department** has been nominated as the Finance Committee Member of Alagappa University.

Scholars/Students:

- ✚ Research Scholars received their Ph.D. degrees in the year of 2019-2020
- ✚ A Research Scholar has been awarded the Senior Research Fellowship by the Indian Council of Medicinal Research (ICMR), New Delhi

- ✚ 9 Research Scholars have received meritorious fellowship from Govt. of India and renowned agencies besides International Travel grant
- ✚ 10 Ph.D. students were lauded with meritorious awards for their research work in national and International Conferences.



11th National Symposium cum Workshop on “Recent Trends in Structural Bioinformatics and Computational Aided Drug Design” || [SBCADD’2019] 12th-15th February, 2019



Seminar Hall



Class Room



Computational Facility



CADD Lab



Sophisticated Lab

Department Facility



Experimental Lab



FPLC



Structural Biology Lab



Crystallization Lab



UGC Innovative Facility



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), Karalkudi
Account name	: Bioinformatics and Drug Discovery Society
Account number	: 36993002251
IFSC Code	: SBIN0000855

Scan & Register



CONTACTUS

President

Prof. D. Velmurugan , SRMIST, Chennai

Secretary General

Prof. Sanjeev Kumar Singh

Email: secretary.bidds@gmail.com

Ph: +91-4565-223342



Membership Details

- **Eligibility for Membership:**

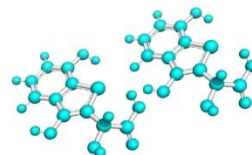
B.Sc., M.Sc., Ph.D. or equivalent degree in science and actively engaged in research or teaching in the field of Life science.

- **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.bids@gmail.com

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

