ISCB-SC RSG India

CBInd 2023-24

Computational Biology India Symposium

Program Booklet

10th Jan 2024 | Hybrid Mode

Symposium Organizing Committee

Govinda Rao Dabburu (Chair)

Mrittika Adhikary (Co-Chair)

Aakriti Jain

Nikita Ray

Ashitha Washington

Symposium Volunteers

Rubi Jain

Sabyasachi Bakshi

Rashi Sharma

Nithya Kruthi

Acknowledgements:

Sponsors : ISCB & ISCBSC

Faculty Advisors of RSG India : Dr. Manish Kumar, Prof. Manisha Goel

Mentors : Pradeep Eranti, Dr. Sohini Chakraborti

Keynotes & Esteemed Professors : Dr. Saugata Hazra, Dr. Imtaiyaz Hassan, Prof. R. Sowdhamini

Students & Faculties Department of Biophysics, University of Delhi :

Dr. Suman, Dr. Hemalata, Dr. Sumit, Kamakshi, Neha, Rashmita, Sachin, Amber

Foreword

Message from the ***RSG India Team (Aakriti, Ashitha, Govinda, Mrittika, Nikita)***

As we bid farewell to a remarkable year, we wish to take a moment to reflect on the incredible journey we have undertaken together towards building and fostering a space that unites budding researchers and enthusiasts and spreads awareness of the excellent scope of the interdisciplinary field of computational biology and bioinformatics.

Throughout the year, RSG India has been dedicated to organizing events that foster learning, collaboration, and networking. Our workshops, webinars, and conferences have provided platforms for professionals and enthusiasts to come together, share insights, and explore the latest trends in computational biology and bioinformatics. The heart of RSG India lies in its vibrant and engaged community. We are grateful for the enthusiasm and active participation of our members who have made every event, discussion, and initiative a resounding success. Your passion fuels our commitment to advancing the frontiers of science and technology.

Looking ahead, we are excited about the possibilities that the coming year holds. The RSG India team is dedicated to continuing its mission of promoting cognizance of computational biology and bioinformatics in our country. We aim to expand our reach, collaborate with more experts, and create opportunities for the next generation of researchers to thrive.

We extend our heartfelt gratitude to all the contributors, sponsors, volunteers, and community members who have played a vital role in making this year exceptional. Your support has been instrumental in our collective success, and we look forward to continued collaboration in the future.

As we turn the pages of the calendar, let us carry the spirit of collaboration, discovery, and innovation into the coming year. Together, we can make a lasting impact on the world of computational biology and bioinformatics.

*Message from **Prof. Manisha Goel** (Faculty Advisor, RSG India)*

It has been a pleasure and a privilege to be associated with ISCB-RSG India for the last one year. It is really impressive to see the enthusiasm of the young researchers that are part of the RSG team in conducting activities as per the mandate of ISCB. They have not only come up with a variety of novel outreach activities but have also worked synergistically to maximize the impact of such activities. The execution has been flawless and the participation of the younger students exploring career avenues in the field of bioinformatics has been heartening. I personally have been able to learn so much more just by being associated with this younger generation of computational biology sleuths. I wish them the very best to continue with similar momentum in the coming year.

*Message from **Dr. Manish Kumar** (Faculty Advisor, RSG India)*

It has been one year since I became part of RSG-India as a faculty advisor. As the year draws to a close, it culminates with a symposium that I am optimistic will be a resounding success. There could not be a more heartening conclusion. The role played by the RSG-India team members has been an indispensable factor in ensuring these remarkable achievements. I would like to extend my sincere congratulations and deep gratitude to the RSG-India team for the spectacular success over the past year. I hope that all stakeholders will continue to stay in touch and utilize this event as an opportunity to establish new friendships and collaborations.

Programme Schedule

10th Jan 2024 , Venue: Biotech Auditorium, University of Delhi South Campus, New Delhi (& Online)	
10:00 - 10:15	Introductory Remarks
10:15 - 11:15	Keynote Address **Dr. Imtaiyaz Hassan, Jamia Millia Islamia**
11:15 - 11.30	Tea break
11:30 - 12:00	Departmental & Networking Activity
12:00 - 13:00	Talks of Early Career Researchers/Students
13:00 - 14:30	Lunch + Poster Session
14:30 - 15:30	Keynote Address **Dr. Saugata Hazra, IIT Roorkee**
15:30 - 16:00	ISCBSC & RSG India Activity
16:00 - 17:00	Talks of Early Career Researchers/Students
17:00 - 17:30	Prizes and Concluding Session

Abstracts of talks by keynotes & Early Career Researchers

in-silico, in-vitro & *in-vivo* approaches for studying enzyme beta-lactamase: Understanding strategies taken by Hazra Group to control Antibiotic Resistance (ABR)

Saugata Hazra*[a,b]

Email: saugata.hazra@bt.iitr.ac.in, saugata.iitk@gmail.com

[a] Department of Biosciences and Bioengineering, Indian Institute of Technology Roorkee, Uttarakhand, 247667, India

[b] Centre for Nanotechnology, Indian Institute of Technology Roorkee, Roorkee, Uttarakhand, 247667, India

Abstract:

Addressing microbial infections with antibiotics faces significant challenges due to the rapid emergence and spread of antibiotic resistance, posing a substantial clinical threat. This concern is particularly pronounced in developing countries, where promoting proper hygiene and adherence to appropriate medication regimens must be intensified at the grassroots level. Innovative approaches are imperative to counteract drug-resistant strains of deadly pathogens. Penicillin and other beta-lactam antibiotics are widely prescribed for antibacterial therapeutics. Their primary mode of action involves inhibiting transpeptidase enzymes involved in bacterial cell wall biosynthesis. However, a key hurdle in combating bacterial resistance is the production of beta-lactamases, enzymes synthesized by bacterial pathogens to confer resistance against beta-lactam antibiotics, such as penicillins and cephamycins. Beta-lactamases break down the antibiotic structure, rendering them ineffective.

The current presentation aims to elucidate the state-of-the-art challenges associated with bacterial resistance and demonstrate a multilevel approach to comprehending beta-lactamase enzymes. This approach is crucial for developing new-generation therapeutics that minimize the risk of drug resistance. The key topics covered in the presentation include an integrated computational approach to identify promising beta-lactamase candidates for further investigation, supported by the following case studies. a) Understanding novel mutations responsible for drug resistance. b) Employing a multilevel approach to decipher enzyme mechanisms. c) Design, development, and optimization of novel diagnostics.

In summary, this work provides a comprehensive overview of beta-lactamase enzymes, outlining their mechanistic intricacies. The efforts discussed have culminated in designing and developing advanced diagnostics and therapeutics, contributing to effectively managing antimicrobial resistance.

Integrative Transcriptomics & miRNAome: Engineering Agronomic miRNA Candidates

Rubi Jain, Namrata Dhaka*, Pinky Yadav, Manoj Kumar Sharmac, Md Danish#, Shalu Sharma#, Sonika Kumari#, Ira Vashisht, R.K. Brojen Singh, Rita Sharma
Jawaharlal Nehru University

Brassica juncea is an allotetraploid that originated through the hybridization of B. rapa and B. nigra. It is a crucial edible oilseed crop and is presently cultivated across the world. Seed size is a pivotal agricultural trait in oilseed Brassicas. However, the regulatory mechanisms underlying seed size determination in *B. juncea* is poorly understood. In this study, we integrated both transcriptional and miRNA dynamics involved in the determination of seed size in *B. juncea*. We performed a comparative transcriptomic analysis using developing seeds of two varieties, small-seeded Early Heera2 (EH2) and bold-seeded Pusajaikisan (PJK). Out of 1,12,550 transcripts annotated from both the varieties, 27,186 and 19,522 were differentially expressed in the intra-variety and inter-variety comparisons, respectively. Functional analysis using pathway and transcription factor enrichment revealed that cell cycle- and cell division-related transcripts were upregulated during later stages of seed development in the PJK variety but downregulated at the same stages in the EH2 variety. Further, we investigated the expression patterns of cell division, cell cycle, phytohormones, and transcription factors related transcripts using K-means clustering. We also identified a total of 326 miRNAs, including 127 known and 199 novel miRNAs from seed stages of these varieties. Among these, 103 miRNAs (62 known and 41 novel) exhibited differential expression between EH2 and PJK during both the stages of seed development. Further, we detected a total of 13,854 putative miRNA-target transcripts modules. These findings shall unravel crucial candidates suitable for marker assisted breeding and engineering of varieties with improved seed size and oil content in *B. juncea*.

Accurate disease diagnosis with the help of AI

Pranay Agarwal, Kanika Rathi, Sakshi Sharma
Amity Institute of Biotechnology

Our research work focuses on empowering Clinical Labs and Doctors through Advanced AI based Medical Diagnosis Models. Our groundbreaking technology is dedicated to transforming the medical diagnostic landscape by leveraging cutting-edge artificial intelligence (AI) technology. Our primary focus lies in empowering healthcare professionals and patients by offering reliable insights and expedited decision-making processes.

By harnessing the power of AI algorithms, we are developing models. These models utilize comprehensive parameters and cutting-edge image analysis techniques to accurately diagnose heart diseases, liver cirrhosis, and brain tumors, and many more. Our ultimate goal is to enhance patient care, streamline the diagnostic process, and empower both clinical labs and patients alike.

Our research also involves tailoring other services as well to meet the needs of both clinical laboratories and Doctors. By offering our advanced diagnostic models to clinical labs, we alleviate the workload burden faced by healthcare professionals. Our models will significantly reduce the time and effort required for accurate diagnosis, allowing clinical labs to focus on essential tasks and improving overall efficiency. Simultaneously, patients benefit from our models' accuracy and speed that facilitate early intervention and personalized treatment plans.

Our technology will emerge as a leader in the field of medical diagnostics by harnessing the potential of AI and machine learning. Through our models, we will provide accurate, efficient, and non-invasive diagnostic solutions to clinical labs and patients. By streamlining the diagnostic process, we aim to enhance patient care, improve treatment outcomes, and support healthcare professionals in delivering optimal medical interventions. With our innovative technology, we strive to shape the future of medical diagnostics and make a positive impact on global healthcare.

Data reuse: A neglected approach in sustainable data management

Manisha Aswal, Manish Kumar
Department of Biophysics, University of Delhi South Campus

Background

Data management primarily rely on three major approaches that includes data generation which means creation of fresh data, data analysis where the raw data get converted into some meaningful information and data storage where the raw/analysed data is stored. Tirelessly working in these three aspects, but the reuse of data already stored in public databases to enhance downstream analysis has not been highlighted or touched so far.

Objective

To Develop a genome assembly pipeline for bacterial isolates we reused the genomic data available on repositories. Public database contains a huge number of draft/complete genomes for particular bacterial species. These genomes are merely used in further studies. By considering reuse this genomic data, we developed a genome assembly pipeline, named as de-novo reference-based guided genome assembly, that uses both de-novo and reference based approaches. The closest reference was selected from the public repository genomic data.

Method

In this pipeline, pre-processed short-sequence reads were assembled into contigs using the de- novo assembly approach. The assembled contigs are then scaffolded using a reference genome selected on the basis of lowest Mash value and at least 75 % alignment value of contigs. Benchmarking showed a significant increase in the N50 value of assembly using our
approach in comparison to either de-novo or reference based assembly.

Result

Using this pipeline three Escherichia coli isolates from river Yamuna, were assembled and we obtained maximally increment in N50 value leading towards completeness of genome assembly. Also, this pipeline could be easily applied for other bacterial genomes.

TRN analyses reveal cultivar-specific pathways associated with GQS under Drought Stress in Rice

Vaishali Singh, Mukesh Jain
Jawaharlal Nehru university

G-Quadruplex in transcriptome under Drought stress response in Rice is a detailed process regulated via a complex transcriptional regulatory network(TRN). To understand the molecular mechanisms/pathways regulating G-Quadruplex formation under drought stress response in Rice, we thoroughly analyzed transcriptome dynamics during drought response in two cultivars with opposing differences (drought-sensitive, IR64, drought-tolerant, N22). Our analysis identified drought-specific GQSes expression for a significant ratio of the genes in each cultivar. More than 50% of the total GQSes genes revealed significant differential expression in N22 compared to IR64. We found different drought-specific modules of coexpressed genes. Comparative analysis indicated differential drought-specific GQSes of some modules between the two cultivars.
Similarly, we assembled transcriptional regulatory networks(TRN) and recognized important details determining drought-specific GQSes. The results presented that metabolic pathways and biosynthesis of secondary metabolites during GQSes play a specific role in N22(drought-tolerant). Further, we identified quantitative trait loci-associated GQSes-candidate genes containing single nucleotide polymorphisms in the TSS+500bp sequences that differentiate IR64- and N22(drought-tolerant) rice cultivars. The outcomes provide a beneficial resource to examine the function of candidate genes regulating drought-specific-GQSes in Rice.

Impact of polycystic ovary syndrome on women's reproductive outcomes

Ashitha Washington
National Institute of Technology-Calicut

Polycystic Ovary Syndrome (PCOS), impacting 10% of women, has significant reproductive and metabolic implications. Linked to obesity, insulin resistance, and cardiovascular disorders, PCOS presents with irregular menstrual cycles, elevated androgen levels, and ovarian cysts. Increased endometrial cancer (EC) risk suggests potential molecular pathway convergence with ovarian cancer.

The rising PCOS prevalence highlights the need for diverse large-scale studies across
populations. PCOS exhibits four phenotypes, complicating diagnosis and treatment. Current therapies focus on lifestyle changes and symptom relief medications. PCOS origin involves genetic and epigenetic factors, including steroidogenesis-related gene
variations and fetal development epigenetic changes.

Despite declining interest, India's 373 research publications stress regional PCOS variations, necessitating phenotype-based studies. A comprehensive research approach, integrating insilico methods, epidemiology, biomarker identification, and phenotyping, is vital for PCOS understanding and control. Proposed research, using existing datasets, aims to enhance early detection, personalized treatment, and prognostic outcomes.

The study analyzes GSE155489 and Expressiondata_2, identifying 878 significant genes in PCOS patients, indicating disrupted bidirectional communication between oocytes and cumulus cells (CCs). The early endometriosis dataset reveals 26 differentially expressed CC genes, suggesting endometriosis I/II dysregulation. Common genes (CXCL3, CXCL1, NRP2, and CCL20) in endometriosis, PCOS, and endometrial cancer implicate immune response, inflammation, and disease progression. Further research is recommended to validate findings and understand gene functions.

Antifungal Activity of Allyl Methyl Sulfide against Candida albicans: In Vitro and in silico approach

Ziaul Hasan[1*], Asimul Islam[2] and Luqman Ahmad Khan[1]

1. **Department of Biosciences, Jamia Millia Islamia, New Delhi, India-110025**
2. **Centre for Interdisciplinary Research in Basic Sciences, Jamia Millia Islamia, New Delhi, India, 110025**

Background: Across the world, there is a major problem with antifungal medication resistance that is emerging along with an increase in their toxicity. The search for new, more potent medications is necessary. Allyl methyl sulphide (CH2=CHCH2SCH3) is a colourless liquid with a garlic-like odour. It is present in plants such as onions, garlic, and chives and is generated by some bacteria and fungus. Examining AMS's antifungal ability against the human fungal infection Candida albicans is the goal of this investigation.

Methodology: The growth pattern, time kill kinetics, hydrolytic enzyme secretion, morphological investigations, adhesion, and biofilm formation were all examined in in vitro anti-Candida research. Using InstaDock software for molecular docking and the AMBER software package for MD simulation experiments, the AMS-protein interactions with five virulence-associated antifungal targets (Als3, Bcr1, Plb1, Sap2, and Tec1) were evaluated.

Results: AMS exhibited fungicidal properties at 400 µg/ml against Candida albicans, with a minimum inhibitory concentration (MIC) of 200 µg/ml. As demonstrated by growth curve and time kill kinetics experiments, fungal growth was totally inhibited in C. albicans at the corresponding MIC values. Using microscopically monitored buccal cell epithelial tissues, AMS treatment prevents yeast from transitioning into hyphae and from adhering to them. Following AMS treatment, C. albicans showed a significant reduction of extracellular proteinase secretion, phospholipase secretion, and biofilm formation. Human red blood cells (RBCs) shown minimal toxicity to AMS, indicating that it may be a useful substitute for antifungal medications that are currently prescribed. Although stable hydrophobic interactions were observed with

all target proteins, AMS gave a good docking score with Plb1 (-4.0 kcal/mol) and Tec1 (-3.7 kcal/mol). Complexes formed with both these proteins showed stable RMSD profiles except with Bcr1.
Conclusion: Adhesion, biofilm development, and morphological transition are all inhibited by AMS, which binds to proteins essential to Candida pathogenicity. It is safe and extremely effective in treating invasive candidiasis. To fully comprehend its mechanism of action and precise target areas, more research is necessary. The current research must be supported by in vivo and molecular investigations.

Abstracts of Poster presentations

Posters are available in the virtual poster hall on our website
http://rsg-india.iscbsc.org/please-click-here-for-poster-hall/

Glu513-induced collapse of hydrophobic barrier promotes light-induced Jα-helix unfolding in AsLOV2

Syeda Amna Arshi, Manisha Chauhan, and Amit Sharma
Jamia Millia Islamia

The C-terminal Jα-helix of the Avena sativa's Light Oxygen and Voltage (AsLOV2) protein, unfolds on exposure to blue light. This characteristic seeks relevance in applications related to engineering novel biological photoswitches. Using molecular dynamics simulations and the Markov state modeling (MSM) approach we provide the mechanism that explains the step-wise unfolding of the Jα-helix. The unfolding was resolved into seven steps represented by the structurally distinguishable states distributed over the initiation and the post initiation phases. Whereas, the initiation phase occurs due to the collapse of the interaction cascade FMN-Q513-N492-L480-W491-Q479-V520-A524, the onset of the post initiation phase is marked by breaking of the hydrophobic interactions between the Jα-helix and the Iβ-strand. This study indicates that the displacement of N492 out of the FMN binding pocket, not necessarily requiring Q513, is essential for the initiation of the Jα-helix unfolding. Rather, the structural reorientation of Q513 activates the protein to cross the hydrophobic barrier and enter the post initiation phase. Similarly, the structural deviations in N482, rather than its integral role in unfolding, could enhance the unfolding rates. Furthermore, the MSM studies on the wild-type and the Q513 mutant, provide the spatiotemporal roadmap that lay out the possible pathways of structural transition between the dark and the light states of the protein. Overall, the study provides insights useful to enhance the performance of AsLOV2-based photoswitches.

Digging through the class A β lactamase literature applying multi-level analysis

Enakshi Das[1] Dr. Saugata Hazra2,*****

Beta-lactam compounds, known for their strong healing powers, became crucial in treating soldiers during World War II. However, bacteria fought back by using Beta-lactamases, protective enzymes that made these compounds less effective. Unfortunately, using antibiotics, especially those containing Beta-lactams, without caution has led to a big problem called antimicrobial resistance (AMR). Beta-lactamases cleave the amide bond of beta-lactam-based antibiotics, rendering them ineffective & play a crucial role in causing nosocomial infections.

This study looks closely at Class A Beta-lactamase, which has a specific serine active site. β-lactamases are classified according to the scheme of Ambler et al. into four classes, A to D, based on their amino acid sequences. Particularly those in class A contributed to treatment failures in hospital-acquired infections.

Our investigation goes through six main steps: understanding gene and protein sequences, figuring out protein structures, studying how drugs and proteins interact, observing how proteins behave, and looking at interactions in the protein network. In the next part, we discover how these variations interact with six types of Beta-lactam agents: Penicillin, Cephalosporin, Carbapenem, Monobactam, MBI, and BATSI. Our custom automated docking procedure helps these interactions happen, leading to simulations.

The story we create from all this work aims to give us a solid understanding of antimicrobial resistance (AMR). The Hazra Lab keeps a carefully organized collection of this data to add to the Class A Beta-Lactamase compendium. This big effort will change how we see AMR, bringing in new ideas and a powerful tool against harmful bacterial infections.

An insight on how CHT7 restrains it's CXC domain from quiescence repression

Manisha Chauhan , Syeda Amna Arshi , Naveen Narayanan , Haseeb Ul Arfin and Amit Sharma
Jamia Millia Islamia

Microalgae, under nutrient rich conditions, provide biomass. Whereas, nutrient deprivation leads to accumulation of biofuel feedstock, but cells enter quiescence. Net enhancement in feedstock, therefore relies on the precision of the quiescence regulator. In Chlamydomonas reinhardtii, CHT7 is a central regulator of quiescence. Surprisingly, rather than using its own DNA binding domain (DBD) for the regulatory activities, CHT7 recruits external transcriptional regulators using its non DBDs. To ensure smooth functioning, CHT7's DBD must rapidly switch to inactive form. Modifications in DNA binding profiles of DBDs due to non DBDs are seen in transcription factors of many organisms. The switching mechanism discussed could therefore be a generic approach of timely regulation of individual components of the complex transcriptional machineries. Our test results show limited ability of CHT7_CXC to withstand steric forces and provide insights to why and how algal cells may hold back CHT7_CXC's indulgence in quiescence repression.

Systems, methods and devices to detect drug-resistance: BL Testers

Niteesh Kumar Pandey, Subhecchha Baidya, Kunal Dhankhar, and Sugata Hazra

For on-site detection of drug-resistant bacteria, Hazra-Lab developed 3 types of BL Testers; 1. BL-tester Basic, 2. BL tester Advance, 3. BL-Tester Environmental. BL-tester Basic has 3 components, sample preparation vial, BL Tester vial, and dye-containing pouch. Antibiotic was used to screen resistant bacteria in BL tester basic. It can work with, milk, urine, and soil samples. BL-tester Advance would be based on bacteria culturing to reduce the detection time i.e. about 2 hrs. It can work with clinical samples such as body fluids (saliva, pus, blood, etc). BL Tester Environmental, system could detect drug-resistant bacterial presence within a 30-minute of span. This system can work to detect drug-resistant bacteria in wastewater, river water, ponds, and sewage samples. BL Environmental work on 4 types of filter chambers, filter size could be from 1mm to 0.45µm diameter to concentrate bacteria. Chromogenic dye has been used, in every BL Tester which can change its color from yellow (λmax 390) to red (λmax 486) in the presence of drug-resistant bacteria.

The total duration to detect drug resistance was 5 hours for BL tester Basic, while BL tester advance took 2 hours and Environmental took only 30 minutes. The naked eye visualizes results and can be analyzed by an untrained person. The intensity of the color (red) was directly proportional to drug-resistant bacterial load in the samples. BL Testers are easy, fast, reliable, and less costly systems to detect drug-resistant bacteria in clinical and non-clinical samples.

Network Biology-Unraveling The Biological Pathways Using Computational Biological Tools

Pigili Akhil Kumar , E Bharat Raju , P D R Satish
DNR COLLEGE (A)

This paper delves into the intricate realm of epidemiological networks and their pivotal role in modeling the spread of infectious diseases within populations. Leveraging network theory and computational modeling, we explore how contact networks, social interactions, and spatial dynamics collectively shape the dynamics of disease transmission. The paper emphasizes the significance of understanding the underlying structure of these networks in predicting and controlling the diffusion of pathogens.Through a comprehensive review of current research and methodologies, we discuss the application of network theory to epidemiology, highlighting how complex interactions between individuals contribute to the dynamics of contagion. Furthermore, we investigate spatial aspects of disease spread, considering the impact of geographical proximity, travel patterns, and population density on transmission dynamics.The paper also addresses the challenges and opportunities in utilizing epidemiological networks for predictive modeling. We explore recent advancements in data-driven approaches, integrating real-time data and leveraging computational simulations to enhance the accuracy of spread predictions. Additionally, we discuss the implications of these models for public health interventions and policy decisions, emphasizing the potential for targeted strategies in disease containment.As the global landscape continues to grapple with emerging infectious threats, a nuanced understanding of epidemiological networks and disease spread modeling becomes paramount. This paper contributes to the ongoing discourse by synthesizing current knowledge, identifying gaps in research, and proposing avenues for future exploration in the quest to unravel the intricate web of contagion.

Literature mining based profiling of angiotensin-converting enzyme 2

Neelam Krishna, Shivani Tyagi, Pramod Katara
Research student

COVID-19, caused by the zoonotic coronavirus SARS-CoV-2, is not the first coronavirus infection, before this, two severe coronavirus infections were already faced by humans in different parts of the world. COVID-19 is found to be more severe than its previous counterparts and causes respiratory syndrome along with some other pathophysiology effects. The main human protein used by SARS causing coronavirus (SARS-CoV and SARS-CoV-2) is angiotensin-converting enzyme 2 (ACE2), a key member and regulator of RAS. Coronavirus shows a significant affinity with the ACE2, spike protein of the virus participates in this crucial interaction, and initiates the infection cycle of SARS. This ACE2 plays a very significant role in RAS, which directly affects the pathophysiology of humans, mainly respiratory and cardiovascular diseases. Blockage or down-regulation of ACE2 can easily block the virus entry in the cells, but due to the other important role of ACE2, the human system cannot afford its suppression or blockage. Due to its importance, it is required to understand the physiology and pathophysiological role of the ACE2, which can help to develop therapy against SARS. This report provides a detailed account of ACE2 and helps to understand it, which will help to plan a possible way to fight against SARS-CoV-2 and other coronaviruses.

Computational Docking Study of Azadirachta indica for the Treatment and Management of PCOD/PCOS

Sounh Sansar, Khushi Dulwani, Sumiksha Kumariari
Amity University

Background

Polycystic Ovary Syndrome, or PCOS, is a prevalent hormonal condition that usually affects women throughout their reproductive years. Among women, it is one of the most prevalent endocrine abnormalities. PCOS can cause several health problems, including infertility. Although the precise origin of PCOS is unknown, a mix of environmental and genetic factors is likely involved. Key characteristics of PCOS include irregular menstrual cycle, hyperandrogenism, polycystic ovaries, insulin resistance, and metabolic issues. Treatment for PCOS is specifically designed to address symptoms such as hirsutism, irregular periods, and reproductive issues. It frequently involves medicine, such as birth control pills or insulin-sensitizing pharmaceuticals, together with lifestyle changes, such as controlling weight through food and exercise. Current treatments provide only transient relief, highlighting the need to explore untapped therapeutic possibilities, especially those derived from medicinal plants. The neem tree, Azadirachta indica, is well-known for its therapeutic qualities, and there is growing interest in its possible use to treat PCOS, or polycystic ovarian syndrome. According to preliminary research, neem's anti-inflammatory, antioxidant, and anti-androgenic properties may be useful in the treatment of PCOS symptoms. In response, this study concentrates on Azadirachta indica, to identify phytochemicals that have the potential to serve as effective therapeutics for PCOS.

Methodology

Utilizing computational tools and methods, the screening of 56 phytochemicals from Azadirachta indica was done against TNF-α and TNF Receptor 2. The molecular docking study confirmed their potential as candidates for the treatment of PCOS.

Results

Out of the 56 phytochemicals, 19 exhibited promising results. Notably, Scopoletin (docking score: -7.972) and Nimocinolide (docking score: -6.898) emerged as particularly promising candidates for further investigation.

Conclusions

This research sheds light on the potential of Azadirachta indica-derived phytochemicals as novel therapeutics for PCOS. The identified compounds, especially Scopoletin and Nimocinolide acetate, exhibit promise for further research. These findings contribute to the exploration of alternative treatments for PCOS, emphasizing the potential of natural compounds in addressing this complex hormonal disorder.

A Comparative Study on Post Monsoon Flora within and in vicinity of GPCOE Campus

Pradnya Dicholkar, Anisha Gawde, Diksha Naik Mandrekar
Goa University

Backgroud - The project was carried out with the goals of documenting the diversity of the campus, comparing it with the surrounding area diversity and comparing the native species to the exotic species of plants within and around the campus of college.

Methodology - It was a post monsoon survey conducted on a lateritic plateau. Photographs of every plant were taken and the identification was done with the help of local floras and literatures. The scientific names, native place and families were gathered from "POWO".

Result - A total of 106 vascular plant species belonging to 56 families were recorded. Fabaceae, Asteraceae and Apocynaceae were dominant families. There are a total of 78 different plant species i.e. 68% in the college campus belonging to 33 families dominated by Fabaceae and Asteraceae families. In the area around the campus, there are 36 species, i.e. 32% species dominated by Fabaceae and Apocynaceae family. 7.6% similarity was discovered between vicinity and campus. When all plants were considered, 39% of native species and 61% of exotic species were discovered. The species endemic to India were also found - Lepidagathis prostrata Dalzell, Eriocaulon sp, Jasminum auriculatum Vahl, Glyphochloa acuminata (Hack.) Clayton

Conclusion - Exotic invasive species can be detrimental with regards to native plants. Though the exotic species should be allowed to grow, but the introducing and adding of new species should be avoided as they affect the survival of the native plant diversity. This data provide key information for planning and executing right conservation strategies by local management to protect native flora.

Docking Studies on Piper nigrum phytochemicals to treat vitiligo.

Yukti Sabikhi, Meghna, Sounh Sansar, Anshika Singh, Cheena Dhingra, Seneha Santoshi, Hina Bansal Centre for Computational Biology and Bioinformatics, Amity Institute of Biotechnology, Amity University, Noida 201303, Uttar Pradesh, India

Background

Vitiligo is a common depigmenting skin disorder which has affected 0.5-2% of the population worldwide. There is a selective loss of melanocytes which results in a chalky skin. Proteins JAK and CDK1 are the two most common receptors for effective therapeutics for vitiligo. Protein JAK1 belongs to Janus Kinase Family and binds cytokine receptor through amino terminal FERM domains and link them to molecules of the STAT family. The serine/threonine kinase CDK1 forms a heterodimer with cyclin B1 called CDK1/CyclinB1. Piper nigrum also known as black pepper is a commonly used Indian spice has the properties to treat vitiligo. It has anti-carcinogenic and anti-inflammatory properties. This research summarizes the current knowledge on vitiligo and its treatment using Piper nigrum plant.

Methodology

The protein JAK1 and CDK1 were docked with 267 phytochemicals from Piper nigrum using Schrödinger Maestro Suite (version 13.2.138) along with Prime MMGBSA and ADME Analysis.

Result

Out of 267 phytochemicals, 8 showed promising results. Notably , Guaiacol(-6.256), Benzyl Alcohol(-6.054),Carvacrol(-6.036),(E)-Piperolein A(-6.610),Benzyl benzoate(-6.315), and 4-Carvomenthenol(-6.082) emerged as promising candidates for the further investigation .

Conclusion

This research highlights the potential of Piper nigrum derived phytochemicals as novel therapeutics for Vitiligo. The identified compound exhibit promises for further research. These findings contribute to the exploration of alternative treatments for vitiligo, emphasizing the potential of natural compounds in addressing this autoimmune disorder.

Exploring Natural Compounds as Inhibitors of Monkeypox Virus Cysteine Proteinase

Prashant Kumar Tiwari
Sharda University

Monkeypox is a serious viral illness that is rarely seen but is spread from person to person and from animals to humans. The Cysteine proteinase, an essential enzyme involved in the replication of the monkeypox virus (MPXV), is one of many possible therapeutic targets for MPXV. The primary function of this enzyme is to cleave the precursor polyprotein into the distinct proteins required for viral assembly. Researchers are actively engaged to develop potential drugs that can inhibit the proteinase and stop the spreading of the MPXV. In this study, virtual screening, molecular docking, molecular dynamics simulation, and free binding energy calculations were used in order to explore the potential of 569 phytochemicals from a different variety of plants that could inhibit the proteinase of the MPXV. Based on the docking score, the top four compounds (Unii-CQ2F5O6yiy, Lithospermic acid, Kaempferol, and Rhamnocitrin) displayed docking score values ranging from -9.5 to -7.4 kcal/mol and were used for further analysis. Out of these, Unii-CQ2F5O6yiy displayed the docking score of -9.5 kcal/mol, indicating the highest binding to the proteinase. Unii-CQ2F5O6yiy had the most stable and consistent RMSD with < 3 Å. Hence, Unii-CQ2F5O6yiy could be used as potential antiviral agents for further experimental validation against MPXV.

Inhibition of Mycobacterium tuberculosis RpfB by natural compounds: a computational study

Mandeep Chouhan
Sharda University

The majority of the world population (around 25%) has latent Mycobacterium tuberculosis (Mtb) infection, among which only 5–10% of individuals develop active tuberculosis (TB), and 90–95% continue to have latent tuberculosis infection. This makes it the biggest global health concern. It has been reported that the resuscitation-promoting factor B (RpfB) is an exciting potential target for tuberculosis drug discovery due to its significant role in the reactivation of latent TB infection to an active infection. Several attempts have been made to investigate potential inhibitors against RpfB utilizing in-silico approaches. The present study also utilized a computational approach to investigate microbially derived natural compounds against the Mtb RpfB protein which is a very cost-effective This evaluation
used structure-based virtual screening (SBVS), drug-likeness profiling, molecular docking, molecular dynamics simulation, and free-binding energy calculations. Six potential natural compounds, viz. Cyclizidine I, Boremexin C, Xenocoumacin 2, PM-94128, Cutinostatin B, and (þ)1-O-demethylvariecolorquinone A were selected, which displayed a potential binding affinity between -52.39 and -60.87 Kcal/mol MMGBSA score and docking energy between -7.307 Kcal/mol to -6.972 Kcal/mol. All the complexes showed acceptable stability (<2.7 Å RMSD) during 100 ns MD simulation time except the RpfB protein-xenocoumacin 2 complex. This result exhibited that the selected compounds have high efficiency in inhibiting the Mtb RpfB and can be taken into account for additional in vitro and in vivo experimental validation.

Supporting Molecular Level Data in Hazra Lab using Biological Assays

Rajsekhar Adhikary, Saugata Hazra

Antimicrobial resistant (AMR) is one of the most concern in present days and it may leads to the next pandemic in the world. The functional analysis and specific mode of actions should be elucidated to combat this genetic marker and the future pandemic. The primary aims of this study is elucidation of biofilm related genes, their evolution and protein analysis, characterization of the β-lactamase variants with their drug interaction analysis in in vitro conditions and to develop alternate way of therapeutic and diagnostic systems that reduces the antibiotic dependency. The first work here presented about the isolation, characterization and whole genome analysis of the pathogenic bacteria from hemodialysis cuffed catheter tips of infected patients. The second work here presented are the end point analysis of the beta lactamase variants on the basis of their mortality, macromolecular localization by fluorescent microscopy. The third part is the analysis of antimicrobial efficacy and mode of action of designed drug especially boronates and nanoparticles. This entire multidimensional approach will encompasses the entire AMR study.

Leukaemia

Debanjali Adhikary
Amity University

Abstract: Leukemia is an amalgam of cancers and its also called blood cancer. Many people have lost their life due to this cancer.Abnormal growth of cells is called cancer. In simple language we can say that they are actually the abnormal WBC cells which are not fully developed is called leukemia cells. Leukemia cells grow rapidly than as compared to normal cells. The abnormal cells survive longer, build up in larger numbers and enter the bloodstream. In 1811, Peter Cullen defined a case of splenitis acutus with unexplainable milky blood. Alfred Velpeau defined the leukemia associated symptoms and observed pus in blood vessels 1825.In 2012, 3,52,000 people were affected by leukemia and 2,65,000 deaths occurred. AML is the most common type of acute leukemia in adults. CLL the most common chronic adult
leukemia.Chronic leukemias are rare in children.

Molecular Docking and ADME Studies of curcuminoids as human histone deacetylase inhibitors

Annuja Anandaradje[1], Bikashita Kalita[2], Mohane Coumar[2], Sandhiya Selvarajan[1]
1. Department of Clinical Pharmacology JIPMER;
2. Department of Bioinformatics Pondicherry University.

Introduction: Diffuse large B cell lymphoma (DLBCL) is a highly heterogeneous malignant tumour type, in which deregulation of histone deregulation worsens prognosis. Although substantial progress has been made in the development of synthetic HDACi, high toxicity limits their clinical application. This demands the discovery of natural HDACi. Curcumin, a natural polyphenol and a bioactive compound of Curcuma longa is a proven pan HDAC inhibitor exploited in various anticancer treatments. Yet the potential of other curcuminoids is left unexplored.
Objectives: (i) To virtually screen curcuminoids against human HDAC class I, II and IV enzymes and to predict by computational approach the drug likeness property of curcuminoids and approved HDAC inhibitors.
Methods: Homology modelling followed by docking was performed to understand the protein -ligand interactions and binding efficiencies. Further, the study ligands with low binding energy were predicted for pharmacokinetic properties and Lipinski's rule of 5.
Results: Our study revealed that BDMC followed by DMC and curcumin had high inhibitory effect. All of the chosen ligand molecules, with the exception of Romidepsin adhered to Lipinski's rule of five.
Conclusion: The outcome of the present research strengthens the relevance of these compounds as promising lead candidates for the treatment of DLBCL which could help pharmaceutical professionals in further designing of more potent natural drug candidates.

ISCB Regional Student Group India

ISCB Student Council

ISCB-SC RSG India

CBInd 2023-24

Computational Biology India Symposium

10th Jan 2024 | Hybrid Mode

Venue : Biotech Auditorium, University of Delhi South Campus, New Delhi - 110021

CONTACT US

http://rsg-india.iscbsc.org/