ISCB REGIONAL Student GROUP
Bangladesh

ISCB Student COUNCIL
INTERNATIONAL SOCIETY FOR COMPUTATIONAL BIOLOGY

1st RSG Bangladesh CompBio Symposium

Computational Biology for Adapting 4IR

March 10th – 11th, 2023

Bangladesh Reference Institute for Chemical Measurements

Organized by

ISCB RSG-BANGLADESH

Welcome to the 1st ISCB RSG-Bangladesh CompBio Symposium 2023

Dear CompBio Enthusiasts,

We extend a heartfelt welcome to you all to the fist ever CompBio / Bioinformatics Symposium in Bangladesh, the 1st ISCB RSG-Bangladesh CompBio Symposium 2023, on behalf of the organizing team of the International Society for Computational Biology (ISCB Regional Student Group (RSG) - Bangl;adesh.

First and foremost, we would like to thank you who registered to attend the symposium, and we are thrilled to have such an encouraging and diverse community in Bangladesh. Thank you very much!

We have created a comprehensive program that will provide opportunities for networking and learning together by sharing knowledge. We are proud of the fantastic scientific program available for you as part of the first edition of the ISCB RSG-Bangladesh CompBio Symposium, presenting opportunities for students and early career researchers in the form of oral talks and poster networking sessions.

In addition to these formal presentations, we have planned two tutorial sessions, the 1st ever Bioinformatics Olympiad in Bangladesh, and a career-oriented speech from the pioneers in this field at the symposium.

ISCB RSG-Bangladesh's mission is to bring together scientists from computer science, molecular biology, mathematics, statistics, chemistry and related fields to provide an intense multidisciplinary forum for disseminating the latest developments in bioinformatics / computational biology in an in-persion environment. We hope the platform will foster new dialogues, collaboration, and learning opportunities for the Bangladeshi CompBio community.

All of this is possible because of your active participation, support from the community and hardworking, enthusiastic volunteers.

We do hope that you enjoy your participation in the 1st ISCB RSG-Bangladesh CompBio symposium!

Syed Muktadir Al Sium - Symposium Chair
Sanjana Fatema Chowdhury - Symposium Co-Chair

EVENT SEGMENTS

Tutorials | Bioinformatics Olympiad | Keynotes | Invited Talks | Oral Presentations | Poster Presentations | Networking | CompBio CV Bank | Job Fair | Internship Opportunity

EVENT SCHEDULE

1st ISCB RSG Bangladesh CompBio Symposium 2023: Program Timeline		
TIME (UTC+6)		**Timeline**
Start	**End**	
		Day 01 - March 10, 2023 (Online)
09:00	12:30	Basic Bioinformatics Tutorial
12:30	16:00	Prayer and Lunch Break
16:00	17:00	The Art of Writing A Scientific Abstract: Dos and Don'ts
		Day 02 - March 11, 2023 (BRiCM)
08:30	09:00	Gifts, Kit & Food Coupon Collection
09:00	10:30	Welcome Speech, Guests' Speech and Words from Pioneers
10:30	10:50	Keynote
10:50	11:10	Tea Break
11:10	13:00	Oral Presentation Session | Poster Judgement
13:00	14:00	Networking | Prayer & Lunch Break
14:00	15:00	Bioinformatics Olympiad
15:00	16:00	Networking | Poster Visiting
16:00	16:20	Invited Talk
16:20	16:50	Advisor Talk
16:50	17:30	Closing Ceremony | Announcements of the Prize winners
17:30	17:45	Final remarks & Group Photo

Honorable Guests

Professor Dr. Md. Aftab Ali Shaikh, Chairman, BCSIR
Dr. M Sarwar Jahan, Member (Science & Technology), CSO & Director, BCSIR Dhaka Laboratories
Dr. Mala Khan, DG, BRiCM
Prof. Dr. Zeba Islam Seraj, Department of BMB, DU
Prof. Dr. Md. Tofazzal Islam, IBGE, BSMRAU
Dr. Md. Salim Khan, CSO & Director BCSIR Rajshahi Laboratories

Keynote & Invited Talk

Prof. Dr. M. Sohel Rahman, CSE, BUET
Prof. Dr. Khondaker A. Mamun, CSE, UIU

Tutorial Instructors

Dr Farzana Rahman, Assistant Professor, Computer Science, Kingston University London, UK
A.S.M. Rubayet-Ul-Alam, Assistant Professor, Dept. of Microbiology, JUST

Judge Panel

Dr. Md. Murshed H Sarkar, Senior Scientific Officer, BCSIR
Dr. Mustak Ibn Ayub, Assistant Professor, DU
Dr. Sabrina M Elias, Assistant Professor, IUB

Dr. ADA Shahinuzzaman, Senior Scientific Officer, BCSIR
Md. Ibrahim Mia, Assistant Professor, DU
Dr. Mohammad Tanbir Habib, Global Health Fellow, ideSHi

Organizing Team

Chair - Syed Muktadir Al Sium, SO, BCSIR
Co-Chair - Sanjana Fatema Chowdhury, SO, BCSIR
Find the full organizing team here:
rsg-bangladesh.iscbsc.org/symposium2023/organizing-team

Sponsors & Partners

Sponsor - ISCB Student Council; Venue Sponsor - BRiCM; Support - BCSIR; Outreach Partner - STEM Community IUB, Life Sciences Club, IUB, BSMRMU Science Club

POSTERS LIST

P-01

Cardiovascular disease detection using machine learning algorithms

Maria Binte Belal[*1], *Md. Asaduzzaman*[2]
[1]*Daffodil International University*, [2]*University of Rajshahi*

Heart disease and other cardiovascular disorders have surpassed all others as the leading cause of mortality worldwide during the last several decades. Given the many potential causes of heart disease, it is essential to develop effective, efficient methods for making an early diagnosis and taking prompt action to treat the illness. In the healthcare industry, data mining has become more popular as a method for evaluating massive datasets. Researchers use a variety of machine learning and data mining approaches to analyze large, complicated medical datasets to help healthcare practitioners in making heart illness predictions. This research proposes a model that makes use of various supervised learning methods, including the Decision Tree, the Random Forest, the K-Nearest Neighbor, the XG Booster, the Support Vector Machine, the Gaussian Naive Bayes, the Bernays Naive Bayes, and the Logistic Regression, as well as two hyper-parameter optimization strategies, the Grid Search CV and the Randomized Search CV, and three feature selection strategies, the Univariant selection, the Model It makes use of the preexisting UCI collection of people with heart illness. Keeping score in Cleveland. The dataset has 1025 samples with 14 different characteristics. All of these are essential for the proper operation of different algorithms. The goal of this research is to determine how likely it is that participants will develop heart disease. The findings suggest that the Univariant selection method provides the maximum reliable outcomes.

P-03

Innovative nano solver

Md.Asifur Rahman Shaon[1]
[1]*University of Dhaka*

In the era of nanotechnology, we will introduce you to nano-microbiology for solving SDG 6 and adapting 4IR. We choose this because Worldwide, 785 million people lack access to basic drinking water, and 701 million lack basic sanitation facilities. So, we try to design different types of nano solvers using microorganisms (BIOINFORMATICS ANALYSIS) based on nano-microbiological techniques. The main function of those nano solvers is to purify dirty water and reduce pollution. Nanoparticles will be produced by microbes via a bottom-up technique that contains the metal solution and microbes(proteins, membrane, enzymes) and also a sensor(IN SILICO METHOD) that will be capable of sensing actual contaminant, temperature, Ph, organic and inorganic materials in water. So that, our nano solvers will be able to do their function according to the water environment. Our one type of nano solver is made up of double-layer microbial content with a

central carbon metal that acts like a filter. It is capable of maximum organic and particulate adsorption, high filtration capacity, and also maintains low-pressure drop. Another type of nano solver will function in distribution lines of water because it contains a particle that is synthesized from microbes that inhibit bacteria and other organisms, thereby reducing the probability of leakage of pathogenic microbes downstream. Our final type of nano solver will protect against contamination in the reservoir of water by converting toxic materials to non-toxic materials. The capping of the microbial proteins over the metallic nanoparticle surface provides stability to the biosynthetic procedures that would be checked out via PYMOL, SWISS-MODEL, etc. The cost of production of the nanoparticles can be decreased to 1/10th in comparison to the chemical synthesis protocols because of the use of computational biology. Besides, adding fermentative bacteria with nanoparticles can produce dihydrogen and biofuels from the waste materials of water that can play a crucial role in adapting 4IR in our country. So, it can be called green technology due to its clean, safe, non-toxic effects.

P-04

Liver disease prediction using machine learning algorithms

*Senzuti Sharmin**[1]
[1]*Asian University for Women*

Liver disease is a significant public health concern in the Asia Pacific. South Asia appears to have the most cirrhosis deaths globally, with almost 442,000 deaths, followed by the Western Pacific region with around 253,000 deaths. Cirrhosis has led to the death of more men than women, with men accounting for almost 70% of the deaths (Koike, 2020). The diagnosis of liver disease is costly and complicated. The recent advancement of Artificial Intelligence (AI) and Machine learning (ML) plays a significant role in disease detection and prediction of many phenomena. It makes Machine Learning an excellent technique for predicting liver disease prediction. A dataset of Indian liver disease patients was collected from the Kaggle respiratory to perform the Machine learning techniques. This research follows six well-known machine learning algorithms: Logistic Regression, Gaussian Naive Bayes, Random Forest, Decision Tree, Support Vector Machine, and k-Nearest Neighbor to predict liver disease. A comparative study of the algorithmic performances is performed to identify the best practical algorithm in the clinical decision system. The performance of different classification models is evaluated by four metrics such as accuracy, precision, recall, and f1 score. The result shows that LR gives the highest accuracy and f1 score, SVM shows the highest recall and f1 score, and GaussianNB gives the highest precision.

P-05

An in-silico approach to discover efficient natural inhibitors to tie up Epstein-Barr virus infection

*Ayan Das**[1], *Mumtaza Mumu*[1], *Tanjilur Rahman*[1]

[1] *University of Chittagong*

Epstein-Barr virus (EBV) belongs to the herpes virus family and is also named as human herpesvirus 4. EBV is a widespread virus and causes infectious mononucleosis with symptoms like fever, fatigue, swollen lymph nodes and spleen, swollen liver and many more. Additionally, it causes different lymphocyte associated non-malignant, premalignant and malignant diseases. No proper treatment procedure or therapeutic drug is available for EBV induced infections and diseases. In this study, we have searched for proper natural compounds to inhibit EBV glycoprotein L (gL) and block EBV fusion to host cells. We have applied computational approaches including molecular docking and in silico ADMET analysis. We docked 845 natural compounds against gL and found 404 compounds that able to bind effitienty with gL active site and may inhibit gL. Considering binding scores, interaction characteristics, and pharmacokinetic properties, four best compounds acting as most efficient inhibitors were obtained against gL. Compounds with PubChem CID: 4835509, CID: 2870247, CID: 21206004 and CID: 51066638 showed greater docking scores and also non-toxic for human body. These findings can open a new way to an effective drug design against EBV as well as associated infections and diseases.

P-06

Mutational effects of non-synonymous SNPs in Human CDK5: A computational and molecular dynamic studies

Shafiqul Islam[*1], *Jahirul Islam*[1], *Md. Shahadat Hossain*[1], *Md Ackas Ali*[2], *Md. Rimon Parves*[1], *M. Obayed Ullah*[1], *Mohammad A. Halim*[1,2]

[1]*Division of Infectious disease and Division of Computer Aided Drug Design, The Red-Green Research Centre, Dhaka 1215, Bangladesh*

[2]*Department of Chemistry and Biochemistry, Kennesaw State University, 370 Paulding Avenue NW, Kennesaw, GA 30144, USA*

The cyclin-dependent kinase 5 (CDK5) is a serine/threonine kinase that plays a vital role in various cellular processes and functions. Although studies have reported the fact that genetic mutations in CDK5 leads to various neurological disorders and cancers, there is a lack of an extensive study on how the deleterious non-synonymous SNPs (nsSNPs) disrupt its phenotypic effects. In this study, our goal is to discover the structural and functional impacts of nsSNPs in CDK5 by applying computational approaches for identifying deleterious nsSNPs and molecular dynamics (MD) simulation to gain a deeper understanding of the magnitudes of harmful effects. Our results indicated that three most deleterious nsSNPs (R50W, D184E, and R274H), have a noticeable impact on the structure and functions of CDK5. The substitution of D184E facilitate to open the activation loop confirmation might cause pathophysiological role. Also, the R274H alterations caused significant structural changes in the kinase domain of CDK5, including the formation of new coils and turns and the disruption of existing helices and sheets. These changes could potentially affect the kinase activity of the protein. Furthermore, the R50W changes caused a

significant increase in the flexibility of the activator binding domain, which could affect its ability to interact with other proteins. Molecular dynamics simulations revealed higher overall flexibility, decreased intramolecular hydrogen bonds, and lower content of regular secondary structures for R50W, D184E, and R274H mutants when compared to the wild-type structure. In the case of R50W and R274H, loss of the total number of H-bonds may affect the ATP binding site in the catalytic cleft at the interface between the N and C lobes. Together, these findings propose CDK5 as a possible candidate for the development of neurodegenerative diseases and uterine corpus endometrioid carcinoma, and provide structural insights into how disease-susceptible nsSNPs could affect protein structure stability, function, and the interaction network.

P-07

In silico identification of de novo and conserved microRNAs in the genome of the model organism *Marchantia polymorpha*

Nasrin Sultana[1], Mahmudul Hasan Rifat[1], Rahnuma Nurain Tahsin[1], Zannatul Musammat Asfia Islam[1], Ponchom Chandra Bhowmik[1], Mst.Sumaiya Sadia[1]*

[1]Sylhet Agricultural University

The liverwort *Marchantia polymorpha*, one of the well-known study plants in plant biology, is gaining popularity as a new model system. Due to its ease of use in the lab, haploid life cycle, high frequency of transformation, and small genome size, it is frequently used as a model organism for physiological, metabolic, and genetic investigations as well as for evolutionary study (about 280 Mb). As for plant immunity, *M. polymorpha* can tolerate high levels of lead in soils along with other heavy metals, which can be used to determine the genesis and evolutionary processes of plant defense mechanisms. Phylogenetic analysis of land plants shows that it occupies an important position for studying gene regulation. Compared with other terrestrial plants, it has simple gene networks that are involved in a diverse range of biological functions. For the purpose of studying the function of genes, any desired gene can be targeted by miRNAs. MicroRNAs are an important class of short RNAs (sRNAs) that regulate stress, immunity and growth in flowering plants. The discovery of multiple novel and conserved miRNAs has provided an ideal opportunity to further our understanding of the role of miRNAs in the evolution of terrestrial plants. MiRNAs generate precursor RNAs with the particular hairpin structure that regulate the expression of relevant target genes by binding to reverse complementary sections and causing cleavage or translational inhibition of the target RNA. Here, we present an overview of the miRNAs found in liverwort and suggest methods for studying their function in *M. polymorpha*. The *Marchantia polymorpha* genome's 33,722 non-redundant ESTs were allowed to be compared to 3514 known miRNAs from flowering plants for EST-based homology searches, which led to the prediction of 5 potential miRNA candidates from five different miRNA families. The putative miRNAs were made up of 22 nucleotides with (A + U) content in their pre-miRNAs varying from 39% to 60% and MFEI values between -0.52 and -0.95. The study employed a comprehensive computational

methodology, including genetic analysis of specific gene targets, to locate and characterize the conserved miRNAs in the *M. polymorpha* genome.

P-08

An alternative method to detect urinary tract infections through the algorithms of machine learning.

Sadia Islam Badhan[*1], *Afia Nowshen*[1]
[1]*BRAC University*

A review has been done to put forward a computational method on detecting urinary tract infection (UTI) of patients rather than using conventional urine testing. Our focus is to decrease the high rate of diagnostic errors happening in case of UTI and suggest a method of identifying UTI causing organism specifically for emergency cases and primary care where the organism is not yet noticed but the patients start to suffer from UTI or UTI related diseases. Rather than regular urine culture tests which is time consuming and error prone, the concept of machine learning can be used to help detect infectious organisms in UTI patients. In the study, we have acknowledged and collected relevant research papers between 2016 to 2021 where information was gathered for different categories of UTI samples, and further systematic documentation has been conducted under areas of sampling, demographic information (age, sex, etc.), vitals, laboratory results, urinalysis, current outpatient medications, past medical history and physical exam findings. Models have been prepared using different algorithms of machine learning. Data including patient medical history and urine samples were collected, analyzed and matched with initial database setup that includes biological data set of different infectious organisms to compare with the sample. Reports show that the machine learning predictive method has more accurately diagnosed positive urine culture with a less false negative ratio and can be re-categorized from a false negative to a true positive. Furthermore, improved sensitivity was observed when compared to the documents of UTI diagnosis. However, previous research has demonstrated inadequate diagnostic performance for both individual laboratory tests and prediction tools. Different algorithm of machine learning such as random forest, extreme gradient boosting, adaptive boosting, support vector machine, elastic net, neural network, and logistic regression can be used to slowly reduce the labor and save time of UTI tests and decrease the possibility of inaccurate results of conventional methods. The method can be used to detect the susceptibility rate of organisms to drugs avoiding the misuse of antibiotics specifically for patients with co morbidities.

P-09

In silico structural and functional annotation of *Lactobacillus plantarum* hypothetical protein

Pronay Das[1]
[1]*University of Chittagong*

Lactobacillus plantarum is a gram-positive probiotic bacterium, that naturally found in our mouth and gut. It also found in fermented food like yogurt, kimchi etc. It helps to break down foods, absorb nutrients and control "bad" microbes in our digestive tract. *L. plantarum* has recently been used in the medical profession to treat a variety of chronic and cardiovascular diseases, including Alzheimer's, Parkinson's, diabetes, obesity, cancer, hypertension, difficulties involving the urinogenital system, liver disorders, and others. Using a variety of computational approaches and tools, this research investigated and characterized the likely functional characteristics of a hypothetical protein from *Lactobacillus plantarum* (Accession no. VTU65449). The FASTA sequence of protein is retrieved from NCBI, determination of subcellular localization, physiochemical properties, function prediction, secondary structure prediction all are predicted by using online tools like PSORTb, ProtParam, NCBI conserved domain, SWISS Model. The targeted protein is consisting in YvpB super family and functions as a Cysteine peptidase (C39 family). Family C39 includes endopeptidases that are involved in the processing and export of bacteriocins. It is a stable hydrophilic and soluble protein due to its negative GRAVY index. Further analysis predicts, this protein can be used in various clinical aspects.

P-10

Bioinformatics Workshop Fiesta 2020/22: Introduction to Python

*Aakib Bin Nesar**,*
North South University

This abstract describes the workshop that was conducted by the author, as an instructor, for the Bioinformatics Workshop Fiesta (BWF) 2020/22. BWF was organized by the Asia-Pacific Bioinformatics Network (APBioNET), Association for Medical and Bioinformatics, Singapore (AMBIS), Perdana University, Malaysia and Bezmialem Vakif University, Turkey. It was a joint effort that aimed at enhancing bioinformatics skills and competencies in the community. This fiesta spanned a proposed pathway of 15 workshops. The workshop titled, "Introduction to Python" conducted by the author was part of the "Essential" pathway level and the workshop that inaugurated BWF 2020/22. This workshop consisted of 8 sessions, each spanning for 4 hours, once every week. Each session was divided into two parts: A & B, where Session A was spent on covering the theoretical part of the topic and B was spent using that theoretical knowledge into hands-on live coding exercises. The major challenge of this workshop was that it was conducted online via Zoom meetings. The author utilized the Covid-19 lockdown to become proficient in bioinformatics programming using Rosalind and used that enthusiasm into structuring this workshop without following the conventional programming workshops, which proved to be an innovative pedagogical method. Sessions 1 to 6 were designed based on 2 Rosalind bands: Python village and Bioinformatics Stronghold and Sessions 7 and 8 were based on the band Bioinformatics Armory. All these bands consisted of coding problems that were synonymous with the day's topic such as in the topic "Repetition" where the data structure Dictionary was taught, it was shown that in the coding problem "Translating RNA into Protein" an RNA codon table can be built using a

dictionary. This proved to be an effective method as it was seen that by the end of the workshop, every participant was confident of their programming skills as well as showed more enthusiasm to solve bioinformatics problems using python beyond their workshop lectures.

P-11

Bacterial detoxification of tannery waste water

Mst. Saoda Ahmad[1], Mritteka Rahman Rupa[1], Moushifa Mim[1], Tasnim Hosen Tanha[1], Shoaib Saikat[1], Rabiul Hasan[1], MD. Mehedi Hasan Yeamin[1], Hafsa Jahan[1]*

[1]Department of Biochemistry and Biotechnology, University of Barishal

Mismanagement of tannery waste has become one of the most pressing problems of Bangladesh. Chromium, tannin, lead, sulfide, ammonia, cadmium, and other toxic substances are released during the processing step but are not truly detoxified before being dumped in environmental resources like soil and water. Through the application of CRISPR biotechnology, this study intends to develop a genetically modified (GM) bacteria that can concurrently detoxify the hazardous elements such as chromium (Cr6+), tannin, lead (Pb2+), and ammonia (NH3+) present in tannery effluent. The genes that code for the degrading enzymes of these toxic compounds are incorporated into the genome of the GM bacterium, enabling it to remove the harmful effects of these substances from the polluted water and environment. Escherichia coli (E.coli) was found to have a greater specific rate of Cr6+ reduction at lower cell densities, with the highest reduction rate of 86 mg Cr6+ h-1mg-1 dry weight occurring at a cell density of 3 x 10^8 cells mL-1. The hexavalent chromium detoxification will be achieved through the use of the chromium reductase enzyme encoding gene ChrR of E. coli strain K12. For tannin detoxification, the hydrolyzing activity of *Lactobacillus plantarum* will be used. Lead detoxification will be carried out through the use of the lead-tolerant bacterium Pseudomonas aeruginosa. Nitrosomonas europaea's denitrifying abilities will be used to detoxify ammonia. Using the CRISPR biotechnology method, this study introduces a novel feature of the bioremediation of harmful chemicals and heavy metals in tannery waste water. This paper theorized a solution that can be explored to find its implementation feasibility to solve the concerning problem.

P-12

In silico screening of anti-Zika virus compounds to target NS2B-NS3 protease protein of Zika virus influx in the human body using computational tools

Rahat Alam[1], Mahdi Mubin Shaikat[2], Sanjida Ahmed Srishti[2], Nusrat Jahan Lily[2], Hamja Hasanat[3], Tabassum Mounita[4], Minhaz Zabin Saif[4], Abdus Samad[5], Foysal Ahammad[5].*

[1] Department of Genetic Engineering and Biotechnology, Jashore University of Science and Technology,

[2] Department of Mathematics and Natural Sciences, BRAC University,

[3] School of Life Science, Independent University,

[4] School of Health and Life Sciences, North South University,

[5] *Department of Genetic Engineering and Biotechnology, Jashore University of Science and Technology*

ZIKA virus is a recent outbreaks of worldwide belongs to Flaviviridae family that can cause neurological disorder in central nervous system. ZIKA virus single-stranded RNA genome encodes large precursor single polyprotein including 10 viral proteins which is responsible for viral replication when this large single polyprotein is cleaved by NS2B-NS3 protease which have NS3 serine protease needs to cofactor NS2B. For this criteria, NS2B-NS3 protease has been reported an excellent drug target in which effective Flavonoids or compounds can bind to inhibit its cleavage activity.A library of 52 ligands was constructed. From the library on two ligands showed up as effective in the protein binding. These two phytochemicals were selected based of their ADME and toxicity profile. On the basis of molecular optimization, molecular docking and molecular dynamic simulation feature over 200 nanoseconds. The order for target specificity towards 5LC0 receptor is predicted as PubChem CID: 56649692 > PubChem CID: 7267140. With -5.321 (Kcal/mol) binding affinity, and based on the RMSD, RMSF value and the interaction with the protein 5LC0 through hydrogen bond and hydrophobic interactions from the analysis of molecular dynamic simulation; ligand (PubChem CID: 56649692) was the most stable ligands towards the macromolecule.To estimate the best therapeutic efficacies of the designed aromatic ligands, an in silico and in vivo integrative research is to be conducted prior to approaching any clinical trial as Zika Virus drugs.

P-13

Prolonged use of proton pump inhibitors (PPIs) may incline to toxicity, cognitive and behavioral disorders and hinder cancer treatments: In silico study

*Medha Sultana[1], Arifa Farzana Tanha[*2,4], Most. Buni Akter[1], Naima Khondkar[1], Khadiza Nur Rahi[1], Jurana Jahan Deepti[3], Tasnima Haque[4], Maruf Hasan[5], Asif Ahmed[6], Mohammad Mahmudur Rahman[4,7,8]*

[1]Department of Microbiology and Immunology, Bangladesh University of Health Sciences, Dhaka, Bangladesh

[2]Department of Community Nutrition, Bangladesh University of Health Sciences, Dhaka, Bangladesh

[3]Department of Biochemistry and Cell Biology, Bangladesh University of Health Sciences, Dhaka, Bangladesh

[4]Research and Analysis Wing, Health and Nutrition Organization, Dhaka, Bangladesh

[5]Department of Biomedical Engineering, Military Institute of Science and Technology, Dhaka, Bangladesh

[6]Biotechnology and Genetic Engineering Discipline, Khulna University, Khulna Bangladesh

[7]Department of Medical Biotechnology, Bangladesh University of Health Sciences, Dhaka, Bangladesh 8Health and Nutritio Organization, Dhaka, Bangladesh

Proton-pump inhibitors (PPIs) decrease stomach acid production and are among the most regularly prescribed treatments in the world. They accomplish this by permanently blocking the H+/K+ ATPase proton pump in the stomach. The World Health Organization has classified proton-pump inhibitor drugs as essential medicines. However, numerous nations have reported a surge in PPI usage in recent decades. This rise is attributed to the widespread use of PPIs have the common misconception of having minimal side effects. Furthermore, multiple studies have revealed widespread incorrect PPI prescription, as a result, patients with no indication may constitute the majority of users in many societies. The objectives of the study were to revealed the major adverse effects of PPIs through in silico analysis. Chemical structures of PPIs were obtained from different databases. Absorption, distribution, metabolism, excretion and toxicity analysis were conducted with several bioinformatics tools. Gene expression pattern changes due to PPIs were also predicted. We searched the targets of PPIs other than proton pumps. Drug-drug interactions were correspondingly projected. Finally, molecular docking analysis were conducted to know whether PPIs were acted as agonist or antagonist to several receptor they bind. Low clearance and long half-life would make PPIs to stay longer time in body and can interact with several proteins and drugs. High hepatotoxicity was predicted along with the changes in gene expression pattern in hepatic cells. PPIs also found as carcinogens and may facilitate the expression of oncogene like fatty acid synthase. PPIs also found as modulator of androgenic, dopamine and GABA receptors. PPis mostly interferes the cancer drug absorptions. In silico analysis predicted that long time use of PPIs may create toxicity and have risk of cancer initiation and progression in liver and other organs, modulate cognitive and behavioral characters and hinders several cancer treatments.

P-14

Molecular docking approaches to screen out dipeptidyl-peptidase 4 inhibitors form twelve edible plants to treat diabetes

Naima Khondkar[*1], *Most. Buni Akter*[1], *Khadiza Nur Rahi*[1], *Jurana Jahan Deepti*[2], *Medha Sultana*[1], *Farhana Faruque Tule*[1], *Arifa Farzana Tanha*[3], *Tasnima Haque*[3] *and Mohammad Mahmudur Rahman*[3]

[1]*Department of Microbiology and Immunology, Bangladesh University of Health Sciences, Dhaka, Bangladesh*

[2]*Department of Biochemistry and Molecular Biology, Bangladesh University of Health Sciences, Dhaka, Bangladesh*

[3]*Health and Nutrition Organization, Dhaka, Bangladesh*

Dipeptidyl-peptidase 4 (DPP4) is a 110 kDa glycoprotein that is present on the surface of many different types of cells. A number of substrates, such as cytokines, growth factors, neuropeptides, and the incretin hormones, are preferentially cleaved by this exopeptidase to provide N-terminal dipeptides. There is a significant dysregulation in the expression of DPP4 in a number of disease

states, including inflammation, cancer, obesity, and diabetes. The inhibition of DPP4 by the gliptin family of drugs has attracted significant interest for the treatment of type 2 diabetic patients because the incretin hormones glucagon-like peptide-1 (GLP1) and glucose-dependent insulinotropic polypeptide (GIP) are important regulators of post-prandial insulin secretion. In this study, we have retrieved phytochemicals (from Allium cepa, Allium sativum, Azadirachta indica, Cinnamomum zeylanicum, Musa sapientum, Beta vulgaris, Momordica charantia, Aloe vera, Annona squamosa, Coriandrum sativum, Embellica officinalis, and Camellia sinensis) and control drug (sitagliptin, linagliptin, vildagliptin) from zinc and pubchem databases. DPP4 3D structure were downloaded from PDB database. Autodock vina tools were used to dock ligands and enzyme. Control medicines had affinities ranging from -9.2 to -7.5. Stronger affinity values below -7.5 were chosen from the screening findings. Out of the 243 phytochemicals tested, 79 were bound at or above -7.5 afinity. Theaflavin 3,3'-Digallate (-11.3) from tea had the best binding. Among the 79 phytochemicals, 43 are from tea (Camellia sinensis), 17 are from aloe vera, 9 are from neem (Azadirachta indica), 4 are from amla (Embellica officinalis), 2 are from sugar apple (Annona squamosa), and 1 is from coriander (Coriandrum sativum) and bitter gourd (Momordica charantia). Despite the fact that ADMET and molecular dynamic studies are still being conducted, preliminary results indicate that healthy plant consumption may suppress DPP4 enzyme and be advantageous to diabetic patients using GLP1 or GIP medecation.

P-15

Molecular docking approaches to screen out Human Maltase Glucoamylase (MGAM) inhibitors form twelve edible plants for the treatment of diabtes

Most. Buni Akter[*1], Medha Sultana[1], Naima Khondkar[1], Khadiza Nur Rahi[1], Jurana Jahan Deepti[2], Farhana Faruque Tule[1], Arifa Farzana Tanha[3], Tasnima Haque[3] and Mohammad Mahmudur Rahman[3]*

[1]Department of Microbiology and Immunology, Bangladesh University of Health Sciences, Dhaka, Bangladesh

[2]Department of Biochemistry and Molecular Biology, Bangladesh University of Health Sciences, Dhaka, Bangladesh

[3]Health and Nutrition Organization, Dhaka, Bangladesh

Traditional sulfonylureas, biguanides, glinides, thiazolidinediones, -glucosidase inhibitors, glucagon-like peptide-1 (GLP-1) receptor agonists, dipeptidyl peptidase IV (DPP-4) inhibitors, and sodium-glucose cotransporter 2 (SGLT2) inhibitors are among the medications used to treat type 2 diabetes. Since 1990, -glucosidase inhibitors have been used to reduce postprandial glucose levels caused by type 2 diabetes. -Glucosidases play an important role in the human metabolic system and are found mostly in families 13 and 31. Maltase-glucoamylase (MGAM) is a glycoside hydrolase from the glycoside hydrolase family 31. Human Maltase Glucoamylase (MGAM) catalyzes the final glucose-releasing stage of starch digestion; blocking MGAM would cause glucose absorption into the circulation to be delayed. Thus inhibition of MGAM could be benefical

for diabetes patient. Twelve edible plants (Momordica charantia, Aloe vera, Annona squamosa, Coriandrum sativum, Embellica officinalis, and Camellia sinensis) have shown to antidiabetes activities. In this study, we screened out phytochemcials from these plants that can be act as MGAM inhibitors. Phytochemical along with known MGAM inhibitors (salacinol and kotalanol) structures were obtained from zinc and pubchem databases. MGAM 3D structure were downloaded from PDB database. To dock ligands and enzymes, Autodock vina tools were employed. The affinity of the control medicines ranged between -6.4 and -5.6. Stronger affinity values below -5.6 were chosen from the screening findings. A total of 73 phytochemicals out of 130 were bound at or above -5.6 afinity. Procyanidin B1 (-10.2) from tea (Camellia sinensis) and sugar apple binded the best (Annona squamosa). There are 38 phytochemicals from tea, 14 from amla, 8 from aloe vera and sugar apple, and 2 from bitter gourd among the 73. Despite the fact that ADMET and molecular dynamic investigations are still being conducted, preliminary results indicate that healthy plant consumption may suppress MGAM enzyme and be advantageous to diabetic patients.

P-16

Screening of bioactive components from six plants α-amylase inhibitors for the treatment of diabetes

Medha Sultana[1,] Naima Khondkar[1], Most. Buni Akter[1], Khadiza Nur Rahi[1], Jurana Jahan Deepti[2], Farhana Faruque Tule[1], Arifa Farzana Tanha[3], Tasnima Haque[3] and Mohammad Mahmudur Rahman[3]*

[1]*Department of Microbiology and Immunology, Bangladesh University of Health Sciences, Dhaka, Bangladesh*

[2]*Department of Biochemistry and Molecular Biology, Bangladesh University of Health Sciences, Dhaka, Bangladesh*

[3]*Health and Nutrition Organization, Dhaka, Bangladesh*

In diabetes individuals, the enzymes α-amylase breakdown the carbs and raise the postprandial glucose level. This enzyme can be inhibited to manage postprandial hyperglycemia and lower the risk of developing diabetes. Six edible plants (*Momordica charantia*, *Aloe vera*, *Annona squamosa*, *Coriandrum sativum*, Embellica officinalis, and *Camellia sinensis*) have shown to antidiabetes activities. In this study, we screened out phytochemcials from these plants that can be act as α-amylase inhibitors. Phytochemical along with known α-amylase inhibitor (acarbose) structures were obtained from zinc and pubchem databases. α-amylase 3D structure were downloaded from PDB database. To dock ligands and enzymes, Autodock vina tools were employed. The affinity of the control medication was -9.2. Screening results with a higher affinity on or below -9.2 were chosen. Out of the 130 phytochemicals tested, 19 were bound to the active site of -amylase. Theaflavin 3,3'-Digallate (-10.8) from tea had the best binding. 14 phytochemicals belong to tea (*Camellia sinensis*), two to coriander (*Coriandrum sativum*), and one each to amla (Embellica officinalis) and aloe vera. Despite the fact that ADMET and molecular dynamic studies

are still being conducted, preliminary results indicate that healthy tea drinking may suppress -amylase enzyme and be advantageous to diabetic patients.

P-17

Multi-omics bioinformatics approach for the development of new antimicrobials

Nasrat Ahmed Yousha[*1]
[1]*BRAC University*

The effectiveness of current antibiotics is decreasing with the growing antimicrobial resistance (AMR) crisis.The Lack of molecular understanding on various and intricate mechanisms underlying microbes' antibiotic resistance is one of the major causes of AMR phenomenon. This existing problem creates the need for prospective research toward molecular analysis of resistance mechanism in microbes and the discovery of novel antimicrobial compounds for therapeutic purposes. In this regard, modern and technologically advanced computational approaches give a new dimension to antimicrobial drug discovery. In this study, different bioinformatics approaches were reviewed focusing on 'omics technologies' to find potential antimicrobial agents. This project examined the use of bioinformatics to study the mechanisms of action in microorganisms as well as the search for new antimicrobials. All the information was collected from relevant research literature between the years (2012-2022). Results demonstrated that omics approaches (genomics, transcriptomics, proteomics and metabolomics) could be opportunistic for the discovery of new antimicrobial drugs. These approaches can generate a great deal of data which gives us the ability to analyze the underlying molecular mechanism and identify potential antimicrobial targets. Implementation of the latest omics technologies could significantly accelerate the discovery and development of these antimicrobial compounds. Experts have suggested the use of multi-omics bioinformatics as an integral part of antimicrobial drug discovery. However, the challenges in the application of omics technologies to antimicrobial drug discovery need to be addressed for the prevention of antimicrobial resistance. New developments in bioinformatics tools and the appropriate use of bioinformatics resources could show effective results in this aspect.

P-18

Screening of bioactive components from plant-based food through molecular docking as Angiotensin-II Type I Receptor Blockers (ARBs) to reduce several noncommunicable diseases complications

*Mohammad Mahmudur Rahman**[1,2], *Tasnima Haque*[1,2] *and Mohammad Nurul Islam*[1,2]
[1]*Department of Botany, University of Dhaka*
[2]*Health and Nutrition Organization. Dhaka, Bangladesh*

Renin Angiotensin System is an essential regulator of several physiological systems and plays a vibrant role in pathophysiology of diverse organ activities. In several non-communicable diseases, elevated level of Angiotensin-II (AngII) is observed. Activation of Angiotensin-II Type-1 Receptor (AT1R) by AngII is blamed for several disorders in different organs and tissues. Studies showed that AT1R antagonist improve several non-communicable diseases complications including diabetes, cardiovascular diseases, kidney disorders, cancers etc. Food derived bioactive components could be potential AT1R-Blocker (ARB).Molecular docking tools were used to screen bioactive components from different plant-based foods. AT1R three-dimensional structure was derived from PDB-database. A total 1,00,000 ligand structures were acquired from ZINC-database. Several bioinformatics tools were used to prepare protein and ligands before docking. Autodock and allied bioinformatics tools were used for final screening, and analysis. Three synthetic drugs Losartan, Olmesartan, and Telmisartan were used as ligands for control docking. Control ligands showed average binding energy of -7.381 kcal/mol (-6.83 to -8.846 kcal/mol). Among 603 ligands a total 267 were screened whose binding energy were below -7.381 kcal/mol. Catechin(4a->8)gallocatechin(4a->8)catechin of different pod-vegetables, guava, and green tea showed lowest binding energy (-11.634 kcal/mol) to dock AT1R. Phytochemicals from ginger, black tea, pea, lichee, onion, coffee, jackfruits, citrus fruits, garlic, tomato, cabbage, cinnamons, berries, lentils and carrots also bound with AT1R.
These screened photochemicals need to be studied further in dry and wet labs to confirm. This study indicates several diabetes complications can be lessened by taking nutrient-rich foods.

P-19

Molecular docking and pharmacological property analysis of phytochemicals from *Clitoria ternatea* as potent inhibitors of cell cycle checkpoint proteins in the Cyclin/CDK Pathway in cancer cells

Ananna Saha[*1], *Asad ullah*[2]
[1] University Malaya
[2] Jahangirnagar University

Cancer comprises a group of diseases which are involved in the aberrant growth of the cells causing disruption of normal body function. Due to the lack of proper sophisticated treatments this nasty disease leads to the death of most of the patients affected with it. Moreover, treatments like chemotherapy involve other post-treatment complications which make them unfavorable for extended use. Medicinal plants possess many phytochemicals of great therapeutic value and many of them are effective in killing cancer cells. These compounds working by variety of mechanisms and in most of the cases exhibit their anticancer potentiality by inhibiting many proteins involved in cell growth and division. Molecular docking is a computational approach which facilitates the finding of the best molecule from a group which may bind with the highest affinity with the intended target by providing a virtual biological system. This process works on the basis of specific algorithm and involves scoring function to rank the molecules that fit with the target. This study

has been designed to investigate the potentiality of four phytochemicals from *Clitoria ternatea*—Kaempferol, Myricetin, P-Hydroxycinnamic acid and Quercetin as inhibitors of two cell cycle checkpoint proteins—Cyclin Dependent Kinase-2 (CDK-2) and Cyclin Dependent Kinase-6 (CDK-6) in Cyclin/CDK pathway. Quercetin and Myricetin docked with higher affinity with CDK-2 and CDK-6 respectively. Drug likeness property analysis and ADME/T test impose computational approach to investigate physicochemical and pharmacological properties of candidate drug molecules. P-Hydroxycinnamic acid performed well in both drug likeness property analysis and ADME/T than Quercetin and Myricetin. So, P-Hydroxycinnamic acid is the best finding of this experiment.

P-20

Genomic insights into the plant growth promoting novel fungus *Aspergillus welwitschiae* (Oc_Streb1) and its comparative genomics

Nishat Tamanna[*1], *Arifa Akhter Airin*[1], *Md. Iyasir Arafat*[1], *Rifat Ara Begum*[1], *Md. Rakibul Islam*[1], *Zeba I. Seraj*[1]

[1]*Department of Biochemistry and Molecular Biology, University of Dhaka*

Aspergillus welwitschiae (Oc_streb1), an endophytic fungus, isolated from the wild halophytic rice Oryza coarctata, showed to improve growth parameters of commercial rice BRRI Dhan 28 under no stress and 900mM NaCl stressed conditions. For understanding its mechanism of enhancing plant growth at the genetic level, we sequenced the whole genome of this masterly fungal isolate. Genome assembly and gene annotation was conducted using SPAdes, BRAKER2 & AUGUSTUS. The completeness of the gene prediction was assessed with BUSCO. ANI based clustering placed it with the Aspergillus welwitschiae species with a similarity score of over 98% whereas >97% similarity with A. niger strains was found. The final genome assembly was 38 Mbp in size, consisting of a total of ~12,000 protein coding genes. 3,118 SSR were predicted in the Oc_Streb1 genome. We further analyzed the CAZymes families, and secondary metabolite clusters in the Oc_Streb1 genome. The results improve our understanding of the novel Aspergillus welwitschiae (Oc_streb1) genome and will assist in future investigations on the genetic basis of other plant growth promoting endophytic fungi.

P-21

Prognostic significance analysis of KPNA2 in Head and Neck Squamous Cell Carcinoma (HNSCC): An in-silico approach

Susmita Barua[*1], *Uschash Sikder*[1], *Tasnim Sultana*[1], *Silvia Naznin Etu*[1], *Abu Tayab Moin*[1]

[1] *Department of Genetic Engineering and Biotechnology, University of Chittagong, Chittagong-4331, Bangladesh.*

Karyopherin alpha-2(KPNA2) is a bi-directional nucleocytoplasmic transport protein necessary for the transportation of cargo proteins in between cytoplasm and nucleus. Many of the cargo proteins of KPNA2, such as Chk2, NBS1, E2F1 etc, are associated with tumor formation and cancer progression. HNC being the seventh most common cancer has been responsible for around 4,50,000 deaths in 2018 globally. Head and Neck Squamous Cell Carcinoma (HNSCC) accounts for around 90% of total HNC cases. In the early phase, HNSCC patients usually exhibit none to minimal clinical symptoms, because of which more than half of the cases are diagnosed at later stages. This necessitates the development of new specific diagnostic and prognostic biomarkers to facilitate early detection and treatment methods. In this study, our in-silico gene expression analysis shows overexpression of KPNA2 in HNSCC cells compared to normal cells. Furthermore, the overexpression was found to be related to the promoter methylation aberration, copy number changes and resulted in the poor prognosis and survival outcome of patients. Finally, co-expression, correlation and gene ontological analysis were done to identify the pathways related to the progression of HNSCC. To conclude, this study proposes that KPNA2 can be considered as a potential prognostic biomarker of HNSCC for the perception of diagnostic and therapeutic strategies in the near future.

P-22

An immunoinformatics approach to design a multi-epitope vaccine candidate against Mokola virus (MOKV)

Mohammed Sajjad Hossain Bappi[*1], Iqbal Hossain Nafiz[1], Farjana Akter Shahin[1]*
[1]*University of Chittagong*

Mokola virus (MOKV) is an RNA virus belonging to the genus Lyssavirus, which was first isolated from Shrews in Nigeria. Similar to rabies, MOKV can also be transmitted by animal scratches and bites. Currently, there is no vaccination available for humans or animals against MOKV. Despite having similarities, vaccination against Rabies doesn't provide protection against MOKV. Therefore, In this study, the entire proteome of the MOKV was examined using the immuno-informatics methods to develop a potential multi-epitope-based vaccination. Globally available protein sequences were retrieved from Uniport in FASTA format. Protein antigenicity and allergenicity were examined using Vaxijen and Allertop respectively. Non-antigenic and probable allergen proteins were excluded from further analysis. Afterward, Selected proteins were evaluated for both T-cell and B-cell epitope prediction using the IEDB server. Then, probable epitopes were selected from the entire set of epitopes based on their antigenicity, non-toxicity and non-allergenicity. These selected B and T cell epitopes were joined together with the help of linkers and poly-histidine tag H6. Protparam and Soluprot found admissible physical and chemical properties of the constructed vaccine. In the end, several immunoinformatics tools and Molecular Docking simulations verified the efficiency of the designed vaccine against MOKV.

P-23

An in silico approach for evaluating *Caenorhabditis elegans* as a model organism for inorganic arsenic toxicity assessment: a hypothetical study.

*Mumtaza Mumu**[1], *Ayan Das*[1], *Rahul Sharma Rag*[1];
[1]*University of Chittagong.*

Caenorhabditis elegans, also known as roundworms are nematodes that share many characteristics with human despite of distant phylogenetic position. The applicability of *C. elegans* to investigate mutations or gene expression modulations induced by heavy metals in human is still enigmatic. In this study, we screened the open-access GEO of NCBI server and gathered differential expression analysis (DEA) data on *C. elegans* and human individually, in the presence of inorganic arsenic contamination. We conducted functional enrichment analysis of 95 dysregulated genes from *C. elegans* and 263 dysregulated genes from two different human cell lines (HepaRG, PrSPCs) using Enrichr server. Only three of the dysregulated genes of *C. elegans* showed direct orthology to three dysregulated genes from both human cell lines. Again, overall 14.56% of the overexpressed/underexpressed gene products from *C. elegans* found to be orthologous to several human proteins. These data analysis show the high similarity between *C. elegans* and Homo sapiens and reveal the high possibility of heavy metal contamination assessment on *C. elegans* as a model organism. The study hypothesizes the possibility of using *C. elegans* in assessing arsenic toxicity in human and urges for further wet lab research to enquire the expression of orthologous proteins in human in presence of the inorganic arsenic contamination.

ORAL TALKS LIST

O-01

Drug repurposing and computational modeling of potential therapeutic targets of *Mycobacterium tuberculosis* provides insights into anti-tuberculosis drug resistance

Md. Al Amin[*1], Tasnim Pasha Kimu[1], Md. Arju Hossain[1], Shahin Mahmud[1]*

[1]Department of Biotechnology and Genetic Engineering, Mawlana Bhashani Science and Technology University, Tangail, Santosh-1902, Bangladesh

Hundreds of thousands of people per year die from antibiotic-resistant tuberculosis, posing a threat to the entire world. Mycobacterium tuberculosis (Mtb) is a microscopic, rod-shaped, non-motile, strictly aerobic bacterium responsible for tuberculosis. Investigations on how Mycobacterium tuberculosis evades medicines and eventually develops resistance could lead to the creation of innovative therapies and diagnostics. Here, we carried out an extensive analysis of 338 Mtb whole genome sequences through Abricate in order to find antibiotic resistance genes (ARGs), uncover gene-drug and protein-protein interactions, as well as identify regulatory pathways and repurposing drug for the evaluation of potential therapeutic candidates. The coverage and size of the chosen genomes were ≥ 40x and ≥ 4.2 Mbp separately. We detected 32,377 ARGs in 338 genomes from six different ARGs databases, and only 101 ARGs were found to be unique. Additionally, by examining the mechanisms of resistance, we discovered majority of ARGs induced resistance by antibiotic target alteration (62.50%), antibiotic inactivation (23.08%), antibiotic efflux (9.62%), antibiotic target protection (1.92%), and resistance by absence (0.96%). Using twelve distinct techniques, we outlined six hub-proteins (esxA, esxB, esxH, eccE3, mbtK, and eccC3) that are shared by the study populations. Pathway analysis disclosed two vital constituents, primary metabolic process and nitrogen compound biosynthetic process are the most enriched pathways in Mtb that influence resistance. Besides, we suggested some repurposing drug against mbtK resistance protein (PDB ID: 1YK3). Based on five individual gene-drug interaction databases, four drug candidate including Orelabrutinib (-10.1 kcal /mol), Piperacillin (-10.3 kcal/ mol), Piroxicam_cinnamate (-10.9 kcal/mol), and Rilzabrutinib -11.7 kcal /mol) exhibited greater binding affinity compare to binding score of already resistance antibiotics cefepime (-7.3 kcal/mol), Ceftriaxone (-7.4 kcal/mol), Ciprofloxacin (-6.7 kcal/mol) and BOG (-7.1 kcal /mol) control ligand. These, drug mechanisms can be evaluated to explore antibiotic stimulatory effects and Mtb isolates revealed an increased frequency of ARGs resistance mechanisms which must be accounted for in future study. Lastly, the identified hub-proteins may be utilized to develop and design innovative therapies against multi-drug resistance (MDR) Mtb.

O-02

In silico study on the effect of missense mutations of MDM2 in Glioblastoma

Azwada Tabassum[*1], Ashim Kumar Bepari[1]*

[1]*North South University*

Mutation in the human E3 ubiquitine Ligase, MDM2, negative regulator of tumor suppressor protein p53, alters the genes activity, enhancing the tumor progression in glioblastoma. In this study, we aimed to identify the most deleterious nsSNPs (non-synonymous single nucleuotide polymorphism) related to MDM2 gene and identify their structural and functional impact on the protein. Several in silico tools were utilized to identify the nsSNPs in MDM2. The information about nsSNPs on MDM2 was collected from GDC Data Portal. Among the 61 mutations, only the missense mutations (55) were considered for the study. The template MDM2 structure for SWISS-MODEL was collected from RCSB PDB (ID-6Q9L). 11 computational tools were used to identify the most deleterious nsSNPs of MDM2. They are SIFT, FATHMM, PolyPhen 2, PANTHER, SNAP 2, SNPs&GO, Predict SNP, MutPred, Phd Snp, SUSPECT, and PMut. Only the disease causing or most deleterious mutations common in every tool is selected for further study. Structure of both the Wild type and mutated protein was constructed using homology modelling server, SWISS-MODEL. To demonstrate the MDM2 proteins structural conservation, CONSURF tool was utilized. Project HOPE server was utilized to see the effect of amino acid modification on MDM2. The D80Y mutation of MDM2 showed promising results in all the bioinformatics tool. Molecular Dynamics (MD) Simulation was performed for 20ns in this study to understand the dynamic changes in the conformation of wild-type MDM2 and mutant MDM2 (at D80Y) protein structure. The RMSD graph of D80Y depicted that the mutant (D80Y) variant was steadily deviating from the wild type conformation, indicating structural instability. Per residue RMSF value is evaluated where the mutant (D80Y), showed slightly higher RMSF value, implicating instability in the loop region. The compactness of the structure was evaluated by measuring Radius of Gyration (Rg) where the D80Y mutated conformation had higher value, meaning the mutated conformation was adopting expansion. Therefore, after analyzing all the results, the most deleterious mutation was proposed to cause more damage on the progression of glioblastoma.

O-03

Computational epigenetic landscape analysis reveals association of CACNA1G-AS1, F11-AS1, NNT-AS1, and MSC-AS1 lncRNAs in prostate cancer progression through aberrant methylation

Mahafujul Islam Quadery Tonmoy[*1]

[1]*Noakhali Science and Technology University*

Aberrant expression of long non-coding RNAs (lncRNAs), caused by alterations in DNA methylation, is a driving factor in several cancers. Interplay between lncRNAs' aberrant methylation and expression in prostate cancer (PC) progression still remains largely elusive. Therefore, this study characterized the genome-wide epigenetic landscape and expression profiles of lncRNAs and their clinical impact by integrating multi-omics data implementing bioinformatics approaches. We identified 62 differentially methylated CpG-sites (DMCs) and 199 differentially

expressed lncRNAs (DElncRNAs), where 32 DElncRNAs contain 32 corresponding DMCs within promoter regions. Based on Spearman's correlation, a significant negative correlation was observed between 8 DElncRNAs-DMCs pairs. Univariate and Multivariate Cox regression analysis identified 3 (cg23614229, cg23957912, and cg11052780) DMCs and 4 (CACNA1G-AS1, F11-AS1, NNT-AS1, and MSC-AS1) DElncRNAs as high-risk factors for poor prognosis of PC patients. Survival analysis showed that the overexpression of hypo-methylated CACNA1G-AS1, F11-AS1, and NNT-AS1 and down-regulation of hyper-methylated MSC-AS1 significantly lower the survival of PC patients and could be a potential prognostic and therapeutic biomarker. These DElncRNAs were found to be associated with several molecular functions (e.g. GTPase activity, tyrosine phosphatase activity, cis-regulatory region binding, Microtubule binding, kinase activity, ATP binding, translation initiation factor activity, and histone deacetylase activity) whose deregulation can lead to cancer. Involvement of these epigenetically deregulated DElncRNAs in cancer-related biological processes (e.g. up-regulation of the Wilms' tumor 1-associating protein targeted genes, and down-regulation and up-regulation of Histone Deacetylase 3 targeted genes) was also noticed. These findings provide new insights into the understanding of lncRNA regulation by aberrant DNA methylation which will help to clarify the epigenetic mechanisms underlying PC and ultimately reveal the path of future development of lncRNA-based PC-specific biomarkers and therapies.

O-04

Assessment of the association of CYP1A1 gene polymorphisms with the susceptibility of cervical cancer: A case-control study and meta-analysis

*Md Abdul Barek**[1,2], *Mohammad Safiqul Islam*[1,2]

[1]*Department of Pharmacy, Noakhali Science and Technology University, Sonapur, Noakhali-3814, Bangladesh*

[2]*Laboratory of Pharmacogenomics and Molecular Biology, Department of Pharmacy, Noakhali Science and Technology University, Sonapur 3814, Noakhali, Bangladesh*

Cervical cancer (CC) is the second most common type of female malignancy in Bangladesh. Polymorphisms in the CYP1A1 gene have been reported to be associated with CC in different populations. This case-control study with meta-analysis was undertaken to assess the relation of CYP1A1 rs4646903 and rs104893 polymorphisms with the susceptibility of CC. A total of 185 CC patients and 220 healthy controls were recruited, and the PCR-RFLP (Polymerase chain reaction-restriction fragment length polymorphism) technique was applied for genotyping. Again, 42 eligible studies (24 with rs4646903 and 18 with rs1048943) were included, and RevMan 5.3 and Metagenyo web tool were used for performing the meta-analysis. The rs4646903 polymorphism was significantly linked with CC in all association models, namely, additive 1, 2, dominant, recessive, overdominant and allele models (OR=2.41, 4.75, 2.67, 3.61, 2.13, 2.44,

respectively). On the contrary, rs1048943 showed no association (p>0.05) with CC. Haplotype analysis revealed AT and AC haplotypes significantly decreased (OR=0.45) and increased (OR=4.86) CC risk, respectively, and SNPs are in strong linkage disequilibrium (D'=0.912, r2=0.448). Again, rs4646903 carriers with a contraception history and >5 years of taking contraceptives showed an enhanced risk of CC (OR=2.39, OR=3.05). Besides, rs1048943 carriers aged >40 years (OR=0.44), conceived first child aged≤18 years (OR=3.45), and history of contraceptives (OR=2.18) were significantly linked with CC. Our meta-analysis found that codominant 1 (COD 1), codominant 2 (COD 2), codominant 3 (COD 3), dominant model (DM), recessive model (RM) and allele model (AM) in Caucasians and overdominant model (OD) in the overall population are associated with an elevated risk of CC. Our case-control study and meta-analysis summarize that CYP1A1 rs4646903 and rs104893 polymorphisms are correlated with CC risk.

O-05

Predicting hub genes as biomarkers for the prognosis of pancreatic ductal adenocarcinoma by using bioinformatics tools

Tanjilur Rahman[*1], *Pronay Das*[1]

[1]*University of Chittagong*

Among all the other cancers, pancreatic ductal adenocarcinoma (PDAC) is the fourth main cause of cancer-related death in the modern world. PDAC is one of the most aggressive cancer with very poor prognosis due to lack of specific symptoms and well-founded biomarkers. Biomarkers are very critical in cancer diagnosis, surveillance of progression of cancer metastasis and treatment response. Other non-pancreatic cancers have specific well-established biomarkers but there is an absence of biomarkers for PDAC with high sensitivity and better prognostic value. Thus, in this study, we identified some potential hub genes as prognostic biomarkers of PDAC by in silico analysis of differential expressed genes (DEGs). The dataset GSE62165 (n = 131) was retrieved from the Gene Expression Omnibus (GEO) database and DEGs were obtained by using GEO2R which employs GEOquery and limma R packages for producing DEGs. Following that, Enrichr web-server was used to Gene ontology (GO) and pathway enrichment analysis for the DEGs. A protein-protein (PPI) network was established and top 10 hub genes were retrieved using STRING database and cytoscape software respectively. Then protein expression levels of the hub genes in human pancreatic adenocarcinoma were checked and survival analysis was performed to determine clinical significance. A total of 244 DEGs were identified based on p-values (< 0.05) and logFC. Among them, 117 upregulated (logFC > +1) and 127 downregulated (logFC < -1) genes. These DEGs were enriched in extracellular structure organization, platelet aggregation, cell-cell junction, cell-matrix adhesion mediator activity according to GO analyses and also in focal adhesion, pathways in cancers according to KEGG pathway analyses. The constructed PPI network contained 172 nodes and 268 edges. All the 10 hub genes were selected based on their node score (> 10). Among them, 9 genes had high expression level in human PAAD. They also reduced the survival probability. Therefore, these 9 hub genes (ACTB, FN1, ITGB1, ACTA2,

SERPINE1, CFL1, ITGA2, ANXA2, THBS2) were identified for potential biomarkers for better prognosis of PDAC.

O-06

Deciphering the role of novel miRNAs predicted from newly discovered genomic regions of human in collecting duct renal cell carcinoma

Anik Mojumder[*1], *Sazzad Shahrear*[1], *Abul BMMK Islam*[1]

[1]*Department of Genetic Engineering and Biotechnology, University of Dhaka, Dhaka 1000, Bangladesh*

The newly released complete gapless human reference genome, T2T-CHM13, has opened doors to finding new information about the human genome. The newly discovered genomic regions might encode miRNAs that were previously unknown. In this study, we tried to predict the miRNAs from these newly found regions using small RNA-seq data and elucidate their potential role in collecting duct renal cell carcinoma (CDRCC). CDRCC is a rare type of renal cancer having a very poor prognosis. This spreads and progresses faster than other types of renal cancer. After extracting the sequences of newly sequenced genomic regions of T2T-CHM13, we aligned multiple small RNA-seq data to those sequences. Then we performed in silico predictions around the aligned regions and found 156 novel putative miRNAs. We predicted their target mRNAs that are encoded from protein-coding genes and performed enrichment analysis of those genes to find their association with CDRCC. Moreover, we performed differential gene expression analysis using RNA-seq data from a CDRCC study and extracted the differentially expressed genes that are targeted by the novel miRNAs. Here, the pathway and gene ontology enrichment analyses show that the miRNAs can target genes associated with tumor suppression as well as genes that are responsible for cancer progression. Thus, dysregulation of these miRNAs might deactivate tumor suppressor genes and activate proto-oncogenes accounting for the emergence of several cancer pathways. The differentially expressed genes of CDRCC that are targeted by miRNAs enrich multiple signaling pathways that are responsible for cell proliferation, metastasis as well as tumor suppression. A few transcription factors were also found which also showed upregulation in other cancers and might be associated with CDRCC progression. Therefore, we conclude that the novel putative miRNAs, as epigenetic modulators, may have a strong molecular connection with CDRCC as well as other types of cancer due to their targeting of several signaling pathways.

O-07

Integrated bioinformatics analysis for identification of the therapeutic targets of Ibuprofen in lung cancer

Inan Rahman[*1], *Ayan Saha*[2]

[1]*East West University,* [2]*Asian University for Women*

Ibuprofen is a Non-Steroidal Anti-Inflammatory Drug (NSAID) that is vastly used to relieve pain, reduce inflammation and slow down the rising body temperature. Ibuprofen targets various proteins including PTGS2 which has a great impact on cancer. The increased regulation of PTGS2 is also linked with rising cell adhesion, phenotypic changes, resistance to apoptosis, and tumor angiogenesis.The direct protein targets of Ibuprofen were identified from DrugBank. According to the STRING analysis, ibuprofen targets the PTGS2 and BCL2 proteins, which can regulate Small Cell Lung Cancer (SCLC). The genomic data of Ibuprofen in different types of lung cancer was explored by cBioPortal. The comprehensive analysis of tumor-infiltrating immune cells was performed by TIMER. The relationship between the relative expression of PTGS2 in lung cancer was estimated with the help of UALCAN data analysis. PTGS2 expression profiling interactive analysis was performed by GEPIA. PTGS2 expression was correlated with tumor-infiltrating B cell, CD8+T cell, CD4+T cell, macrophage, neutrophil, and dendritic cell in the Lung Squamous Cell Carcinoma (LUSC). A visual summary of alteration across a set of lung cancer samples based on a query of the 2 genes (PTGS2, BCL2) was observed. From the analysis, PTGS2 expression in lung cancer was low and down-regulated. The expression level of PTGS2 was found to be down-regulated compared to normal cells. In a study on mice treated with the drug Aspirin, a low level of PGE2 was found in the plasma as well as in the tumors. On the other hand, the 5′-Adenosine Monophosphate-Activated Protein Kinase (AMPK) level was high (Wong, 2019). AMPK has a great role in cancer prevention as it negatively regulates PTGS2. Ibuprofen is not recommended for lung cancer patients because it inhibits the PTGS2 and BCL2 genes. However, Ibuprofen can be beneficial in cancers that have high levels of PTGS2 expression.

O-08

In-silico design and analysis of Azurin-2-IL-4 fusion protein as an anti-cancer agent targeted to glioblastoma

Syeda Fahmida Ahmed[*1], *Foyez Ahmed Saikat*[1]
[1]*Sylhet Agricultural University.*

Cancer is one of the most serious, puzzling and frightening disease or set of diseases with high incidence and high mortality rate threaten human health and quality of life. Azurin from Pseudomonas aeruginosa is known anticancer bacteriocin, which has the ability to penetrate, specifically human cancer cells and induce apoptosis. Here we employed several linker peptide sequences for construction of the fusion protein and AEAAAKEAAAKA resulted the highest freedom of action against glioblastoma with significant C-score. Moreover, the stability of the constructed fusion protein “Azurin-2-IL-4” identified as 96.03% in favored regions with 0.00% Ramachandran and rotamer outliers. Key feature of this fusion protein was, the binding capacity for its receptor 3BPL with -13.59 global energy without any refinement. Together, these findings of the protein concur that it could be a new antitumor candidate in cancer immunotherapy and can potentially use in cancer treatment as an alternative of chemotherapy and others in clinical trials or studied in-vitro and in-vivo.

O-09

Personalized digital genetic disease detection application

Ashrafi Anjuman Sneha[*1], *Evance John Gomez*[1], *Aurpita Paul*[1], *Rizwana Mehreen Aanila*[1], *Maliha Mehjabin*[1], *Halima Tul Rokeya*[1]

[1]*Department of Life Sciences, Independent University, Bangladesh (IUB), Dhaka, Bangladesh*

The importance of genetic biomarkers in diagnostics is emerging with the discovery of new genetic variants and mutations associated with different genetic disorders every day. Genetic disorders are caused by a change in the DNA sequence, with the possibility of digitizing the genome sequence arising in the near future, comes the prognostic importance of genetic biomarkers in the identification of these disorders through digital means. In this study, a digital mobile application is theorized that will help achieve personalized diagnostics by acquiring an individual's digital genome sequence and placing in cloud computing dependent analysis through a specified server to analyze with genetic biomarkers sequences. Machine learning assisted sequence detecting tools will be used to check for genomic abnormality in the given user sequence. Portable digital genome sequence analyzer is targeted to be rapid, user friendly, and cost effective with maximum security of the user's data. Authentic third-party software will be integrated for precision, with a high accuracy rate and it comes with a data collection for a wide range of genome data including different genetic risk factors linked with several genetic disorders. The application can eliminate the need for stressful trips to the hospital and sample collection. "Sequence IT" will not only make diagnosis more affordable and convenient but also allow users for early detection of diseases.

O-10

Green tea improves working memory and brain function: An in silico *model*

Adittya Sabhayasachi Khan[*1,2], *Rezowana Mannan*[1,3], *Laila Anjuman Banu*[4], *Sohidul Islam*[2] *and Mahmud Hossain*[1]

[1]*Laboratory of Neuroscience and Neurogenetics, Department of Biochemistry and Molecular Biology, University of Dhaka, Dhaka-1000, Bangladesh*

[2] *Department of Biochemistry & Microbiology, North South University, Bangladesh*

[3]*Institute of Epidemiology, Disease Control & Research (IEDCR), Mohakhali, Dhaka-1212, Bangladesh*

[4] *Bangabandhu Sheikh Mujib Medical University, Shahbag, Dhaka-1000, Bangladesh*

Scientific advancements in the past decade have sparked an upswing toward returning to nature. Natural medical derivatives are preferred over synthetic ones due to fewer side effects. Green tea is abundant in bioactive components and vitamins. Although the bioavailability of green tea components seems inadequate by oral administration, they are essential for better health. An in-silico approach was taken to evaluate the correlation of bioactive components of green tea on memory retention, cognitive performance, and the prevention of neurodegenerative diseases that result in memory alterations, dementia, and cognitive dysfunction. The binding of bioactive

components with brain-specific proteins and possible modifications in those proteins due to tea components were illustrated. Four critical brain-specific proteins were evaluated in the present molecular analysis. Cyclooxygenase 1 (COX1), Acetylcholinesterase (AChE), Amyloid-β Precursor Protein (APP1), and Cytochrome P4502D6 (Cyp2D6) were the proteins involved. Their interaction with the bioactive components of green tea was evaluated using computational molecular docking analysis (CMDA). The bioactive molecules were Epigallocatechin gallate (EGCG), L-Theanine, Kaempferol, Coumarin, and Myricetin. The beneficial effect of green tea on memory was prioritized. Noteworthy, CMDA has shown plausible inhibition of proteins known to initiate neurodegenerative diseases, and memory alterations, such as acetylcholinesterase, amyloid-β protein, cyclooxygenase 1, and Cytochrome P4502D6 (Cyp2D6) by kaempferol, myricetin, and EGCG. Our results indicate that EGCG has the highest probability of inhibiting memory-related enzyme AChE in the biological system and thus might have a prominent influence on working memory. In comparison, kaempferol showed significant inhibition of a neurodegenerative disease-related protein COX1. Absorption, distribution, metabolism, excretion, and toxicity (ADMET) prediction strengthened the findings since bioactive components of green tea crossed the blood-brain barrier and influenced short-term memory at low concentrations. In a nutshell, catechins, especially EGCG, flavanol Kaempferol, and myricetin, could lower neuro-inflammation and psychotropic influence while increasing adult neurogenesis, memory retention, cognitive functions, and working memory potential. Significant dosage or concentration in capsulated form might result in long-term effects since both bioavailability and attention to essential components of green tea are scarce.

O-11

Development of multi-epitope based subunit vaccine against Crimean-Congo hemorrhagic fever virus using reverse vaccinology approach

Md. Ashik Imran[1], Md. Rubiath Islam[1], Akash Saha[1], Shahida Ferdousee[1], Moshiul Alam Mishu[1], Ajit Ghosh[1]*

[1]Department of Biochemistry and Molecular Biology, Shahjalal University of Science and Technology, Sylhet 3114, Bangladesh

Crimean-Congo hemorrhagic fever (CCHF) is a viral disease caused by the Crimean-Congo hemorrhagic fever virus (CCHFV) of the Nairovirus genus. CCHF has occurred endemically in several regions of Africa, Southern Europe, and Central and Southeast Asia, with a case fatality rate of 5 to 80%. The World health organization enlisted CCHF as one of the top prioritized diseases for research and development in emergency contexts that making it a public health concern as no efective vaccine is available till date. Therefore, the present study aims to develop an efective multi-epitope subunit vaccine using immunoinformatics and reverse vaccinology

approach against this virus. The B-cell and T-cell epitopes were predicted from structural and non-structural proteins, and fltered by immunogenicity, allergenicity, toxicity, conservancy, and cross-reactivity. The computational analysis revealed that the epitopes could induce an adequate immune response and had strong associations with their respective human leukocyte antigen (HLA) alleles with 98.94% of total world population coverage. Finally, the vaccine with 427 amino acids was constructed by connecting 8 cytotoxic T-lymphocytes, 4 helper T-lymphocytes, and 10 B-cell epitopes with appropriate linkers and β-defensin as an adjuvant. The antigenicity, allergenicity, solubility, and physiochemical properties of the vaccine were evaluated, followed by structural modelling, refnement, and validation. In addition, molecular docking and molecular dynamic simulations revealed a robust binding afnity and stability of the vaccine-immune receptor complex. Moreover, the codons were optimized for its higher expression in Escherichia coli (E. coli) K12 strain followed by in silico cloning. The proposed subunit vaccine developed in this study could be a potential candidate against CCHFV. However, further experimental validation is required to ensure the immunogenicity and safety profle of the proposed vaccine for combating and eradicating CCHFV.

O-12

In silico virtual screening of South African natural compounds against GRK-2 using machine learning based QSAR, molecular docking and molecular dynamics simulation

Md. Asaduzzaman[*1]*
[1]*University of Rajshahi*

Cardiovascular diseases are a group of disorders of the heart and blood vessels that are playing the threatening role against mankind being the most killer diseases of all time. G-protein coupled receptor kinase-2 (GRK2) is considered one of best target for heart diseases for involvement in phosphorylation reaction that eventually block the usual cardiac functionality. A computational method was applied to identify the natural inhibitors against GRK2. A dataset of 308 Bioactive molecules with reported IC50 against GRK2 was obtained from ChEMBL database and utilized in a machine learning assisted quantitative structure-activity relationship (QSAR) study. The best predictive model having R2 value of 0.87599 was generated from 882 types PubChem fingerprints of these molecules and associated in screening of the South African Natural Compound Database of 998 compounds. Top 86 compounds having predictive pIC50 over 5.0 (IC50 = 1×1¬0^-5 nM) was selected for Molecular Docking simulation and ADMET analysis. Top 3 Molecule was selected for Molecular Interaction Analysis and best of them (Bromodeoxytopsentin, Bromotopsentin) were subjected to Molecular Dynamics Simulation for rigidity analysis. Finally, the study finds both Bromodeoxytopsentin and Bromotopsentin could be an effective inhibitor for cardiovascular diseases and a potential candidate for wet lab analysis.

O-13

An immunoinformatics approach for annotation of hypothetical proteins and multi-epitope vaccine designed against the Monkeypox Virus

*Md. Hridoy Ahmed**[1], *Md. Hasan Sayed Rakib*[1], *Nure Sharaf Nower Samia*[2], *Gagandeep Singh*,[3,4], *Vandana Gupta*[5], *Mohammed Faizan Mohammed Mishal*[6], *Alomgir Hossain*[7], *Kamrul Hassan Suman*[8], *Adnan Raza*[9], *Amit Kumar Dutta*[10], *Moriom Akhter Labony*[1], *Jakia Sultana*[11], *Emdadul Haque Faysal*[11], *Sulaiman Mohammed Alnasser*[12], *and Faizul Azam*[13]

[1]*Department of Genetic Engineering and Biotechnology, University of Chittagong, Chittagong, Bangladesh – 4331*

[2]*Department of Life Sciences (DLS), School of Environment and Life Sciences (SELS), Independent University, Bangladesh*

[3]*Kusuma School of Biological Sciences, Indian Institute of Technology, Delhi, New Delhi (India) – 110016*

[4]*Section of Microbiology, Central Ayurveda Research Institute, Jhansi, Uttar Pradesh, CCRAS, Ministry of AYUSH (India)- 284003*

[5]*Department of Microbiology, Ram Lal Anand College, University of Delhi, India 11002*

[6]*IBMBB, University of Colombo*

[7]*Department of Genetic Engineering and Biotechnology, University of Rajshahi, Rajshahi, Bangladesh – 6205*

[8]*Department of Fisheries, Dhaka-1205, Bangladesh*

[9]*Bioscience department, COMSATS university of Islamabad*

[10] *Department of Microbiology, University of Rajshahi, Rajshahi, Bangladesh – 6205*

[11]*Department of Botany, University of Rajshahi, Rajshahi, Bangladesh – 6205*

[12]*Department of Pharmacology and Toxicology, Unaizah College of Pharmacy, Qassim University, Unaizah-51911, Saudi Arabia*

[13]*Department of Pharmaceutical Chemistry and Pharmacognosy, Unaizah College of Pharmacy, Qassim University, Unaizah-51911, Saudi Arabia*

A worrying new outbreak of Monkeypox (MPX) in humans is caused by the Monkeypox virus (MPXV). The pathogen has roughly 28 hypothetical proteins, of unknown function, structure, and pathogenicity. Using reliable bioinformatics tools, we attempted to analyze the MPXV genome, identify the role of hypothetical proteins (HPs) and design a potential candidate vaccine. Out of 28 we identified 7 hypothetical proteins with a high confidence for the presence of conserved domain using multi-server validation. Their physical, chemical, and functional characterizations, including theoretical isoelectric point, molecular weight, GRAVY value, subcellular localization, functional motifs, 3D structures, antigenicity, and virulence factors, were performed. We predicted possible cytotoxic T-lymphocytes (CTL) and helper T-lymphocytes (HTL) epitopes, as well as linear and conformational B cell epitopes, which were combined in a 219 amino acid multiepitope vaccine

with human b defensin as a linker. This multi-epitopic vaccine was structurally modeled and docked with TLR-3. The dynamical stability of the vaccine-TLR-3 docked complexes exhibited stable interactions based on RMSD and RMSF tests. Additionally, in silico cloning of the vaccine was done in an *E. coli* host to confirm the appropriate expression of our final vaccine built. Our results might conform to an immunogenic and safe vaccine, which would require further experimental validation.