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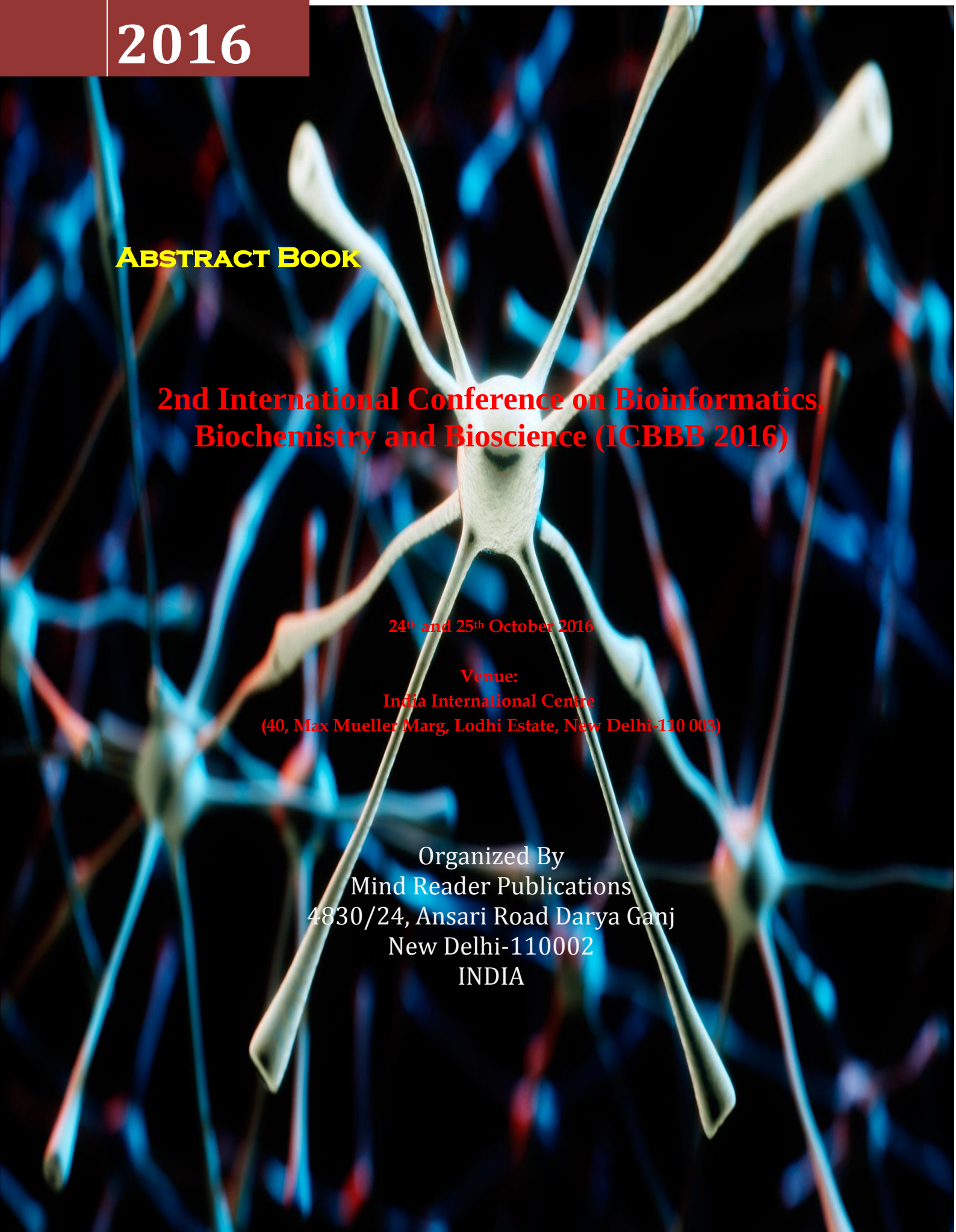

ABSTRACT BOOK

2nd International Conference on Bioinformatics, Biochemistry and Bioscience (ICBBB 2016)

24th and 25th October 2016

Venue:
India International Centre
(40, Max Mueller Marg, Lodhi Estate, New Delhi-110 003)

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Abstract Book

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2nd International Conference on Bioinformatics, Biochemistry and Bioscience (ICBBB 2016)
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ABOUT THE CONFERENCE

The aim objective of the 2016 **2nd International Conference on Bioinformatics, Biochemistry and Bioscience** (ICBBB 2016) is to provide a platform for researchers, engineers, academicians as well as industrial professionals from all over the world to present their research results and development activities in Bioscience, Biochemistry and Bioinformatics. **International Conference on Bioinformatics, Biochemistry and Bioscience** (ICBBB 2016) held in DELHI, INDIA 24th and 25th October 2016.

2nd International Conference on Bioinformatics, Biochemistry and Bioscience (ICBBB 2016)
24th-25th October 2016

Dichotomous Nitric oxide-Release Profiles of Isomeric *N*-nitrosated Secondary Amines Containing an Aromatic Nitrile and a Nitro Group and Inhibition of Human Aortic Smooth Muscle cells Proliferation by the Secondary Amines.

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Abstract

Excessive proliferation of vascular smooth muscle cells (SMC) is an important contributor to the progression of atherosclerosis. Inhibition of proliferation can be achieved by endogenously produced and exogenously supplied nitrogen monoxide, commonly known as nitric oxide (NO). We report herein the preparation of two isomeric families of exogenous nitric oxide-donors, derived from the nitrosation of the corresponding secondary amines. The two families of secondary amines were synthesized using 2,6-difluoro-3-nitrobenzonitrile (2,6-DFNBN) (O family) or 2,4-difluoro-5-nitrobenzonitrile (2,4-DFNBN) (P family) and two equivalents of homologous aliphatic primary amines. QuantitativeN-nitrosation of these diamines was achieved using sodium nitrite and glacial acetic acid in tetrahydrofuran at room temperature. The NO release profiles of each of the N-nitrosated compounds were obtained using Griess reagent, which indicated that NO was released in a slow and sustained manner. The extent of NO release by both families was strongly dependent on the aliphatic chainlength. Unlike our previous findings, the NO release rates of the compounds from the O family decreased with increasing aliphatic chain lengths. On the other hand, the NO release rates of N-nitrosated amines of the P family decreased with decreasing aliphatic chain lengths. In addition both families of amines were found to inhibit proliferations of human aortic smooth muscle cells (HASMC). Details of which will be discussed.

Key Words: Sustained Nitric Oxide Release; Dichotomous NO Release Profiles. Inhibition of (HASMC) proliferation.

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Novel tool for xylan polysaccharides tracking in lignocellulosic biomass and its industrial impacts

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Abstract

Lignocellulosic biomass is a major source for the production of biofuel and several other wood based products. The bioconversion of lignocellulosic substrate to biofuel is a multiple stage process. The enzymatic hydrolysis of the lignocellulosic component to fermentable sugars is a crucial step in this bioconversion. It takes the mixture of complementary (cellulases) and accessory enzyme (hemicellulases). The use of hemicellulases (xylanase) is important to eliminate the significant effect of residual hemicellulose, mostly xylan on the enzymatic hydrolysis of cellulosic component during bioconversion. Xylan has frequentlybeen studied as a physical barrier, which generally cover the outer surface of cellulose fibers and interfibrillar space, limiting the accessibility of cellulase enzymes to cellulose. Hemicellulases are also vital for the prebleaching (biobleaching) of kraft pulp.The redeposition of the xylan on the surface of cellulose fiber during the kraft pulping, inhibit the bleaching process and xylanase enzymes have been found to be most effective for that purpose. However, the cost related to these enzymes are still economically arguable. To make these processes cost effective, it is important to correlate the enzyme loading to the substrate availability.

To do so, one should study the surface chemistry of the lignocellulosic biomass in order to determine that 'up to what extent the surface of cellulose fiber is still covered by hemicellulose, lignin and extractive' after each and every treatment and/or processes. So far tools such as XPS, AFM, ToF-SIMS, gas chromatography, FTIR and various chemical methodologies have been used to study the surface chemistry. However, these standard methods for lignocellulosic biomass analysis are laborious, require specialized equipment, tedious sample preparation and long analysis time. Currently, there are no available toolfor direct, easy and rapid (high throughput) monitoringof xylan on the surface and correlate thisto the amount of xylanaseneeded for optimum pretreatment of lignocellulosicbiomassand/or prebleaching of cellulosic fibers. Considering the importance of the xylan detection in lignocellulosicbiomass, we describe here a novel method, using Carbohydrate Binding Module (CBM) to track xylan on the surface of cellulose fibers which can eventually help to improve the properties of lignocellulosic end products by enhancing bioconversion and/or pulp bleaching by minimizing environment pollutant.

In this study, we have used cellulose fiber from paper industries to demonstrate this novel xylan tracking tool. This tool will help us to optimize the biocatalyst loading and minimize the production cost of the end products of lignocellulosic based industries.

A systems biology approach to study a complex phenomenon of hypoxia

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Abstract

Hypoxia or hypoxiation or ischemia occurs when cells, tissues and organisms receive less than the required levels of oxygen. It may be affect part of the body (localized) or whole body (generalized). It is a complex multifactorial pathophysiological condition which occurs in physiological conditions like wound-repair, embryogenesis, pre-natal birth or in pathological conditions like cardiovascular diseases, stroke, tumorogenesis, inflammation or environmental like ascent to high altitude, deep-sea diving etc. Nearly 2% of the world population representing almost 140 million people reside in high altitudes and are continuously exposed to hypoxia. Different levels and duration of hypoxia cause varying adverse effects from time to time. Inspite of various studies it is still difficult to predict susceptibility and adaptability to hypoxia. We have used a systems biology approach to understand the complex phenomenon. The cellular response to hypoxia involves a coordinated regulation of a myriad of genes at both transcriptional and translational level. There has been intense interest in the cellular response to hypoxia, and a large number of differentially expressed proteins have been identified through various high-throughput experiments. These valuable data are scattered, and there have been no systematic attempts to document the various proteins regulated by hypoxia. Compilation, curation and annotation of these data are important in deciphering their role in hypoxia and hypoxia-related disorders. Therefore, we have compiled HypoxiaDB, a database of hypoxia-regulated proteins. It is a comprehensive, manually-curated, non-redundant catalog of proteins whose expressions are shown experimentally to be altered at different levels and durations of hypoxia. The database currently contains 72,000 manually curated entries taken on 3500 proteins extracted from 73 peer-reviewed publications selected from PubMed. These differentially expressed proteins were used to build a giant core "hypoxia-responsive PPI network" of 603 nodes connected via 4264 edges was built. A backbone network of 24 bottleneck proteins with high Betweenness Centrality and large degree was also identified. The robustness and accuracy of backbone network was validated by 104 test networks. The giant network could be divided into functional subnetworks, each enriched with important and distinct biological pathways. The study is the first methodological network and pathway enrichment analysis and comprehensively describes the global protein-protein interactions; the biological subnetworks and the backbone network regulating the

hypoxic-stress response. In principle, the methodology described may be implemented to understand the molecular mechanisms in other multivariate disorders.

Understanding the changes in expression of HIF responsive genesthrough real time PCR array analysis in lowlander Indian population at high altitude.

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Abstract

Background: Lowland residents adapt to hypoxia at high altitude through a process known as acclimatization. Hypoxia at high altitude is known to directly affect cellular and molecular processes by affecting gene expression.Hypoxia inducible factor(HIF)pathway plays an important role in physiological adaptation to hypoxia and regulates more than 90 genes to its downstream. Present study aim to assess the changes in expression of these genes during high altitude exposure in Indian population.

Observation: The study was carried out on volunteers of lowland Indian population first at basal (800m), followed by high altitude (3200m) exposure (Day 1, 7, 14) & after de-induction (DI) on Day 3. Blood was collected in PAX gene tubes at each time points.RNA was isolated using PAX gene RNA isolation kit (concentration >= 100ng/ul and A260/280 = 1.9-2.1) and run for Real-time PCR on a Human hypoxia PCR array for screening of 84 hypoxia responsive genes. Among these around 20 genes were found to be differentially expressed in terms of fold change with respect to basal. Hypoxia inducible factor-3 (HIF-3), erythropoietin (EPO, helps in erythropoiesis), nitric oxide synthase-3 (NOS-3, catalyze synthesis of nitric oxide responsible for vasodilation) and carbonic anhydrase9 (CA9, very important cellular biomarker of hypoxia and maintain pH) had more than two foldup-regulation in the subjects upon induction. Adenosine A2b receptor (ADORA2B) which belongs to GPCR family is less than 0.5 fold change (2 folddown-regulation) decreased in the population on day 7 and 14.

Conclusion: The study reflects thatthe reduced oxygen partial pressure at high altitudes adversely affects lowlanders and the population senses a considerable amount of stressand hence undergo major changes in HIF associatedgene expression for adaptation purpose.

Keywords: Human hypoxia, RT-PCR, HIF

Analysis of MD simulation trajectories of proteins derived using three forcefields and identification of mobile segments.

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Abstract:

The selection of the forcefield is a crucial issue in any MD project and there is no clear indication as to which of the many available forcefields is the best for protein analysis. Because there are established differences in MD results for different forcefields, we have sought to ask how we could assess common mobility segments from a protein by analysis of trajectories under various forcefields. This is important because, disparate fluctuations appear to be more at flexible regions compared to stiff regions; in particular, flexible regions are more relevant to functional activities of the protein molecule. Therefore, we have tried to assess the similarity in the dynamics using three well-known forcefields ENCAD, CHARMM27 and AMBERFF99SB for 61 monomeric proteins and identify the properties of dynamic residues, which may be important for function. The comparison of popular forcefields with different parameterization philosophy may give hints to improve some of the currently existing agnostics in forcefields and characterization of mobile regions based on dynamics of proteins with diverse folds. These may also give some signature on the proteins at the level of dynamics in relation to function, which can be used in protein engineering studies.

The gross structural features from the trajectories from the 3 forcefields expect for few cases. In all three cases and the correlation in the case of CHARMM –AMBER is better compared to other two combinations. Flexibility index analysis on the proteins indicated that the secondary structural elements might not have any role in the difference in the flexibility index. In addition, the flexibility index in the case of CHARMM and AMBER simulations are more varied than in ENCAD.Although secondary structures are well preserved during the simulations, the tertiary interactions are lost in many proteins and may be responsible for the difference in the some of properties among forcefields. Comparison of simulation results to experimental structures in terms of sRMSF, secondary structures, average ASA and average radius of gyration indicates that the simulations results are on par with the ones derived from

experimental structures. Based on the threshold of nRMSF and conformational properties, we have evaluated the properties of rigid hinge residues and corresponding mobile residues.

In addition, functional relevance of proteins is depicted considering the dynamic mobile residues from each protein from each forcefield simulation with the residues important for the function. It is observed that the number of residues found to be mobile is more in number whencompared to experimental B-factor data.

HOMOLOGY MODELING AND PROTEIN INTERACTION MAP OF CHRNA7 NEUROGENESIS PROTEIN

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Abstract

CHRNA7, protein is a neurodevelopment protein involved in differentiation and neurogenesis, this protein is also named as nicotinic acetylcholine receptors (nAChRs), cholinergic receptor, nicotinic, alpha 7 (neuronal) . The protein encoded by this gene forms a homo-Oligomeric channel, is a major component of brain nicotinic receptors displays that are blocked by and sensitive to alpha-bungarotoxin.studeies shows involvement of CHRNA7 protein in neurological diseases such as Alzheimer's disease , Neuroblastoma , schizophrenia , Neuroblastoma .Till date no structure of CHRNA7 is deposited in PDB database, since protein structure is related with functionality of protein ,in this paper we have done homology modeling of CHRNA7 protein and binding site prediction using Schrödinger software suite .Further protein –protein interaction analysis is done by using string database that shows connection and involvement of this protein in other neurological diseases in reference to pathways. This study can be further used for docking and drug development process and also for pathway mapping that gives insight into function of CHRAN7 protein

Keywords—CHRNA7,neuronal development disease,homology modeling,Schrodinger softwae,proteim interaction

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Assessing the Environmental Exposure and Diversity of the Human Nostril Microbiota by High Throughput Sequencing of 16S rDNA Amplicons

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Abstract

Human body houses trillions of microbes, which form the human microbiota that is susceptible to change due to environmental exposures (e.g. pollution), thus leading to diseases. Therefore, studies related to interaction and deviation of these microbial communities in response to change in the environmental conditions are essential to establish a baseline for health and disease conditions. As compared to culture-based methods used earlier, the application of next generation sequencing has made the microbial identification more accurate and efficient. Especially, the 16S rDNA sequencing has emerged as a low cost and highly reproducible method to study variations in microbial populations. In this study, we have investigated the microbiota of the nostril of 10 individual residing in Kuwait. Thebacterial diversity through 16S rDNA sequencing was determined using the Next Generation Sequencing on Illumina MiSeq platform and variations at intra and interpersonal levels were studied in responses to changes in climatic conditions and weathers, i.e. summer, winter and dust storms. The results suggest that environmental variations greatly affect the types of microbes inhabiting the human nostrils.

This work was supported by Kuwait University Research Administration grants RM01/13 and SRUL02/13.

The Nature of Proteins in Arena viruses

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* **ABSTRACT**

The genome of Arena virus comprises of two single stranded RNA molecules of negative polarity. The virus belongs to the family of Arenaviride and found to infect rodents and humans. These viruses are the causative agent of severe hemorrhagic fever in humans. In the present work we tried to analyze the protein sequences of twenty serotypes of arenavirus at atomic level. The carbon percentage of the proteins retrieved from Uniprot database was calculated using a dynamic programming code. This was further subjected to plotting and statistical analysis. The result indicates that there is a specific threshold of carbon percentage in all the proteins. The analyses reveal a clear cut rise in the carbon atom percentage of the Glycoprotein precursor (GPC) proteins for the twenty serotypes of arenaviruses. The maturation of the envelop GPC is the most important step of arenavirus life cycle. An elevation of carbon content in this protein incriminate that carbon does play an important role in the protein function and can be further used for its characterization.

Keywords: Arena viruses, carbon, Glycoprotein precursor, protein.

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Psychosocial management and online intervention for improving Quality of Life in Cancer Patients.

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ABSTRACT

There is considerable evidence suggesting that cancer patients suffer from substantial and long-term psychological distress associated with different forms of cancer and its medical treatment. An estimated 90% of patients with cancer experience at least moderate pain at some point in their illness, and 42% of patients receive inadequate palliation. Aside from impairing quality of life, uncontrolled pain can contribute to depression, increase the likelihood of suicide, and decrease patient acceptance of potentially beneficial therapy. Psychosocial interventions have proven efficacious for helping Cancer patients and families confront the many issues that arise during this difficult time. There is a need for psychosocial interventions for men with cancer to promote adaptive coping with the challenges and distress associated with diagnosis, treatment and recovery. Interventions are needed that help to overcome barriers to psychosocial treatment such as limited face-to-face psychosocial support services, a shortage of adequately trained professionals and geographical distance. Establishing the information needs of partners and family members of cancer patients is an important, but as yet neglected, area of research. The psychosocial impact of a cancer diagnosis and subsequent treatment, followed by consideration of what appropriate treatment of this level of patient. The interventions to treat distress and improve quality of life in cancer patients are widely available, highly effective, and standardized. This will be followed by a review of the literature detailing the efficacy of psychosocial treatments for cancer patients, and a summary of the literature on medical cost offset, supporting the notion that psychosocial interventions are not only effective, but also economical. Outcomes generally assessed include: psychological functioning, primarily anxiety and depression, and overall quality of life.

KEYWORDS: *Psychosocial interventions, Quality of Life, Psychosocial management, cognitive behavioral therapy for Pain, Emotional Outcomes.*

Computational studies of SPECT Protein (A potential target of *plasmodium*) using molecular modeling and screening of lead compounds.

Supriya Srivastava, Seneha Santoshi and Puniti Mathur

2nd International Conference on Bioinformatics, Biochemistry and Bioscience (ICBBB 2016)
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Abstract

Malaria, a scourge of mankind, imposes a huge socioeconomic burden in tropical countries. Emergence of multi-drug resistant malarial parasites impels us to explore novel drug targets. Liver infection is an obligatory step in malarial transmission, but it remains unclear how the sporozoites gain access to the hepatocytes, which are separated from the circulatory system by the liver sinusoidal cell layer. It is known that, a novel microneme protein, named sporozoite microneme protein essential for cell traversal (SPECT), is produced by the liver-infective sporozoite of the rodent malaria parasite *Plasmodium berghei*. Targeted disruption of the SPECT gene greatly reduces sporozoite infectivity to the liver. The SPECT protein is also present in *Plasmodium falciparum* and is a promising antimalarial drug target. Since the crystal structure of SPECT protein of *Plasmodium falciparum* is not yet available, we aim to determine the 3D structure of SPECT protein in *Plasmodium falciparum* and screening of natural molecules for interaction with the protein using molecular docking and High Throughput Virtual Screening methods. We have constructed the three-dimensional structure of the protein using homology modelling method. SPECT protein of *Plasmodium berghei* 4u5a (pdb id) used as a template for model development. The constructed model revealed appreciable measures when validated. The overall quality of the model, stereochemical values and non-bonded interactions were evaluated using PROCHECK and ERRAT. The PROCHECK results showed 90.9% of backbone angles were in allowed regions with G-factors of -0.16. Ramachandran plot analysis revealed no residue in the disallowed region, 8.0% residues in additionally allowed regions and 1.1 % residues in generously allowed regions. The ERRAT score was 85.714% that is within the range of high quality model. After the development of the model the structure was studied for interaction with the entire library of compounds present in ZINC database of natural compounds. Since nothing was known about the active site of the target protein. The binding site was predicted using sitemap and the entire library was screened against the target. From the entire library of compounds, 276784 compounds were screened using HTVS for the first level of screening. The binding affinity of the compounds was further studied using "Extra Precision" (XP) algorithm of Glide Docking. On the basis of docking scores, 164 compounds were selected for further analysis. The Binding affinity was further calculated using MMGBSA. The interaction studies using molecular docking and MMGBSA revealed appreciable docking scores and ΔGbind. 10 compounds were selected as promising leads with appreciable docking scores in the range of -11.401 to -10.516 kcal/mole and ΔGbind score from -90.092 to -76.152 kcal/mol

Our data generates evidence that the screened compounds indicate a potential binding to the target and need further evaluation. Also the analysis of interaction of these compounds can be exploited for better and efficient design of novel drugs against the said target.

IDENTIFICATION OF NOVEL INHIBITORS AGAINST POTENTIAL TARGETS OF *SALMONELLA ENTERICA*

2nd International Conference on Bioinformatics, Biochemistry and Bioscience (ICBBB 2016)
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ABSTRACT

Salmonella enterica, a rod shaped gram- negative bacterium is a major cause of salmonellosis worldwide inducing enteritis and typhoid fever. There are several drugs and remedies available but as few strains have developed drug resistance it is essential to identify potential drug targets. Subtractive genomics/ proteomics approach have led to potential and novel drug targets. The study includes the structure identification and inhibitor designing against three potential drug targets CDP-6-deoxy-D-xylo-4-hexulose-3-dehydrase, CDP-4-dehydro-6-deoxyglucose reductase and 4-hydroxy-3-methylbut-2-enyl diphosphate reductase. The structures of CDP-6-deoxy-D-xylo-4-hexulose-3-dehydrase, CDP-4-dehydro-6-deoxyglucose reductase and 4-hydroxy-3-methylbut-2-enyl diphosphate reductase were predicted and validated generating 91.5%, 91.5% and 94.5 % accuracy respectively. High Throughput Virtual Screening (HTVS) resulted in 6001 inhibitors for CDP-6-deoxy-D-xylo-4-hexulose-3-dehydrase, 5922 inhibitors for CDP-4-dehydro-6-deoxyglucose reductase and 5375 inhibitors for 4-hydroxy-3-methylbut-2-enyl diphosphate reductase against the ZINC drug database. Eventually docking studies were performed to identify the top 10 inhibitors**.**

Keywords: *Salmonella enterica*, Structure prediction, Docking, Inhibitor.

Biosynthesis of titanium dioxide nanoparticles and study the anti-bacterial property and the toxicity of TiO2 nanoparticles on *E. coli*

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Abstract

Here, I present a low-cost, eco-friendly and reproducible microbes *Bacillus subtilis* mediated biosynthesis of TiO2 nanoparticles. Titanium dioxide nanoparticles synthesized using the bacterium, *B. subtilis*, from titanium as a precursor, which were confirmed by TEM analysis. The morphological characteristics states spherical shape, with size of individual and few aggregate nanoparticles as 30-40 nm.

Microbial resistance represents a challenge for the scientific community to develop new bioactive compounds. Here the antibacterial effect of TiO2 nanoparticles on Escherichia coli strain was investigated, which was confirmed by CFU (Colony-forming unit). Further, growth curve study of E.coli

Hb101 in the presence and absence of TiO2 nanoparticles was done. Optical density decrease was observed with the increase in the concentration of TiO2.

Nano materials are known to inactivate cellular enzymes and DNA by binding to electron-donating groups such as Carboxylates, Amides, Indoles, Hydroxyls, Thiols, and etc. They cause little pores in bacterial cell walls, leading to increased permeability and cell death. This shows that TiO2 nanoparticles have efficient antibacterial effect and have potential to be used as an antibacterial agent for different purposes.

Keywords – *Escherichia coli Hb101, TiO2 nanopart*

EXTRACTION OF ACETYLCHOLINEESTERASE INHIBITORS FROM *IXORA COCCINEA* AND THEIR EFFECT ON ZEBRAFISH (*Danio rerio*)

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ABSTRACT

Alzheimer's is a chronic neurodegenerative disease which in advanced stages causes loss of bodily functions and ultimately leads to death. This is caused due to amyloid plaques, neurofibrillary tangles and decrease in the amount of the neurotransmitter acetylcholine (ACh) in the brain. The reduction in ACh is caused due to the increased activity of acetylcholinesterase (AChE) enzyme which degrades it to Acetic acid and choline. In pursuit of an inhibitor for the aforementioned enzyme, the plant *Ixora coccinea* was chosen. Here, zebrafish (*Danio rerio*) was used as a model due to its repertoire in neurological studies and genetic orthology with humans. Methanolic extracts of the plant were analysed by GCMS method and the *in silico* and *in vivo* experiments were performed. The *in vitro* and *in vivo* studies showed a depletion in enzyme activity on incubation with the plant extract. The outcome of the project showed that the plant contained inhibitors for AChE and could be used as a potential drug to treat Alzheimer's disease.

Key words: Alzheimer's, acetylcholine (ACh), acetylcholinesterase (AChE), zebrafish, GCMS.

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Virtual screening & Docking studies to identify natural inhibitor againstMitogen activated protein kinase kinase 4- Atherapeutic approach for prostate cancer

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Abstract

Prostate cancer is one of the most commonly diagnosed forms of cancer along with second leading cause of death due to cancer in men. Most of the deaths were recorded due to prostate cancer metastasis. Mitogen activated protein kinase kinase 4 (MKK4) has been reported as prometastatic which involves in tumor formation. It is a dual-specificity protein kinase which directly phosphorylates serine, threonine, and tyrosine residues. It playsan important role in mitogen activated protein kinase (MAPK) signaling pathway. Itactivates c-Jun N-terminal kinase and p38 MAPK. Crystal structure of MKK4 is available in PDB. In the present study the crystal structure of MKK4 is retrieved from the protein data bank and high throughput virtual screening and docking studies is been carried out with the natural compound database to identify a novel inhibitor against MKK4. After the virtual screening of ZINC database 1071 compounds were obtained which were further carried out for SP and XP docking.91 compounds were obtained from XP docking. The results of docking were confirmed by determining their binding energies. ZINC13547925 has been selected for further study based on MM/GBSA score.ZINC13547925 had shown glide energy -47.829 kcal/mol. The MM/GBSAscore ascertained the binding efficiency of the ZINC13547925 to be-16.626 kcal/mol. This compound promises to be a potential inhibitor against MKK4, and can be examined for its stability using molecular dynamic simulation approaches, and further validated in wet-lab experimentations.

Acclimatization of potent nitrifying and denitrifying bacterial strains

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Abstract

Water pollution through industrial discharges, which is mainly in the form of effluent or wastewater, is one of the biggest problems. Nitrogen containing compounds released into environment can create serious problems, such as eutrophication of rivers, deterioration of water quality and potential hazard to human health, because nitrate in the gastrointestinal tract can be reduced to nitrite ions. In addition, nitrate and nitrite have the potential to form nitrogenous compounds, which are potent carcinogens.

Microbial treatment systems can be used to overcome this issue which has advantage of being simple in design and low in cost as compared to the traditional chemical treatments. Nitrifying and denitrifying bacteria are involved in the degradation of nitrogenous compounds. Screening of nitrifying and denitrifying potent bacterial strains were carried out by using acclimatization process through semi continuously maintained shake flask technique over a period of six months. The acclimatized stains could be further used for bioremediation of nitrogenous compounds.

Keywords: Acclimatization, Bioremediation, Nitrogenous compounds, Screening.

Acclimatization of potent fungal strains for the degradation of municipal solid waste

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Abstract

Solid waste of each municipal corporation is diversified in nature and highly dependent on the type of area from where it has been collected and there are many options for handing and disposing of these wastes. Composting is the natural biological process in which degradable part of waste is transformed to a stable material with excellent characteristics for application on soils.

This makes the recycling of organic waste as soil amendments a useful alternative to incineration, landfill or rubbish dumps. For sustainable development of potent fungal strains, the microbial community requires critical adaptation by acclimatization process through semi- continuously maintained shake flask technique. During the experiment, the bulk cell mass was exposed to periodic simultaneous acceleration in quantitative content of individual selected nutrient as a substrate. The acclimatization program was conducted for about six month and the developed fungal strains were characterized for ecofriendly, sustainable, efficient composting process.

Keywords: Acclimatization, Adaptation, Composting, Municipal Solid Waste.

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Antibacterial activity of novel synthetic thiazole derivatives

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Abstract

In recent years, due to widespread and frequently usages of antibiotic has led to the rapid emergence of drug-resistant microbes against well known antibacterial agents. In this regard, development of synthetic molecules with novel targets represents an attractive approach. In the present study, we describe the synthesis, biochemical characterization and antibacterial activity of structurally thiazole derivatives namely DPT1 - DPT 7. These DPT compounds are hydrophobic in nature with a molecular weight ranging from 350 to 480 Da. The structures of the DPT compounds were confirmed by IR, mass, ^{1}H, and ^{13}C NMR spectra and elemental analyses data. We observed that DPT compounds showed antibacterial activity against *Staphylococcus aureus*, *Escherichia coli, Enterococcus faecalis*, *Vibrio cholera*, *Listeria monocytogens*, *Bacillus antracis* and *Streptococcus pyogens* in the concentration range of 3.91 to 31.25μM, both in liquid as well as solid media. The time kill kinetics of DPT6 (R=Cl and R_1=CH_3) against *S. aureus and E. coli* showed that the killing was rapid and concentration dependent. The killing was associated with change in the surface morphology of *S. aureus* and *E.coli* cells, as indicted by Scanning Electron Microscope studies of the treated sample. Notably, a combination of non-antibacterial conc. of DPT6 showed a synergic effect in killing *S. aureus* and *E. coli* cells with drugs rifampicin and kanamycin. Taken together, these compounds represent a good template for further design and development of new antibacterial agents.

ISOLATION AND CHARACTERIZATION OF β –SITOSTEROL AND ITS ANTIMICROBIAL ACTIVITY FROM *COMIPHORA WIGHTII*– A RARE MEDICINAL PLANT

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Abstract

Medicinal plants have been in use for the eradication of human sufferings since ancient times. In light of their established therapeutic efficiency, the pharmaceutical industries started to use crude extracts of medicinal plants for manufacturing drug. Commiphora wightii is a flowering plant in the family Burseraceae. Many biological effects have been demonstrated on lipid metabolism, thyroid hormone homeostatsis, female reproductive tissues, and endogenous nuclear hormone receptors. Gum of guggul used in incense, lacquers, varnishes, and ointments, as a fixative in perfumes, and in medicine. Therapeutic uses include treatment of nervous diseases, leprosy, muscle spasms, ophthalmia, skin disorders, ulcerative pharyngitis, hypertension, ischaemia, and urinary disorders. The isolated compound was colourless powder, which was further subjected to IR, NMR for proper characterization and elucidation of the structure. The compound was concluded as β-Sitopsterol.

Key words: Antimicrobial activity, β-sitosterol, Medicinal plants

Comparison of two molecular techniques Polymerase chain reaction and Flourescence *in situ* Hybridization (FISH) for diagnosis of bacterial symbionts in insects.

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Abstract

Identification of bacteria in insects is of major importance for understanding the benefits or losses provided by these bacteria to the host species. These interactions between bacterial endosymbionts and their hosts are important for host's ecology, evolution and fitness. In this study, we have used Polymerase reactin (PCR) and Flourescence *in situ* hybridization (FISH) for identification and localization of bacterial endosymbionts in insect pest whitefly. The insect species is of much importance as it destroys the agricultural crops and horticultural plants worldwide, causing huge economic damages. In this study, the present data represents a comparative analysis for endosymbiont detection using both approaches. For PCR, the bacterial 16S rRNA gene specific primers were used for detection of symbionts, while for FISH, Locked Nucleic Acid (LNA) probes for specific bacterial endosymbionts were used. FISH indicated that the primary endosymbiont *Portiera* was present in all the samples as also detected by PCR. On the contrary, detection of secondary endosymbionts by FISH was significanty higher to detection by PCR. The infection frequency of secondary endosymbiont *Wolbachia* (χ^2=3.25, P=0.05), *Rickettsia* (χ^2=6.13, P=0.01) and *Arsenophonus* (χ^2=6.85, P=0.01) as detected by FISH was significantly higher as compared to

detection by PCR. These results showed the superiority of FISH analysis in detecting bacteria with an added advantage of localization within the insect body.

SICKLE CELL SHAPES THE LIFE

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ABSTRACT

Sickle haemoglobin is a structural variant of normal adult haemoglobin results from a single amino acid of beta globin molecule (β 6Glu→Val). Sickle cell is most common pathological haemoglobin variant in the world. The solution at pH6.75 was prepared from four different chemicals. Populations were screened using solubility test. 20 µl oxygenated blood sample from each subject was mixed in 2 ml solution. 2 ml intravenous blood was drawn from positive samples for further analysis. Electrophoresis of all lysates confirmed patterns differentiation for various haemoglobin variants. The data includes castes and communities, scheduled castes and scheduled tribes in Maharashtra.In Maharashtra, HbS gene ranges from 0 to 35 % among different populations that includes castes, communities and tribes. Some tribal groups exhibit as high as 35 % sickle cell gene. Among the scheduled castes the HbS ranges from 0 to 12 %. In other caste groups HbS ranges from 0 to 16 % while among Brahmin and Muslim populations it ranges from 0 to 4.5 % and 0 to 3 % respectively. Sickle cell present in high frequency among the scheduled tribes as compared to other ethnic groups- castes, scheduled castes and communities. In India some tribal populations exhibit very high frequency (up to 62 percents) of sickle cell gene.

The present study is based on empirical data. The study of sickle cell anaemia can be used as useful genetic marker. The high magnitude of sickle cell gene has been located from South India followed by Central, Western with sporadic cases from Eastern India.

Antihaemolytic Activity of *Cordia africana* Bark (Boraginaceae)

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ABSTRACT

Different parts of *Cordia africana* Lam are used in traditional medicine for treatment of different ailments which include use of the leaf for eye infection, headache, and dizziness, nose bleeding and vomiting during pregnancy. Bark extract is taken against fatigue, root decoction is used for jaundice and schistosomiasis, wood ash is used in certain skin disease. The fruit is reported to be rich in vitamin C, polysaccharides and phenolic compounds. This work is aimed at investigating the effects of the bark extracts on the human erythrocyte stability. *In vitro* antihemolytic activity was evaluated by inducing hemolysis using hypo-saline solution containing (3 %) concentration of sodium chloride solution. NaCl (0.9%) and ascorbic acid were used as negative and positive control respectively. The extract showed varied antihaemolytic activities. At 11 mg/mL, the methanol extract of *C. africana* bark showed maximum percentage inhibition of 98.0 ± 0.35 with IC_{50} = 4.8 mg/mL while ethyl acetate extract showed 69.7 ± 2.00 percentage inhibition with IC_{50} = 6.7. Constituents of the extract detected included flavonoids, glycosides, alkaloids anthraquinones and tannins. The results of this study validate the numerous uses of *Cordia africana* bark in traditional medicine.

LEVELS OF BIOGAS PRODUCED FROM FREE – GRAZING FARM ANIMALS' DUNG IN BAGWAI AGRICULTURAL AREA, KANO - NIGERIA

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ABSTRACT

Bagwai local government area is one of the non-metropolitan locations and an important agricultural area of Kano state. And so the aim of the project is to bring an alternative, environmentally-friendly source of energy for processes that require energy in a bid to developing the area from the readily – available resources. In this, free- grazing farm animals' dung was used as the organic source. Different retention times were used, bacteria involved in the production were investigated and the pH of the slurry before and after the biogas production was measured. Results indicated the presence of *Escherichia coli, Bacillus megaterium, Salmonella* spp *Bacillus licheniformis, Bacillus pumilus, Bacillus brovis, Bacillus alvei, Bacillus lentus, Staphylococcus aureus Yersinia enterocolitica, Proteus vulgaris and Pseudomonas aeruginosa*. Average PH changed from 6.7 – 3.5 for most of the digesters. A highest capacity of 3.21dm^3 was obtained after 11 days while the after 19 days the volume kept declining until the end of the experiment with 0.83dm^3 capacity. Results were significant at 0.05 confidence level.

Keywords: Biogas production, Animals dung, Bagwai, Kano.

Preventive role of Curcumin against hepatotoxic effects of Methotrexate and Cyclophosphamide

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Abstract

Chemotherapy acts by killing cells that divide rapidly. This means that it also harms cells that divide rapidly under normal conditions i.e. bone marrow cells, gastrointestinal tract, hair follicle, etc. resulting in most common side effects. In the present case, we have studied the hepatotoxic effects of two common anti-cancer drugs - Cyclophosphamide and Methotrexate. Methotrexate is used to treat various types of cancer and some autoimmune diseases. As a prodrug, it is converted in the liver to the active form that has chemotherapeutic activity. It integrates a subgroup of substances named alkylating agents, which are effective against slow-growing tumors that damage cells at any phase of cellular growth. Methotrexate's therapeutic and toxic effects are a result of its ability to limit DNA and RNA synthesis by inhibiting dihydrofolate reductase and thymidylate synthetase. It enters cells through an active transport system used by folate and binds to and inhibits the enzyme. This enzyme maintains reduced folate by recycling dihydrofolic acid which has been produced during thymidylate synthesis. Dihydrofolate reductase reduces folic acid to tetrahydrofolate, an essential co-factor in the synthesis of purine nucleotides. In the present study, Swiss Albino mice (Mus musculus) were injected with sublethal doses of Cyclophosphamide and Methotrexate with varying dosage and exposure periods. Mice were tested for hepatotoxicity by estimating the common biochemical parameters. The highest toxic dose was treated with Curcumin supplementation, which reduced the toxic effects. The present study will help in better understanding of side effects of usage of these common chemotherapeutic drugs and measures to prevent these side effects.

Keywords — Methotrexate, Cyclophosphamide, hepatotoxicity, Curcumin

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Evaluation of the antioxidative potential of Bee Products: Pollen and Bee Bread against *Staphylococcus aureus*

2nd International Conference on Bioinformatics, Biochemistry and Bioscience (ICBBB 2016)
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Infected Balb/c mice

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Abstract

Pollen is the male plant reproductive part and is a rich source of proteins, collected by worker honey bees for the rearing of their larvae. Before feeding pollen to its larvae honey bees add some enzymatic secretions and store it in the cells of the comb as '**bee bread'**. It was investigated whether water extract of pollen and bee bread exerts antioxidative effect against *Staphylococcus aureus* infected BALB/c mice. The *in vivo* liver damage of BALB/c mice weighing between 25 to 30 g was induced by intraperitonial injection of *S.aureus* ($5x10^6$ CFU/ml bacterial solutions). All the animals were sacrificed on the 16th day by decapitation. *S. aureus* induced toxicity produced oxidative stress in mice which caused increase in *Lipid peroxidase* (LPO) and decrease in *Glutathione* (GSH), Chloramphenicol acetyl transferase (CAT), *Superoxide dismutase* (SOD), Glutathione S transferase (GST), Glutathione peroxidase and glutathione reductase levels. The treatment with pollen and bee bread during the present study caused decrease in the level of LPO and increase in other antioxidant enzymes which showed the positive effect of both bee products pollen and bee bread against bacteria and compared with antibiotics Ampicillin and Amoxycillin as positive control. The study concluded that the water extract of pollen and bee bread had protective effect against *Staphylococcus aureus* induced toxicity in mice liver.

Key Words: antioxidative potential, pollen, bee bread, intraperitonial, *Staphylococcus aureus*

Expectation – Maximization algorithm for protein – ligand complex of HFE gene

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Abstract

In the field of pharmaceutical sciences and biomedicine, the issue of protein stabilization presumes meticulous importance. It plays a significant role in purification, formulation, and storage. Suitably folded proteins are usually stable during expression and purification. The interaction between ligands and proteins generally produces changes in protein thermal stability with changes in the midpoint denaturation temperature, enthalpy of unfolding, and heat capacity. The stability of eleven mutations of the proteins corresponding to HFE gene are identified using Random forest and Support vector machine. Various parameters like Half-life period, Aliphatic index and GRAVY are computed using online webservers. Based on the machine learning techniques and the parameters the ligands for HFE proteins are obtained. The contact surface area between ligand atom and protein atoms are also identified. The expectation – maximization algorithm was done on the contact surface area to test whether there exist any change in the destabilizing contact between the ligand atom and protein atoms.

Keywords— Hemochromatosis, Random forest, Support vector machine, expectation – maximization algorithm.

Docking studies of Hemochromatosis protein with various compounds of the medicinal plants

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Abstract

Hemochromatosis is a genetic disorder which leads to the accretion of iron in parenchymal organs leading to organ toxicity. Normal absorption of iron from daily food is 10% whereas people with hemochromatosis diseases can absorb iron four times more than the normal absorption. There is no proper medication and clinically proved medicines have side effects. Hence an alternative methods is

the extraction of bioactive compounds from the medicinal plants to recognize the novel target. 17 compounds from 13 medicinal plants with 81 properties were collected from database. 81 properties with certain specific conditions were checked for accuracy using various machine learning techniques. The compounds that satisfies the pharmacological properties are docked with the mutated protein of hemochromatosis. The free energy, and the interaction analysis were also discussed.

Keywords— Hemochromatosis, bioactive compounds, medicinal plants, docking , Epigallocatechin -3 gallate,Aloin.

Rotation Forest Ensemble Algorithm for the Classification of Phytochemicals from the Medicinal Plants

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Abstract

Drug Discovery from Medicinal plants is an important area in current research. This area of research has been providing important source of new drug leads. Plant extracts are proved as main source for many drugs. A major part of traditional therapy uses plant extracts or the associated active principles. Many of the traditional medicines are made as a result of applying some small synthetic modifications of naturally obtained substances. But most of the modern medicines are using synthetic substances instead of natural substances obtained from medicinal plants. In the study different compounds and their properties which are proved as vital for a decision to conclude the acceptability for a drug are considered. A machine learning predictive algorithms are applied to classify the compounds to the defined classes. The accuracies of the different classification algorithms are analyzed. The study shows the significance of Rotation Forest ensemble algorithms in the classification of medicinal plant compounds. The other algorithms analyzed are Decision Tree, Random Forest and Naïve Bayes. The Random Forest tree based ensemble outperformed the other algorithms in this study.

Keywords: Medicinal Plants - Chemical compounds –Drugs - Machine Learning – Classification- Rotation Forest-Accuracy measures.

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CYTOTOXICITY, APOPTOTIC ACTIVITY AND PHYTOCHEMICAL ANALYSIS OF RHIZOME EXTRACT OF *AMOMUM PTEROCARPUM* THWAITES

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ABSTRACT

Cytotoxic and apoptotic effect of aqueous rhizome extract of *Amomum pterocarpum* was analysed using *Allium cepa* assay. *A. cepa* roots were exposed to various concentrations (0.1%, 0.05%, 0.01% and 0.005%) of the extract for 24 h. Mitotic index and chromosomal aberrations were analysed. Several clastogenic and non clastogenic abnormalities were observed. Apoptotic effect was analysed using Evans blue test. In general a positive correlation has been observed between concentration of the extract and cytotoxic and apoptotic activities. Preliminary phytochemical analysis using standard methods showed the presence of bioactive constituents like alkaloids, steroids, flavonoids, terpenoids, phenols and tannins. The cytotoxic and apoptotic activities of *Amomum pterocarpum* rhizome extract thus reveals its therapeutic potential.

KEYWORDS: *Allium cepa, Amomum pterocarpum*, Apoptotic, Cytotoxic, Mitotic index

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In-silico modelling of DTNBP1, NRG1 and AKT1 gene target of Schizophrenia for protein structure analysis

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Abstract

Schizophrenia (SZ) is a chronic mental and heritable disorder mainly recognized by neurophysiological impairment and neuropsychological abnormalities and is strongly associated with three genes viz; dysbindin (DTNBP1), neuregulin (NRG1) gene and AKT1 (v-akt murine thymoma viral oncogene homolog1). The three genes are present on different chromosomes besides other genes associated with Schizophrenia, but the exact cause for this disease is not known. In the present work, through

bioinformatics techniques the analysis of the above three genes was performed. The primary analysis (molecular weight, pI etc.) of proteins obtained from these genes was done through Protparam server, for secondary and tertiary structural analysis SOPMA, SOSUI, TMHMM were used. Homology modelling was done using Phyre 2 server with structural validation through Rampage server. These 3D models can further be used for drug development against this particular disease.

Keywords— Schizophrenia, Dysbindin, Neuregulin, AKT1, SOPMA, SOSUI, TMHMM.

Effect of NaCl Stress on Physiological Parameters of four Rice varieties (*Oryza sativa* L.)

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ABSTRACT

Plants in natural and agricultural conditions are continuously exposed to several biotic and abiotic stresses such as drought and salinity. The objective of this study was to compare the salinity tolerance of four locally cultivable different varieties of rice varieties (Niranjan, Ranjan, Swarnamasuri and Maharaja) to assess their biochemical responses like reducing sugar, proline and malondialdehyde content and morphological effect like shoot and root growth rate. The response against stress showed a gradual reduction in shoot growth in all four varieties of rice was decreased 57.3-80.6% and 69.7-79% in 200mM of NaCl concentration in comparison to control on 10 days and 15 days span respectively. In biochemical estimation the proline accumulation, reducing sugar accumulation and malondialdehyde content there were sharp increase in all varieties of rice with respect to the increasing level of salt stress but the rate decreases as the time of exposure is increased. As in case of Maharaja variety the proline accumulation increase was 4.6 times and slowly reduced to 3.6 times, similarly for malondialdehyde content increase was 1.6 times and became 1.4 and also in reducing sugar accumulation the trend was 1.4 times and reduced to 1.1 times in 200mM of NaCl concentration with respect to control in 10days span and 15days span respectively. This study reveals all the four locally cultivable rice varieties of rice seedlings were trying to cope up as the time of salt exposure is increased.

Key words: Rice, Salt Stress, Reducing sugar, proline, lipid peroxidation

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Molecular Docking studies of Resveratrol Against Neurodegenerative Diseases

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Abstract

Neurodegenerative diseases refer o the impairments in human body which arise due to progressive degeneration of nerve cells. In such cases, neurons undergo the structural as well as the functional damage. Parkinson's disease, Alzheimer's disease, amyotrophic lateral sclerosis, multiple sclerosis and systemic lupus erythematosus are major neurodegenerative diseases. The most common reason of neurodegenerative disease is the excess generation of free radicals inside the body which results into a condition called oxidative stress. Neurons are more susceptible to the damage caused by oxidative stress as compared to the other tissues of the body. In this paper we have done molecular docking of Resveratrol against proteins involved in neurodegenerative diseases six proteins were selected from different neurodegenerative diseases and docking is performed using Schrödinger software. Docking of Resveratrol with protein targets shows good binding affinity of Resveratrol against neuronal diseases. Docking results signifies potential role of Resveratrol against neurodegenerative diseases.
Keywords—Neurodegenerative Disease, Resveratrol, Molecular Docking, Alzheimer's disease, Parkinson's disease

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Removal of Baseline Wander from ECG using CEEMD and Adaptive Morphogocial Function

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Abstract

ECG is a documentation of the electrical activities of the heart and it is used for the identification of a number of cardiac imperfections. Quite ECG signal get tainted by various kinds of artifacts, thus in order

to gain proper information from them they must first be denoised. Baseline wander is one of the most common artifact in ECG. CEEMD shows better denoising performance compared to EMD and EEMD. Results also prove that morphology of an ECG signal drastically improved by using adaptive SE in morphological functions. Proposed method presents a novel approach for the filtering of baseline wander artifact of ECG by using a cascade of CEEMD and morphological functions using adaptive structuring elements. By using this novel approach for denoising of baseline wander artifact, it is ensured that the morphological information present in the ECG signal remains preserved and denoising performance is independent of heart rate and external factors. Proposed method is compared with all latest methods and results prove that proposed method provide far superior denoising and morphological results in terms of output Minimum Square Error, Output Signal to Noise Ratio and Correlation Coefficient.

Index Terms - ECG, Morphological Operators, EMD, EEMD, CEEMD, Baseline Wander.