



International Conference on
**“Recent Advances in Biotechnology, Biomolecules
and Pharmacy RABBP – 2020”**
17th to 19th December, 2020



Organized by
Department of Biotechnology
K.L. University
Greenfields, Vaddeswaram, Guntur District, Andhra Pradesh-522 502

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About Department of Biotechnology, K L University

The department of Biotechnology at K L University was established in the year 2002-03 with an aim to provide scientific and technical solutions to mankind. Biotechnology is a congregation of science and technology which embeds basic principles of Physics, Mathematics, Chemistry and Biology. The department went for accreditation by NBA of AICTE for the first time in 2007, and was accredited for three years. The department also attracts foreign students from Middle east, African countries, Nepal and Bhutan.

The department offers a four year undergraduate engineering degree in Biotechnology with specializations in Medical Biotechnology, Bioinformatics, Industrial Biotechnology and Genetic Engineering. The department offers a post graduate program in Biotechnology, which is embedded with one year project in an industry/research organization. The department offers PhD programs in vivid specializations on a full time and part time basis.

The strength of the department is its very rich treasure of faculty who were drawn from reputed National and International Academic and research organizations. Faculty with good industrial experience and exposure are also a part of our team at the Department of Biotechnology. Faculty with post doctoral research experience and faculty with more than 15 years of experience are feathers in the cap of our department.

The faculty of the department is extensively involved in quality Research and Development. The department over the last three years has acquired projects worth more than 3 crores in the areas of Biofuels, Biomedical research, Genomics, Proteomics, Bioinformatics and food biotechnology in vivid fields of biotechnology funded by prestigious research organizations like DBT, DST, UGC and ICMR. The department also has a couple of women scientists working under DST funded projects. The department has filed patents with IPO in collaboration with industry and a few from sponsored projects.

The department has 7 well furnished and fully equipped state of the art laboratories along with 4 research centres. The department also has its own computer center with latest molecular modelling and drug design software purchased from Schrodinger LLC, USA.

As a part of student centric learning various measures and initiatives are taken to improve the skills of students. These include exposure to guest lectures, industrial training and tours, communication and soft skills, Mini Projects, paper presentations in national level paper contests, class room seminars, placement opportunities, academic and career counseling, certificate courses, live projects in industry, exposure to journals and so on.

Another area of concentration for the faculty is Research consultancy. The department has signed MoU's with various Industries and research organizations for faculty and student training and collaborative research. The department of Biotechnology is collaborating with AIT, Thailand for initiating collaborative research in various areas of Biotechnology.

ORGANIZING TEAM

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Er.KoneruSathyanarayana
President, K L E F



Message

Warm and Happy greetings to all.

I am immensely happy that Department of Biotechnology of our K L University is organizing an **International Conference on Recent Advances in Biotechnology, Biomolecules and Pharmacy (RABBP)** from 17th to 19th December 2020 and is going to discuss on a collection of technical papers in the proceedings.

Department of Biotechnology, K L University continues to march on the way of success with confidence. On this occasion, I wish all the very best.

I congratulate HOD, staff members, students of Department of Biotechnology, Delegates and Participants from different parts of the country and nations for their efforts in participating in this conference and wish the conference all the success.

K. Sathyanarayana



Sri Koneru Raja Hareen
Vice-President



Message

I am glad to learn that Department of Biotechnology, K L University is organizing an **International Conference on Recent Advances in Biotechnology, Biomolecules and Pharmacy (RABBP)** from 17th to 19th December 2020. It is heartening to know that the international RABBP-2020 is being organized with the objectives to strengthen the current national and international scenario of Biopharmaceuticals; scaling up from research to production and their usage; thereby prevention and protection from many deadly diseases/disorders.

I wish the conference all success.

K. Raja Hareen



Dr.L.S.S.Reddy
Vice-Chancellor



Message

I am delighted to know that the Department of Biotechnology of our K L University is organizing an **International Conference on Recent Advances in Biotechnology, Biomolecules and Pharmacy (RABBP)** from 17th to 19th December 2020. It gives me an immense pleasure that a souvenir is also being brought out.

I am sure that it will provide a platform to discuss the research in Biotechnology happening throughout the world. I hope that the participants from all over the country and abroad would interact on the subject for upgrading their knowledge and skills to enhance their utility to the Biotechnology sector.

My best wishes for the success of the conference.

L.S.S. Reddy



Dr.K. Giridhar

Head, Department of Biotechnology

Convenor, RABBP-2020



Message

I, on behalf of the Faculty of Biotechnology feel proud in organizing an **International Conference on Recent Advances in Biotechnology, Biomolecules and Pharmacy (RABBP)** from 17th to 19th December 2020. During the conference, participation of people from different disciplines is expected to take place on common platform and sharing of views with eminent speakers from all over the World This conference will help the students, researchers and academicians to interact with professionals and build the scientific network.

I wish the conference a grand success.

K.Giridhar

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Physico-chemical characterization of fecal sludge for resource recovery

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Abstract:

Over a billion people in urban and peri-urban areas of Africa, Asia, and Latin America are served by onsite sanitation technologies. Until now, the management of faecal sludge resulting from these onsite technologies has been grossly neglected. The appropriate and adequate management of faecal sludge deriving from onsite technologies is imperative for the protection of human and environmental health. The first step in designing faecal sludge (FS) treatment technologies that will meet defined treatment objectives is to characterise the FS to be treated. There is currently a lack of detailed information on the characteristics of FS. However, research is actively being conducted in this field. Failure to quantify nutrients in faecal sludge usually leads to its poor disposal resulting into surface water and groundwater pollution. Therefore, this study was conducted to determine and model the distribution of nutrients in pit latrine sludge as a step towards reuse of available nutrients. Sampling was done at 0.0, 0.5, 1.0 and 1.5 m depths from 31 lined and 31 unlined latrines during rainy and dry season. Physico-chemical characteristics such as chemical oxygen demand (COD), dissolved oxygen (DO), moisture content, temperature and nutrients including ammonia, nitrate, total nitrogen, phosphorus and potassium were determined. Results indicated that COD, temperature and DO decreased and moisture content increased with sludge depth. There was no significant variation ($P > 0.05$) in nutrients and physico-chemical properties except COD. Strong correlations of $R^2 \text{ Adj} > 0.85$ were obtained between modelled and measured values. The relative root mean square error of the predicted nutrients was less than 10%. Results revealed that the model is good estimator phosphorus concentrations in lined pits followed by total nitrogen in unlined pits and nitrates in lined pits.

Keywords: *Latrines, Faecal sludge, Nutrients, Physico-chemical properties, Sanitation*

Crocin inhibits urea-induced amyloid formation by bovine lactoglobulin

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Abstract:

®-lactoglobulin (®-LG), a major whey protein, is able to form amyloid fibrillar aggregates, when subjected to urea-induced denaturation at pH 7.0. Crocin, being a polar carotenoid, was used to investigate its influence on the urea-induced unfolding of ®-LG and formation of amyloid fibrils. Crocin was observed to enhance the stability of ®-LG at pH 7.0 and inhibited the formation of amyloid fibrils when incubated for 12-30 days at 37°C in the presence of 3-5 M urea. The inhibition by crocin on ®-LG amyloid formation in a concentration-dependent manner exhibited a clear correlation between the midpoint of urea denaturation and lag time. Crocin was found to form a complex with ®-LG with K_d of 4×10^{-7} M and it could be considered a potential therapeutic agent in the treatment of protein aggregation phenomena.

Keywords: *Amyloid fibril, Crocus sativus, milk, thioflavin, congo red*

Meta-analysis of gene polymorphism in obesity and type 2 diabetes; where does Indian population stand?

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Abstract:

A gene is said to be polymorphic if more than one allele dominates that gene's locus within a population. In addition to having higher than one allele at a specific locus, each allele must also occur in the general population at a rate of at least 1% to generally be considered polymorphic. Type 2 Diabetes is a type of disorder that is observed due to various gene polymorphisms, a disorder characterized by high blood glucose levels caused by either a lack of insulin or the body's lack of ability to use insulin efficiently. There is a very strong link between the occurrence of Obesity and Type 2 Diabetes in an individual. Gene polymorphisms causing these two types of disorders and in some cases either obesity leading to T2DM or that particular polymorphism causes these disorders directly are reviewed by three approaches i.e., gene data sets retrieval from GWAS catalogue, Opentargets.org and through Manual research article survey. The major aim of this review was to find the gene common to both these types of disorders amongst the World populations with a particular emphasis on Indian Cohorts. We found that the Fat Mass and Obesity (FTO) gene is most prevalent among the Indian Cohorts and also is solely responsible for both the type of disorders.

Keywords: *Type 2 Diabetes mellitus (T2DM), Obesity, Gene polymorphisms, Risk alleles, Indian Cohorts.*

Use of plant extracts on the study of agglutination reactions on RBC antigens

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Abstract:

Animals and plants contain numerous carbohydrate binding proteins of non-immune origin called lectins with the ability to recognize specific sugars existing on cell surface. These lectins have attracted great interest due to their various physiological roles in cell agglutination. Rhesus (Rh) factor is an inherited protein found on the surface of red blood cells. If RBC has the surface protein, it is Rh positive in nature else as Rh-negative in nature. In this project we study the effect of thirty-six various cold water and hot water extracted plants on RBC antigens using agglutination reactions as an alternative to commercial monoclonal antibodies. Plant lectins are widely used for the detection, segregation and characterization of glycoconjugates based on their carbohydrate binding properties. Extensive study of sequence homology and 3-D structure of various plant lectins suggests that they are conserved throughout evolution and thus may play, yet unknown, important physiological roles. Some of the lectins are significant reagents for identification of cell surface receptors in various bacteria, protozoa, and higher organisms.

Keywords – Rh factor, Agglutination reaction, RBC antigens, Plant Lectins.

Identification of mutations in SARS-CoV2 that might lead to structural changes

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Abstract:

A recent report about SARS-COV2 has shown that the genome sequence of the virus has undergone independent mutations leading to genetic diversity and evolution of the virus around the globe. These mutations have led to changes in the viral genome that were previously not observed. Mutations in the genome can change the structure or a function of the protein and identifying and studying the change can help us with the research on a vaccine for the virus. The present study is to identify whether the new mutations lead to any structural changes in the viral proteins. We analysed genes of non-structural proteins (Nsp1-Nsp16) from 50 different regions around the world for the presence of mutations. We have seen different mutation sites for all the non-structural proteins from the various isolates selected out of which we selected two proteins Nsp-12 and Nsp-14 based on the number of major mutation sites and proceeded with structural analysis. The mutated protein structures were compared to the original(wildtype) structures of the protein and evaluated for any change in their structures. Therefore, these structural changes can help in determining any functional changes in the protein and also help in computational modelling of drug components against the virus.

Keywords: SARS-COV2, Nsp-12, Nsp-14, Virus, Nsp16

Improving gut immunity for homeostasis using microbial pack of probiotic supplements

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Abstract:

Probiotics are live microorganisms that have beneficial effects on host health, including extended lifespan, when they are administered or present in adequate quantities. However, the mechanisms by which probiotics stimulate host longevity remain unclear and very poorly understood. Probiotic supplements are needed to determine the effectiveness as a non-chemical approach to promote health and welfare. Our studies focus on the assessment of the molecular impact of probiotic administration involved in homeostasis and immunity. Shrimps received the recommended doses of microbial pack containing *Bacillus* species and *Rhodococcus* species. The fermentation was carried at 37°C for 72 hours under microaerophilic condition. The parameters like pH, microbial load, antioxidant activity (DPPH), acidity and concentration of reducing sugar had been measured. This probiotic pack when used either alone or in combination with traditional dairy starter, significantly improved the nutritional properties and the shelf life of the product. The present work will be valuable to elaborate novel functional food based on these original probiotic properties.

Keywords: *Probiotics, Microbial pack, Immunity, Homeostasis, Shrimps, Microorganisms*

Review on effects of axolotl oocyte extracts on cancer cells & comparison studies on human, axolotl and zebra fish p53 tumour antigens

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ABSTRACT

On the course of finding a solution for the omnipresent disease –cancer, there appears another ray of hope amidst darkness. Axolotl (*Ambystomamexicanum*) is an amphibian belonging to the order urodela known for its exceptional regeneration capacity as well as its resistance to cancer. In the recent studies, the understanding that came into focus is that, the extract obtained from the oocyte of axolotl can induce or result in some epigenetic modification on the cancer cells reactivating certain genes that are silenced. The review part of this project also deals with the procedures followed for the administration of axolotl oocyte extracts in to cancer cells and the types of epigenetic modifications observed. The later bioinformatics part deals with the P53 tumour antigen sequences obtained from Uniprot database and their role in finding different parameters such as identification of common motifs using MEME suite, identification of the conserved domains in each of the tumour antigen sequences by using cdBLAST. The identified motifs are run under smart BLAST to identify the similar organisms that contained these motifs. Finally, to get a holistic understanding of how these individual tumour antigen sequences are related with each other the alignment figures and their percentage identity scores are taken by using Global Align.

Keywords: *Axolotl Oocyte Extracts, P53 tumour antigen, epigenetic modification, MEME suite, smartBLAST.*



The Human Pill

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Abstract:

As complex living creatures on cosmos, we as Human beings are being unfolded to discrete diseases and over a period we are being encountered to invaders. we are the best paradigm of embracing ourselves to diverse hosts. Adaptation and change are where most value can be created among humans in the battle field of diseases. Once we all are amalgamation of different craft of diseases with various forms, in near future becoming an architect of one's disease and sculpting ourselves to battle against deadly diseases and eradicating a disease leads to tremendous road in the field of medicine. Synthetic biology can give us different pathways to mould ourselves with artificial cellular and non-cellular components and paint a canvas of one's own human body machines. It also builds a bridge between external and interior part of our body, it also helps to make chimers and mirror mechanism of organs outside the human body by programming them to target a tumour, decipher the genetic codes. However, we are so pleased to take antibiotics, but soon in near future we may encounter Antibiotic catastrophe. Instead of taking a pill can humans become a human Pill?

Keywords: *Human pill, Synthetic biology, Synthetic creatures, Antibiotic catastrophe.*

Application of biotechnology for genetic improvement in fish farming

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ABSTRACT:

Biotechnology produces robust tools for the feasible development of aquaculture, fisheries and also in the food processing industry. Improvements in biotechnology helps us to realize increased rate of growth in farmed species, improve the nutritional value of aquatic feeds, enhance fish health management, help re-establish and save the environment, expand the wide variety of marine animals and enhance the management and preservation of native stocks. For many years, our understanding of fish breeding demand has enhanced and therefore artificial methods have been developed in induced breeding, by the utilization of synthetic or natural hormones. Cryopreservation of gametes is the most important ex situ methods of conservation of germplasm and has wide ranging applications in aquaculture and fisheries management. Fish produced from aquaculture directly account for over one-fourth of fish consumed by humans. Although, success in aquaculture mainly depends on breeding, feeding and protection from disease. Application of recombinant DNA technology in aquaculture can help to enhance these requirements. As aquaculture assumes an expanding role in meeting consumer demands for fishery products, it's obvious to ensure the safety and quality standards. In aquaculture, many of the potential hazards at the assembly level will be controlled by good fish farm management practices, which control pandemic diseases and improve the protection of the products. Successful fish health management starts with prevention of disease instead of treatment, and this is often accomplished by the execution of integrated measures at the assembly level. This global management will contribute to provide safer fish products. The paper provides a comprehensive review on induced fish breeding, transgenic fish, cryopreservation of fish gametes Gene transfer methods, fish health management and commercial application of fish biotechnology.



Keywords: Biotechnology, aquaculture, Cryopreservation

Insilico approach against KAT6A syndrome and prediction of secondary structures

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Abstract:

KAT6A syndrome is a rare genetic condition as a result of a mutation in the KAT6A gene. That gene produces the KAT6A protein that is instrumental in DNA packaging and the production of other proteins in the cell. It is an extremely rare condition with only 195 patients around the world currently diagnosed with the condition. However, common symptoms often include developmental delay, intellectual disability, gastrointestinal problems (feeding difficulties, constipation, acid reflux), speech and language deficits, vision problems, and hypotonia. Our main aim is to design SiRNA and MiRNA of target gene i.e, KAT6A, calculation of GC% (END MEMO), Heat capacity (Oligocalc) and prediction of secondary structures.

Keywords: KAT6A, GC, Heat capacity

A study exploring the correlation between virulence and genomic and protein mutations in SARS-CoV-2

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Abstract:

SARS-CoV-2 is a single stranded RNA virus causing contagious respiratory and vascular disease called COVID-19, declared a global pandemic by WHO in the Month of March, 2020. Nearly 750000 deaths are claimed by COVID-19 across the globe within a span of 6 months calling for immediate social, scientific, technological, public and community interventions. To understand the correlation, if any, between genome and protein diversity and virulence of COVID-19, a genome and protein sequence-based analysis was undertaken. Three hundred sixty-six SARS-CoV-2 complete genomes were analysed. The four main target proteins, spike, envelope, nucleocapsid and membrane proteins play a prominent role in virus entry, assembly and replication in humans. These target proteins were considered for protein level mutational analysis. Three hundred fifty-six protein sequences were analysed, out of which two hundred fifty-four sequences belong to India, eleven from Italy and ninety-one (out of hundred and one genome sequences deposited) are from China as of June 2020. Unique mutations in these target proteins are identified, India has the highest number of mutations out of three. Most of them are found to be unique mutations and belong to the S1 domain only. Protein stability prediction of the four target proteins is done to know the overall stability change due to these mutations. Structural and functional analysis is to be carried out to understand how these mutations are related to the virulence.

Keywords: SARS-COV-2, COVID-19, Mutations, Virulence

Functional properties of *Coleusambonicus* leaf extract with antimicrobial activity

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Abstract:

The use of traditional medicine in the treatment of infectious diseases is increasing worldwide day by day and focused on replacing the use of synthetic drugs and to combat the growth of multidrug - resistant strains. In the current study, the ethanolic and hexane extract of *Coleus ambonicus* leaves were found to inhibit the bacterial pathogens like *Staphylococcus aureus* FR1722, *Escherichia coli* CFR02, *Shigella flexneri* MTCC731, and *Klebsiella pneumoniae*, and also against fungal pathogen *Candida albicans* ATCC90028. Among these, the crude extract showed prominent result against all the tested pathogens with zone of inhibition around 12 to 14 ± 2 mm. Further, to evaluate the concentration of inhibition, MIC (minimum inhibitory concentration), MBC (Minimum bactericidal concentration) and IC50 concentration was performed. It was perceived that around 20 to 40 ± 0.01 and 10 to 40 ± 0.06 for MIC and MBC was noted, respectively against most of the pathogens by the crude extract. The counts of *E. coli*, *S. aureus* and *Shi. flexneri*, declined drastically at 15, 17.5 and 17.5 mg, respectively for both the extracts of *C. ambonicus*. IC50 concentration of ethanol extract against *E. coli*, *S. aureus* and *Shi. flexneri* was 11.25, 10 and 12.5 mg/ml, respectively, and a concentration of 11.88, 8.0, and 10.62 mg/ml was noticed for hexane extract. The findings showed strong antibacterial activity for the ethanol and hexane leaf extract of *C. ambonicus*. Further research into the isolation and characterization of the bioactive compounds responsible for this possible activity is under process.

Keywords: MIC, MBC, IC50, MBC

ERBB3 receptor docking studies with potential anti-carcinogenic thiohydantoin derivative analogues

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Abstract:

A tumour may be defined as a mass of cells formed by the accumulation of abnormal cells. Under normal conditions, the cells in our body undergo senescence and they are replaced by new cells. This normal cell cycle is disrupted in cancer. Unlike normal cells which die after becoming old, tumour cells keep on multiplying notwithstanding the requirement of the body. As cells continue to get added to the mass, the tumour keeps on proliferating. They are associated with therapeutic resistance having specific targets in various types of cancers including resistance to breast, head, neck, prostate cancer, etc. This study gives the pharmacological investigation of a designed receptor tyrosine-protein kinase erbB-3 interacted to thiohydantoin subordinates which can be used as a potential antagonist as shown by in-silico techniques. The ligands designed were analysed using various techniques, such as molecular property prediction, toxicity, solubility and drug-likeness. The profile of the ligands was studied and they also obeyed Lipinski's rule. PatchDock and SwissDock were used for analysing the in-silico docking. The study of docking was concluded based on two parameters – Atomic Contact Energy and Score.

Keywords: ERBB3, PatchDock, SwissDock

Screening of natural ligands against spike protein of SARS-CoV-2

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Abstract

COVID-19, a new pandemic caused by SARS-CoV-2, was first identified in 2019 in Wuhan, China is a human coronavirus. In the past, MERS and SARS, similar to SARS -CoV-2 resulted in similar symptoms and death. Coronaviruses cause widespread respiratory, gastrointestinal, and central nervous system diseases in humans and other animals, threatening human health and causing economic loss. In SARS CoV-2, genes of major structural proteins are present in the 5'-3' order as spike (S), membrane (M), envelope (E), nucleocapsid (N) protein and hemagglutinin-esterase protein (HE). These viruses use similar mechanisms to enter the host cell that is by binding the viral spike glycoprotein to the host receptor, angiotensin-converting enzyme 2 (ACE2). The SARS CoV- 2 spike protein is cleaved into two subunits, S1 and S2 subunit by Transmembrane protease serine2 enzyme thus facilitating the entry of viral particle into the host cell. Its inhibition blocks virus fusion with ACE2 Angiotensin-converting enzyme 2 and restricts SARS CoV2 pathogenesis. The Receptor Binding domain situated in the S1 subunit initiates the viral infection by binding to the host cell receptor. While the S2 subunit is responsible for viral fusion and entry of the viral genome. In addition to its role in penetrating cells, it is a major inducer of neutralizing antibodies (NAbs). NAbs are protective antibodies that are naturally produced by our humoral immune system. Therefore, understanding the mechanisms involving the Spike protein and the host receptor is crucial in designing accurate drugs or vaccines capable to recognize and neutralize the portion of S protein binding the human receptors. In this study, we considered the SARS-CoV-2 Spike protein as the drug target. Curcumin, ascorbic acid and azadirachtin are naturally occurring phytochemicals and are known to have broad pharmacological properties. Considering these as the ligands, in silico docking is carried out.

Key words: COVID-19, SARS-CoV-2, NAbs

Biological roles of various stress proteins and their clinical implications

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Abstract:

Proteins play a major role within our body. These are nothing more than macromolecules which are formed by amino acids within our body. There are various proteins within a human body and the role that each one of them plays drastically differs from their structure as well as composition. In our paper we would like to look into a specific type of protein known as a stress protein. This group of proteins are responsible for protecting the cells from various stresses such as cold, heat, oxygen deficiency as well as glucose. They mostly help the other proteins function within the normal cells. We will often be able to find high levels of stress proteins within cancer cells. The intrinsic capability of HSP's to protect cells has potential connection as a natural mechanism of organ protection throughout harmful environmental conditions and operative procedures, and within the combat against pathogens. In response to a large style of disagreeable stimuli, there's a marked increase in total HSP synthesis, referred to as the cellular stress response. The strain response is meant to boost the power of the cell to address increasing concentrations of unfolded or denatured proteins.

Keywords – Stress Proteins, Heat shock proteins, Cancer cells, Cellular stress response

Effect of artificial food colours and replacement of artificial food colours with naturally extracted food colour

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Abstract:

Coloring is a significant factor for identifying various foods and for deciding about their quality, and attracting people to experiences with them. Since colouring is typically the most important factor many industries are producing them. In many cases the original colours of the food must be maintained for naturally produced fruits and vegetables. There are many sources from which food colours can be extracted like plants, vegetables, fruits, chemicals, microorganisms and many more. But in present many people are using only chemically extracted food colours those are artificial food colours. These artificial food colours have various adverse effects like causing cancers, destroy nutrients in foods, they can also increase hypersensitivity in children because of these effects they are to be replaced with natural food colours which are directly extracted from natural sources like plants, vegetables, fruits, flowers. There are various methods in extracting natural food colours like Soxhlet extraction, maceration, super critical fluid extraction, microwave assisted food extraction etc. In this we are discussing about various sources of naturally extracted food colours and their extraction method and the efficiency of extraction methods for production of natural food colours from natural source.

Keywords: *Natural food colours, Artificial food colours, Soxhlet extraction, Maceration, Super critical fluid extraction, Microwave assisted food extraction.*

Computing the probability of RNA silencing and quantification of (RNAi) in plant

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Abstract:

RNA Interference is the (post-transcriptional gene silencing) PTGS that probably abrupt the translation process of mRNA into protein by cleaving the mRNA at a specific position. Rna silencing is the best strategy in plants to protect them against many viral infections. An understanding of the process of RNA silencing induces the enhancement of producing many pest and viral-resistant plants. Basically, in this mechanism dicer protein splits the dsRNA into small-length RNA fragments is identified as mi- RNA or si-RNA (small interfering RNA) when this si-RNA combines with the RISC complex then it can cleave the mRNA at a specific site which results in interruption of protein translation.it is a very complex process. But the successful gene silencing requires the prediction of RNAi or micro RNA target sites, which helps to find how efficiently they can act as si-RNA to perform the RNAi interference. There are several online tools and off-target prediction software are available. In this, we can design a specific si-RNA sequence using (si-fi) Si-Rna finder software. si-Fi is a tool that helps to design optimized RNAi constructs that can silence or knock out the specific gene function. This tool helps to predict the efficacy of RNAi sequences and off-target site search, this prediction helps in the practical implementation of si-RNA constructs. si-Fi is free (open source) desktop software that available in Microsoft Windows and can use sequences in standard FASTA format. By using this software, we designed a si-Rna that resists the TMV(Tobacco Mosaic Virus) replication. which can silence the TMVgp2 gene or replicase protein translation. We also predict the off-target sites using si-fi software. To design the better si-RNA sequences for plants, we using si-fi(si-RNA finder)software to design efficient si-RNA and analysis of designed si-RNA.

Keywords: RNA silencing, RNA interference, micro-RNA, small interfering-RNA, PTGS.

Nutritional agonists of (PPAR)- γ : an immunomodulatory approach to control cytokine storm in covid19 patients

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Abstract:

Recent examinations express that multi organ failure is seen in Corona virus infected patients with different pathway. It has been shown in contemplates that elevated levels of cytokines like IL-1B and INF gamma were observed. It is called as cytokine storm with higher convergences of CCL2 and CXCL10. The cytokine storm is trailed by the immune system attacking the body which thus may cause numerous organ abnormalities and conclusive outcome being death. As of now there is no particular treatment of the viral sickness and this methodology is an elective path for focusing on specific qualities that could diminish cytokine storm. In such manner peroxisome proliferators activated receptors (PPARs) have a place with group of transcription factors which are known to manage the inflammatory mechanisms in body. This immunomodulatory approach is intended for focusing on the nutritional PPAR-gamma ligands that can be found in food, further Molecular docking studies were performed. The activation or increased expression levels of PPAR gamma because of chosen agonists may decrease the cytokine storm in Corona virus patients. Thus, this is one such fascinating way to deal with neutralization of the cytokines exorbitantly elevated by use of substances like pomegranate, lemon grass and so on to activate PPARs reliably.

Keywords: *CCL2, CXCL10, Covid19, Cytokine storm, PPARs, Molecular docking*

Statistical optimization of medium components for the production of biosurfactant by *Achromobacterxylos*GSR21

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Abstract:

In this paper the advancement of the basic medium segments for bio-surfactant creation from *achromobacterxylos* strain GSR21 using statistical experimental design. Response surface method (RSM) was utilized to decide the ideal degrees of cycle factors (agar powder, yeast concentrate, $\text{FeSO}_4 \cdot 7\text{H}_2\text{O}$, and KH_2PO_4). Central composite design (CCD) of RSM was utilized to contemplate the four factors at five levels, and bio-surfactant fixation was estimated as reaction. Regression coefficients were determined by regression analysis, and the model condition was resolved. R^2 esteem for bio-surfactant (g/L) was tried to be 0.72, demonstrating that the model fitted well with the exploratory outcomes. Confirmation of the numerical model was led by playing out the investigation with the anticipated upgraded values, and bio-surfactant yield was discovered to be 9.69 g/L. Approval of the anticipated model was fitted 96.9% with the test results directed under the ideal conditions. Agar powder and yeast remove was recognized as effective segments for bio-surfactant (*Achromobacterxylos* GSR21) creation.

Keywords: *Achromobacterxylos*; *Bio-surfactant*; *Central composite design*; *Response surface methodology*.

Molecular docking studies to evaluate small molecule inhibitors of wnt/betacatenin signaling pathway

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Abstract:

The wnt-signalling pathways are a set of signal transduction pathways which begins with proteins passing signals into the cell through its cell surface receptors. There are three major wnt- signalling pathways and all the three pathways are activated by the binding of a wnt-protein ligand to a frizzled family receptor, which passes the biological signal to the disordered protein inside the cell, whereas this project involves canonical wnt pathway. The current study involves screening for ligands which can inhibit beta catering signalling pathway. Curcumin, Cardamonin, FH535 and ICRT-3 were used as ligands for the molecular docking study with beta-catenin binding with Transcription factor -4 receptor. All chosen ligands have exhibited significant binding energies with the receptor. The highest -9.518272kcal/mol with Cardamonin followed by -9.28359kcal/mol with FH535, -8.422604 kcal/mol with curcumin and the least -8.407231 kcal/mol with ICRT-3. All the ligands showed atleast 1 hydrogen bond with the target whereas Cardamonin showed 3 hydrogen bonds with the target Curcumin is a close second forming 2 hydrogen bonds while FH535 and ICRT-3 form only 1 hydrogen bond. The 2D interactions of the ligand and the molecule are visualised by using chimera.

Keywords: *Molecular docking, Wnt-signalling, beta-catenin Tf-4 receptor, Cardamonin*



Novel biomarkers in cancer using Liquid biopsy

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ABSTRACT:

Non-invasive tests used to evaluate blood for cancer cells or DNA, Liquid Biopsy. Liquid Biopsy is applied to cancer screening, early detection, evaluation of tumour heterogeneity, identification of genetic/epigenetic alterations for targeted therapy, observation of dynamic changes, and assessment of drug resistance. Blood-based biomarkers such as ctDNA have great potential for early diagnosis. ctDNA useful as a monitoring biomarker for estimating cancer burden in patients and assessing treatment responses. This meta-analysis study to identify common ctDNA available in various cancers. This ctDNA can be used as a liquid biopsy biomarker so that we can able to identify the risk of causative in early detection.

Keywords: *Liquid Biopsy, ctDNA, Blood-based biomarkers, Cancer cells*

Promoter finding algorithm using deep learning

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Abstract:

Promoters are biologically significant elements in gene transcription which ultimately leads to the translation of the genes into functional proteins. It is not possible to hard code it into programming for classifying and finding what a promoter is and what a non-promoter is. To overcome this problem, we have implemented the concepts of deep learning and artificial intelligence in our work. In Deep learning, there are many types of neural networks such as Artificial Neural Networks (ANN), Convolutional Neural Networks (CNN), Recurrent Neural Networks (RNN), etc. In this particular instance, we have used convolutional neural networks (CNN) along with the Recurrent neural network (RNN) which is a Long short-term memory (LSTM). We have used 1D convolution containing multiple layers of parameters concatenated to a single layer which is an input layer to the LSTM and the final output is an optimised model. In our work as the input data is gene sequences which is linear data. We have used libraries and modules such as TensorFlow, Keras, sci-kit-learn, NumPy, and pandas to model the data and train the data. We have chosen 4 different organisms which are homo-sapiens, mus musculus, drosophila melanogaster, and Caenorhabditis elegans to work on. The data required for the work is taken from the new EPD database and NCBI. The positive dataset is promoter sequences with a length of 151 sequences ranging from -100 to +50. The negative dataset is non-promoter sequences with a length of 151 sequences ranging from +100 to +250. A, T, G, C are assigned with values 1, 2, 3, 4 respectively and data the data is normalised. After training of the data, the model is refined and is used for finding the promoters present in it and set that the confidence percentage is 95. Then using the regular expressions of python the output promoters are classified based on the known motifs.

Keywords: ANN, CNN, RNN, Python, TensorFlow, Keras



Futuristic eye on the effective treatments of HIV-1 infection

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Abstract:

HIV/AIDS being considered as epidemic till date, numerous pragmatic techniques are evolving in-order to prevent the transmission of the virus and regulate the viral load in the infected person. Such pragmatic techniques include the broadly neutralizing antibodies (HIV bnAbs) and cell-gene therapy (CGT). These methods show potential results on the effective decrease of the viral load, thus preventing the transmission. HIV bnAbs and CGT can replace the long-term treatments such as HAART and cascade medications as the results are fast and can be done through passive immunization when compared to the existing treatments. The HIV bnAbs are targeted towards the gp120 envelope protein of the HIV-1 strain whereas the CGT includes the ex-vivo removal of CCR5 from CD4+ T-cells which acts as the main gateway to the HIV.

Keywords: HIV, AIDS, bnAbs, CGT, HAART, Passive Immunization.

Formulation and evaluation of acitretin transdermal gel for the treatment of psoriasis

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Abstract:

Aim: The present research work was aimed to develop a novel gel for Acitretin (Act) to enhance the drug absorption by the topical application, which overcomes the demerits of oral dosage form and conventional gel system of Acitretin (Act). **Materials and Methods:** The gels were prepared with carbopol 934 as a gelling agent used in six different concentrations. Span 20 and Tween 20 were included as emulsifying agents in two different concentrations. Liquid paraffin was used as an oil phase, and methyl and propyl paraben were included as preservatives. Ethanol was used to dissolve the drug for preparing the aqueous phase and Triethanolamine was added at the end of preparation, as quantity sufficient for pH adjustment. **Results:** All the formulated nanogels were screened for the parameters, namely, appearance, pH, viscosity study, Spreadability, swelling index, drug content, and in vitro drug release studies. The optimized formulation ActG-4 showed 81.95% of drug release up to 8 h, and the particle size analysis reported good size range, and the gel was found to be nonirritant and nontoxic which was confirmed by HET CAM test. **Conclusion:** Acitretin (Act) can be successfully formulated as gel for better-sustained effect and can be a suitable alternative approach to the oral dosage forms for the management of Psoriasis.

Key words: *Acitretin (Act), carbopol 934, viscosity.*

Development of new lead molecules for targeting dengue virus based on pharmacophore modelling

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Abstract:

Dengue virus (DENV), a mosquito-borne flavivirus, infects 50 to 100 million people worldwide annually, and 40% of people living in tropical and subtropical areas of Asia, Africa, and the Americas are at risk of DENV infection. Concerning the antiviral strategies to inhibit DENV infection, one of the most obvious approaches is to directly target virus encoded enzymes and other functions. α -glucosidases I and II are endoplasmic reticulum (ER) resident enzymes responsible for the sequential hydrolysis of glucose residues from the asparagine-linked (N-linked) oligosaccharides on glycoprotein precursors. The deoxynojirimycins (DNJs) are iminocyclitolglucomimetics that inhibit ER glucosidases by competing with glucose. Here, in our study, we generated the Pharmacophore from the reported α -glucosidases inhibitors and performed the in-silico screening for identifying the potent inhibitors of the enzyme. By using the in-silico approach, an attempt was made to identify the potential α -glucosidase inhibitors for the treatment of Dengue virus related diseases. Initially a pharmacophore was generated based on the reported inhibitors structures, later Zinc database was screened for similar structures containing the pharmacophoric groups. The selected molecules based on RMSD were subjected drug-likeness based on their Lipinski RO5 violations and Pharmacokinetic data. The shortlisted molecules were subjected for molecular docking studies for finding the binding interactions with the α -glucosidase in MolegroVirtual Docker. Some of the compounds have shown good binding interaction with the target enzyme and not possessing the toxic properties. Further evaluation is needed for the selected molecules to investigate their anti-viral activity.

Key words: *Dengue, Pharmacophore, Deoxynojirimycins, α -glucosidases.*

Phylogenetic analysis of corona virus variants in Indian strains

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Abstract

Covid-19, the pandemic that has ravaged the world for most of 2020, continues to take a massive toll on our lives, health systems. Corona virus, the mutated form of SARS-CoV-2 is showing its continuous mutation in genome. The virus having its roots in Wuhan (China) has covered the planet by its own property to vary itself accordingly. These changes lead to its transmission and pathogenicity due to which the concept of social distancing appeared into the picture. Mutation was predicted as a stabilizing change. In this study, phylogenetic analysis was carried out there by finding the evolutionary relationships among its biological species or other entities. To understand or to analyse this phylogeny among those strains is our point of view. So far, we have downloaded the Indian strains and phylogenetic tree was constructed, looking forward to focus on the mutations in the genome. Thus, by keeping the track on the activity that how the virus is changing into a new subtype, we can thereby develop antiviral drugs or vaccines.

Keywords: *Corona virus, non-synonymous mutation, phylogeny, positive selection*

CFD optimization of continuous stirred-tank (CSTR) reactor for biohydrogen production: A review

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Abstract:

The current worldwide economy and energy gracefully depend widely on petroleum products. This has brought about a remarkable expansion in the climatic carbon dioxide focus from the hyper combustion of petroleum derivatives and disturbing consumption of nonrenewable non-renewable energy source assets. The quick raising ozone depleting substance discharges due essentially to carbon dioxide are viewed as the fundamental offender of a dangerous atmospheric deviation and environmental change. To moderate a worldwide temperature alteration and other natural issues, considerable exertion is being placed in at the worldwide level to investigate sustainable power sources that could supplant petroleum derivatives. To deliver greatest measure of biohydrogen production and to watch the cycle associated with between gas-fluid stream in a lab by the computational liquid elements. By creating progressed impeller configuration has been built and adjust with the computational liquid elements resembling of the ordinary and progressed impeller over an extent of velocities. Numerical results resembled astute affirmed by appraisal of RTD. There will join computational liquid elements resembling with ethanol type aging cycle explore, efficient biohydrogen production by cutting edge impellers with different speed produced different stream design

Keywords: *Biohydrogen production, Continuous stirred-tank reactors (CSTR), Computational fluid dynamics (CFD), Hydrodynamics, Reactor Design.*

Phylogenetic and phylodynamic analysis of SARS-CoV-2

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Abstract:

Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) that emerged in late 2019 is a highly transmissible and pathogenic coronavirus. It has caused a pandemic of acute respiratory disease, named 'coronavirus disease 2019' (COVID-19), which threatens human health and public safety. Phylogenetic analysis is the means of estimating the evolutionary relationships. To assess the evolutionary relationship of species the sequence of a common gene or protein can be used in the molecular Phylogenetic analysis. Branching, tree-like diagram—the Phylogenetic tree is usually depicted from the evolutionary relationship obtained from Phylogenetic analysis. Phylodynamic analysis includes analyzing genetic diversity, natural selection, and population dynamics of infectious disease pathogen phylogenies during pandemics and studying intra-host evolution of viruses. To better understand of the mechanisms that drive spatiotemporal incidence and Phylogenetic patterns of bacterial pathogens Phylodynamics combines the study of Phylogenetic analysis, ecological, and evolutionary processes. In our project, we are going to collect the genomic sequences of coronavirus from various countries and then form an analysis on how much variation each sequence had from one country to another. For this analysis we are going to form a Phylogenetic tree using Clustal Omega and iTOL software.

Keywords: SARS, COVID, Phylogenetic analysis, Virus



Conformational epitope prediction towards B-cells

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Abstract:

By attacking with intense specificity by means of receptors synthesized or expressed on the surface of antibodies, B-cells will annihilate pathogenic molecules that enter an organism. The molecular interaction observed between both the antibody residue (known as paratope) engaged in binding and the interacting region of the target antigen (known as epitope) is the means through which the destruction of pathogen molecules is achieved. The main objective of this work is to achieve improved B-cell epitopes predictions through in-silico studies. The antigen sequence cut into peptides are docked against the IgE antibody and those with the highest docking scores are further studied for the bond interactions. The overlapping sequences of the high score peptides are observed in the whole antigen model to predict their position. The residues at where the bond interactions were found have also been reported for these overlapping peptide sequences. The validation is done by antigen-antibody docking studies to confirm the predicted epitope.

KEYWORDS: *Confirmational, B-cell epitope, IgE antibody, Antigen- Antibody Docking*

Identification of Nipah Virus Fusion (F) And Attachment (G) Glycoprotein Inhibitor Agents Using *In-silico* & *In-vitro*

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Abstract:

Nipah virus (NiV) is a member of the family *Paramyxoviridae*, genus *Henipavirus*, level 4 (BSL4) pathogens. The disease spreads through fruit bats or 'flying foxes,' of the genus *Pteropus*, who are natural reservoir hosts of the Nipah viruses. The virus is present in bat urine and potentially, bat faeces, saliva, and birthing fluids. Presumably, the first incidence of Nipah virus infection occurred when pigs in Malaysian farms came in contact with the bats who had lost their habitats due to deforestation. Recent deadly NiV outbreak in Kerala, India during June, 2018 claimed 17 lives has put India on a high-risk zone for future NiV infections. Misfortune there are currently no drugs or vaccines specific for Nipah virus infection. The purpose of our study involves NiV's attachment (G) and fusion (F) envelope glycoproteins mediated viral binding to the ephrinB2/ephrinB3 cell receptors and virus-cell membrane fusion, respectively. Here my study is how to inhibit the TMD (transmembrane domain) in Niv-F by using drug compounds. Virus cell entry is mediated by the fusion protein, F, in response to binding of a host receptor by the attachment protein. During posttranslational processing, the fusion peptide of F is released and, upon receptor-induced triggering, inserts into the host cell membrane. As F undergoes a dramatic refolding from its prefusion to postfusion conformation, the fusion peptide brings the host and viral membranes together, allowing entry of the viral RNA. We will also see this Computational method for Identification of Nipah virus fusion (F) and attachment (G) glycoprotein inhibitors using *In-vitro* & *In-silico* approaches.

Keywords: Nipah virus, Flying fox, Attachment, Fusion, Domain



The genomic study of different strains of Nipah virus

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Abstract:

Nipah Virus, belongs to the genus Henipavirus, and a member of the paramyxoviridae family, is classified as Biosafety level -4 pathogen. NiV was first identified in Malaysia in 1999, caused by the natural reservoir fruit bats, of the genus Pteropus. This has become a great threat to animals and humans. Later on, it was transmitted to humans too. First outbreak in India was recorded in West Bengal in 2001 and again in May 2018 in Kerala. The main aim of this study is to identify the genomic strains of different proteins of different species.

Keywords: *Nipah Virus, protein structure, pteropus vampyrus, sus scrofa, homosapiens.*

Comparative analysis of PHB producing microorganisms

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Abstract:

Polyhydroxybutyrate (PHB) biosynthesis is one of the important phenotypic characteristics expressed under environmental stress. Biodegradable polymers such as poly (3-hydroxybutyrate) (PHB) have gained much attention in recent years. PHB synthesis relies on important intermediates tricarboxylic acid (TCA) cycle, Glycolysis, Pentose phosphate pathway, biosynthesis of amino acids and Nitrogen metabolism. Using metabolic pathway database (KEGG), we have devised *in-silico* pathway, from which we can infer the metabolic changes among microorganisms which may operate under different conditions. The optimized strategy primarily involves automatic retrieval of the KEGG Orthology (KO) identifiers of user defined organisms from the KEGG database followed by overlaying and visualization of the metabolic genes using the KEGG Mapper reconstruct pathway tool. In this analysis, we found some potential microorganisms such as *Bacillus megaterium*, *Rhizobium elti*, *Pseudomonas stutzeri*A1501, *Bacillus thuringiensis*seroverkonkian, *Halomonas sp.* KO116, *Azotobacter*vinelandiiDJ, *Thiomonasarsenitoxydans*, *Azotobacterchroococcum*, *Methylobacterium*aquaticum, *Pseudomonas fluorescens*, *Burkholderiapseudomallei*1106a, *Legionella longbeachae*, *Methylobacterium sp.*DM1, *Ralstoniasolanacearum*, *Alcaligenesaquatilis*and*Methylobacterium*oryzae which have the necessary genetic machinery for production of PHB either in high or low concentration under adverse stress conditions.

Keywords: *KEGG database, KEGG Mapper, G2KO tool and microorganisms*



Applications of probiotics in Agriculture and Aquaculture

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Abstract:

Since ages agriculture and aquaculture are the two main sectors where every individual depends on the food. The wide use of chemicals for agriculture like herbicides, insecticides, fungicides and for aquaculture like disinfectants, pesticides to control the pests and to increase the production of food leads to the environmental and climatic changes and harm to individuals who consumes it. The purpose of using probiotics in food as they are live microorganisms when taken in adequate amounts helps to maintain a healthy balance of gut bacteria and have wide variety of health benefits. In recent years, there is an increased interest in applications of probiotics in agriculture and aquaculture, the selection of new strains and development of new applications.

Keywords: *probiotics, Agriculture, Aquaculture, Live microorganisms, Environment.*

Identification of Drug and Vaccine Targets of SARS CoV2

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ABSTRACT

Severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2) is an emerging virus that is extremely pathogenic and has caused a recent global pandemic officially called coronavirus disease (COVID-19). Search for drug targets is necessary to develop vaccines/ drugs to control or treat the novel coronavirus (SARS CoV2). We conducted a systematic review to identify major druggable targets in coronavirus (CoV). We analysed all the proteins encoded by SARS-CoV-2 genes, compared them with ORFs and proteins from the coronavirus genomes of other countries. With the help of online tools like ORF Finder, MEME, we considered the Genome of SARS CoV2 of various countries and we identified few major proteins as the drug and vaccine targets. This study will provide drug targets for the further studies related to SARS CoV2, new insights into those drugs currently undergoing clinical studies for possible new drug repositioning strategies for the treatment of SARS CoV infections

Keywords: SARS-CoV-2, MEME, COVID-19, ORF Finder, Clinical studies

Structure based *insilico* screening of inhibitors targeting NSP14 OF SARS COV-2

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Abstract:

Novel coronavirus outbreak was intimidating and many researchers across the globe are working on it. The present work involved designing inhibitors for the nonstructural protein-14 (NSP-14) of SARS CoV-2 by screening natural molecule database. NSP-14 exhibits exonuclease and methyltransferase activity. Exonuclease activity is majorly involved in the fidelity of replication. Most of the previous docking studies involved repurposing of antiviral drugs targeting NSP-14. Due to the lack of a crystal structure of SARS COV-2 NSP-14, a homology model was generated using an easy modeler. The amino acid sequence of SARS COV-1 NSP-14 showed 95% similarity with SARS COV-2 NSP-14 and hence SARS COV-1 NSP-14 crystal structure (5C8S) was used as a template for homology modeling. The developed model was validated using the ERRAT score and Ramachandran plot. The model was simulated using desmond for 100ns and was further refined. 98.7% of the amino acids of the model were found in the allowed regions of the Ramachandran plot. 169658 molecules of OTAVA database were used for screening. Virtual screening was done following HTVS, SP, and XP protocols. 67012 molecules passed through HTVS, of which 33931 sustained SP screening. Finally, 6786 molecules were passed through XP screening. The highest glide score obtained was -6.99 kcal/mol. Further, in-vitro evaluation will lead to the identification of a potent inhibitor targeting NSP-14 of SARS CoV-2.

KEYWORDS: *NSP-14, Virtual screening, Homology Modelling, Exonuclease activity.*

Computational identification and characterization validation of potential peptide vaccine from HHV-8(HIV)

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Abstract:

HHV8 is one of the strains of HIV. Scientifically identified from Kaposi's sarcoma lesions as Human herpesvirus-8, member of gamma-2 herpes virus family. Several diseases such as endemic, transplant related, Classic, rare neoplastic disorders (primary effusion lymphoma [PEL], and solid organ variants), lymphoproliferative disorder known as multicentric castle men's disease [MCD]. The regulation Mechanism of cellular proliferation and apoptosis is disturbed by the HHV8. This study combines numerous approaches to annotate possible effective peptide vaccines that could provide protection against multiple infections caused by HHV-8. Some Tools (NetCTL, ElliPro, Patch dock, Fire dock, PDB, ANTIGEN Pro) are used to predict the peptide vaccines. Prediction of Linear B-cells occurs after interacting with antigen lymphocyte, which differentiate into memory cells and plasma secreting cells, activates the immune system and destroys the pathogen. T Cells play a major role that directly kills the infected host cells and also useful to activate the immune system. Docking is useful to predict the interaction towards small molecules such as ligands (examples: CCL1, CD40, SELPLG). B-cells and T cells and peptide 3D co-ordinates is obtained by tools. Potential peptides were then docked against the MHC molecules to obtain peptide-MHC complexes and post-docking interactions is useful to choose potential candidates for the development of peptide vaccines.

Keywords: HHV8, B-cells, T cells, HIV, MHC molecules, Kaposi's sarcoma

A strategic review on production and purification of asparaginase

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Abstract:

L-Asparaginase (E.C.3.5.1.1.) is one amongst the amidase group, that catalyzes the hydrolysis of L-asparagine and releases L-aspartic acid and ammonia. This characteristic of L-asparaginase inhibits the protein synthesis in cancer cells, making L-asparaginase a chief support of pediatric chemotherapy practices to treat acute lymphoblastic leukemia (ALL) patients. L-Asparaginase is also identified as one of the important food processing agent. The removal of asparagine by L-asparaginase leads to the depletion of acrylamide formation in fried food items. L-Asparaginase is produced by different organisms including microorganisms, animals, and plants, however, only microorganisms that produce a significant amount of this enzyme are of commercial significance. The commercial L-asparaginase for healthcare applications is mainly derived from *Escherichia coli* and *Erwinia chrysanthemi*. Present review provides in-depth information on microbial L-asparaginase bioprocess optimization including submerged fermentation and solid-state fermentation for L-asparaginase production, downstream purification, its characterization, and problems related to the clinical application including toxicity and hypersensitivity. Here, we have focused on the bioprocess techniques that can produce enhanced and economically viable yields of L-asparaginase from favorable microbial sources in the current scenario where there is an urgent requirement for alternate L-asparaginase with less adverse effects.

Keywords: *chemotherapeutic agent, enzyme, fermentation, food processing agent*

Genome-wide identification and characterization of LRR-RLK gene family in Foxtail millet

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Abstract:

Receptor-like protein kinases (RLKs) in plants, Leucine Rich Repeats-RLKs (LRR-RLKs) are engaged with numerous basic organic cycles including development, advancement, and stress reactions in the plants. Here in this study, we aimed at identification and characterization of LRR-RLK gene family in foxtail millet. A total of 537 genes and 79 proteins were identified which were related to LRR-RLK present in the transmembrane region. phylogenetic analysis shows the evolutionary relationships of their respective subclades and families. The distribution of genes on chromosomes shows the diversity of LRR RLKs, most of them were located at the segmental duplicated regions which suggests that they are nearly identical. 68 motifs were identified in 537 SiLRR-RLKs under 0.05 p-value threshold. We've also done protein structure analysis the result of the analysis shows that LRR domain, malectin like domain and protein kinase like domain were the most conserved domains among the 79 SiLRR-RLK proteins. Analysis of biological processes showed that SiLRR-RLKs are involved in 'multicellular organism development', 'tube development', 'anatomical structure development', 'developmental process' and 'multicellular organismal process'. This study could be useful to the foxtail millet crop improvement programme.

Key words: *LRR-RLK, Foxtail millet, Phylogenetic analysis, protein structure analysis*

Genome-wide identification and insilico characterisation of chitinase gene family in Foxtail millet (*Setaria italica*)

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Abstract:

Chitinases are a kind of hydrolases with chitin as a substrate and play a vital role in the plant defence mechanism against fungal pathogens by degrading chitin, a key component of the fungal cell wall. Chitinases are also actively involved in helping plants to persist in stressful conditions as a response to abiotic stresses. Despite its dominant stress tolerance trait, foxtail millets are more prone to blast disease which is caused by a fungal pathogen *Magnaporthe grisea*. In the present investigation, identified and characterized chitinase gene family in foxtail millet (*S.italica*), using different *insilico* tools. we performed genome-wide identification, classification, sequence alignment, gene ontology expression, and 3-D structural analysis of the chitinases in *S. italica*. 40 genes were considered out of 46 genes identified and classified into both GH-18 and GH-19 sub-families under the glycosyl hydrolase family. Among these class-V chitinases appear to be quantitatively high. Many of the genes are actively induced by the defence, low-temperature, drought, and osmotic stress due to particular regulatory elements (TC-rich repeats, MBS, STRE, and LTR) in the promoter region also an average number of genes resulting in the response of stress and other organisms was observed in the expression analysis. This study can be helpful to understanding the functions of chitinases in *S. italica*. This may help in the future study for generating blast-resistant foxtail millet genotypes by enhancing chitinase production.

Keywords: *Foxtail millet, Chitinases, Magnaporthe grisea, defence response, Glycosyl hydrolase family.*

In silico screening of compounds from Indian herbs against Covid-19 by targeting spike protein using molecular docking

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Abstract:

To predict the interaction between a drug molecule and a target protein from a microbe molecular docking analysis is routinely used in modern drug discovery. Drugs which are recognized in this way may inhibit the entry and replication of pathogens in host cells. In today's world SARS-CoV-2 associated coronavirus disease, COVID-19 which is more contagious has become the pandemic disease. This censorious situation needs an effective drugs to treat the infected patients. Since ancient times many infectious diseases have been treated with the herbal medicines. The spike protein of SARS-CoV2 plays an important role in the attachment and pathogenesis of the virus. In this study we focused mainly in the search of ligands among the active components present in herbs for S protein that may serve as efficient medicine for COVID-19. The binding efficiency of some compounds present in herbs with the Spike protein of SARS-CoV-2 are analysed by using molecular docking. The validation of results are done by using docking tools. Based on the binding energies and interactions ligands are scored.

Keywords: SARS-CoV-2, COVID-19, S protein, docking



Understanding the most crucial enzymelike IspH of DXP pathway for directed evolution

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Abstract:

Isoprenoids are the most generous and highly diverse group of natural products. Many isoprenoids have been worn for pharmaceuticals, nutraceuticals, flavors, cosmetics, food additives and biofuels. For high yield production of terpenoid based therapeutics, DXP pathway undoubtedly scrape for the downstream enzymes. The DXS enzyme, the initiator one of this pathway, is axial for the convergence of carbon flux, and is computationally learned for the industrially utilized GRAS bacterium *Bacillus subtilis* to decrypt its vital provinces for aiding the composition of a functionally amended mutant library.

Keywords: *Isoprenoids, DXP pathway, DXS enzyme, bacillus subtilis.*

Transcriptional Factors Suppressing the dehydration in plant abiotic stress conditions

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Abstract:

C-repeat/dehydration-responsive element binding factors (CBF/DREB) the gene factor responsible for the dehydration binding factor transcription factors which play a vital role in improving plant in extreme cold stress resistance and recognize the Dehydrins elements responsible for the promoter of a set of cold regulated genes. The CBF/DREB gene responsible for the suppressing the dehydration belongs to APETALA2 (AP2) transcription family which bind to DRE/CRT elements which allow them to suppress the cold stress conditions. Till now this factor was completely observed and analyzed in *Arabidopsis thaliana* and *Oryza sativa*. This is needed to identify the dehydration responsive element binding factors in other field crops for crop improvement. These factors does not allow to get stressed in cold conditions as the Dehydrins activate the factors and make the plant hydrated along the climates and make it healthy.

Key words: CBF/DREB, *Arabidopsis*, *Oryza*, AP2

Building a machine learning model on breastCancer

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Abstract:

Breast cancer is typically common among women and it is the most significant reason for increasing the speed of mortality among women. Its important to understand that most breast lumps are benign or malignant(noncancerous).Various machine learning algorithms are used for the classification of benign and malignant tumors. Jupyter which is used for the execution of collected data from breast cancer patients. Python and Machine learning algorithms i.e logistic regression algorithm is applied for the predicting the test set results.Data is produced by the samples of the patients who have undertaken and FNA biopsy(Fine needle aspiration).The data contains radius,texture,concave points,compactnessmean,concavitymean,perimeter of the cell.All the techniques square measure coded in python Development environments to appreciate this we have used machine learning categorification methods to suit and perform which is able to predict the separate category of recent input.

Keywords: *Breast cancer, Machine learning,python algorithms,Jupyter, logistic regression algorithm*



Computational evolution of aminotransaminase

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Abstract:

Transaminases are enzymes that catalyse a transaminase reaction between an amino acid and alpha keto amino acid. There are different classifications of transaminases. Our goal is to improve the functional activity of the aminotransaminase enzyme. The active site of the enzyme is responsible for the particular substrate to get attached. When the volume or surface area of the active site is increased different large substrates can be attached and functional activity of the enzyme can be improved. The volume of the active site can be changed by mutations by observing their delta-delta-G values and their stability for that particular mutation. The mutations are done at the active site zone as active site is responsible for the substrate attachment.

Key words: *Enzymes, Aminotransaminase,Delta-G*

Insights of therapeutic mesenchymal stem cells mediated therapy against cancer

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Abstract

Recent studies have suggested that MSC (mesenchymal stem cells) can migrate to tumor specific regions and stem cell based therapies have potential in treating several cancers. Such cells are genetically modified to express certain pro-apoptotic factors, pro-drugs, anti-proliferative agents, therapeutic proteins, and anti-angiogenic agents at the tumor sites. It is also evident that new modalities of cancer therapies are needed immediately which would push this research to the clinic and render MSCs as potential vectors for targeted therapy. The current review focuses on different sources of mesenchymal stem cells used against tumors, the interactions and behavior of MSCs in the tumor microenvironment, and the usage of mesenchymal stem cells as delivery vectors.

Keywords : *MSC , pro-apoptotic factors , anti-proliferative agents , targetted therapy , tumor micro environement.*

A data science approach to bioinformatics

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Abstract:

Computer aided drug design (CADD) which uses the computational advance towards to develop, discover and scrutinize and examine drugs and alike biologically agile molecules. CADD is a specialized stream which uses the computational techniques to mimic drug-receptor interactions. CADD procedures are so much dependent on the tools of bioinformatics, databases & applications. There are so many advantages of computer aided drug discovery; it saves lot of time which is one of the main advantages followed by low cost and more accuracy. CADD required less manpower to work. There are different types of CADD such as ligand and structure based design. Objectives of the Computer aided drug design are to boost up the screening process, to test the rational of drug design, to efficiently screen and to remove hopeless ones as early as possible. In Drug designing the selected molecule should be organic small molecule, complementary in shape to the target and oppositely charged to the biomolecular target. The molecule will interact and binds with the target which activates or inhibits the function of a biomolecule such as a protein or lipid. The main basic goal in the drug design is to forecast whether a given molecule will bind to target and if thus how strongly. Molecular mechanics techniques also used to provide the semi quantitative prediction of the binding affinity. These techniques use machine learning, linear regression, neural nets or other statistical methods to derive predictive binding affinity equations. Preferably, the computational technique will be able to forecast the affinity prior to a compound is synthesized, saving huge time and cost. Computational techniques have quickened the discovery by decreasing the number of iterations required and have often produced the novel structures.

Keywords: Computer aided drug design, Target molecule, Binding affinity and Receptor

Genomic comparison between different genetic disorder of genes

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Abstract:

Comparative genomics immediately brings to mind DNA sequence comparing with Human genes. comparative genes are quite which is applied to the comparison of any organism at the range of different levels genetic basis of Human disease because it includes single gene disorder, multifactorial disorder, mitochondrial disorder, and chromosomal disorder. Here our motives are to grasp the genome function and supply an understand among genetic characteristics and physical characteristics and to know at what mode there is change in chromosome of genes. The main target are going to be here on human disorder genes of diseases comes from different mode of living and environment effect. Technological advances is shown to provision of suitable diagnosis managing and disease therapy for patients.

Keywords: Genomics disorder, Genotype and Phenotype.

Prediction Capability Evaluation of Response Surface Methodology (RSM) and Artificial Neural Network (ANN) in Optimization of Biodiesel Production

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Abstract:

In the present study, the optimization of transesterification process parameters was carried out by using both response surface method (RSM) and artificial neural network (ANN) mathematical model. The prediction and simulating efficiencies of transesterification process parameters were evaluated and compared. The process parameters, such as temperature, methanol to oil ratio, catalyst amount and the reaction time were selected and optimized for biodiesel production. The experiments were planned with a central composite design (CCD) matrix using 2^4 factorial designs. The experimental values obtained through CCD were used to train the ANN model. A performance validation assessment was conducted between RSM and ANN models. ANN models showed a high precision prediction competence in terms of coefficient of determination (R^2), Root Mean Square Error (RMSE), Standard Predicted Deviation (SEP) and Absolute Average Deviation (AAD) compared to RSM model. The amount of catalyst added was identified as the most significant factor for the base catalyzed transesterification. The optimum transesterification conditions were found to be, 60 °C, 7:1 methanol to oil ratio, 1.0 g catalyst load, and 90 min reaction time with maximum biodiesel yield of 88.3%. The results showed that, both models showed good predictions in this study. But, the ANN model having more precise ability to predict the process conditions compared to RSM model.

Keywords: Optimization, Transesterification, Catalyst, Biodiesel, Temperature

Extraction of antioxidants from inedible peels of fruits/vegetables by using solvents: a review

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Abstract:

Daily we consume many fruits and vegetables like oranges, water melon, mango, banana, onion etc. These fruits consist of inedible peels, means these are not fit or suitable for eating. The by-products which are obtained from plant processing industries are the sources of antioxidants which are bioactive compounds. Biomass waste like the fruit and vegetable residues creating serious challenge to the environment. These large amounts of agro-industrial wastes which are generating each year, leading to pollution and economic loss. These things should be disposed in a safe manner. In contrast, these are extremely rich in bioactive components, which have a beneficial impact on health, has led to recovering high value bioactive compounds from such wastes before disposing them. Food and agricultural products processing industries also generate huge amounts of by-products which are rich in phenolics, these are renewable source of natural antioxidants is an attractive possibility. In order to reduce the negative impact on environment green solvents are used to extract the chemicals and antioxidants present in fruits and vegetable in edible parts. Green solvents are non-toxic, non-volatile, recyclable, biodegradable, and may not involve a high energy cost of synthesis. Replacement of a harmful solvent by a greener alternative in a separation process is not trivial and, in some cases, novel challenges and limitations can arise due to the different physicochemical properties of the solvents considered. In this review we are discussing about the extraction techniques in which green solvents are used in extraction process.

Keywords: *Plants, biomass, green solvents*

Molecular Dynamic Screening of New Pancreatic Lipase Inhibitors Targeted to Obesity

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Abstract:

Obesity renowned as the new world epidemic of 21st century is a multi-factorial metabolic syndrome that has become a ground cause of several co-morbid disorders including osteoarthritis, type 2 diabetes, gout, hypertension, stroke, gallbladder diseases and some cancers affecting population irrespective of their ages. Targeting the nutrient absorption and digestion is a viable strategy that is widely accepted with the successful exploration of Orlistat, a monopoly anti-obesity drug that functions as an inhibitor of pancreatic lipase (PL) which hydrolyzes the excess dietary fats. Despite its supervene, Orlistat therapy has been limited because of its unavoidable side effects such as vitamin absorption deficiency and greater incidence of gastrointestinal discomforts. Thus, the current study is focused at High Throughput Screening (HTS) that involves molecular dynamic computational methodologies in identification of the new pancreatic lipase inhibitors that are much more efficient and also producing no to very minimal side effects. The best hit molecules were screened from the natural molecules database and structurally modelled and subjected to Molecular Dynamic Simulations (MDS) using various *insilco* protocols and are further evaluated through the *invitro* procedures in 3T3-L1 cells.

Keywords: co-morbid, anti-obesity, PL, HTS, MDS.

Review on production of biofuel from microalgae: A novel source of sustainable green energy

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Abstract:

Fuel is one of the most commonly used sources of energy in the world today. Biofuel production from renewable sources is generally regarded one of the most sustainable solutions to petroleum-based fuels and a feasible means of sustainability for the environment and the economy. One of the biggest problems with fossil fuels is that they are a scarce natural resource, as petroleum, the natural product from which most fuels are refined, takes millions of years to form, and are non-renewable and unsustainable. Microalgae have emerged as an alternative renewable feedstock for biofuel to replace petroleum based fuels. Many algal species contain high lipid content (50 -70% of dry weight) and need easy cultivation, including reduced freshwater and land area needs compared to conventional crops used for biofuels. There are some technological advances recently developed for biodiesel extracted from microalgae through cultivation, harvesting, pretreatment, lipid extraction, and transesterification sub-systems, for the high yield of biofuel content. This article is to provide a comprehensive review on various methods available for microalgae cultivation, culturing parameter; biomass harvesting and lipid extraction methods from microalgae were discussed.

Keywords: *Biofuel, Microalgae, Cultivation, Harvesting, Extraction.*

Mefenamic acid loaded redox-active injectable hydrogel enhances therapeutic efficacy

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Abstract:

Despite the substantial therapeutic efficacy of Mefenamic acid (MA), a few toxicity issues and inadequate reactive oxygen species (ROS) scavenging efficacy considerably limit its success. Oral administration reposed serious toxicity issues compared to subcutaneous or transdermal administration of MA. In addition, a few drug delivery systems (DDS) employed till date showed only partial toxicity reduction and improvement in therapeutic efficacy of the drug. To address this issue, a robust ROS scavenging hydrogel which can be subcutaneously injected has been designed. MA has been encapsulated in polyion complex (PIC) by dialysis method and redox-active injectable gel (RIG) prepared by increasing ionic strength and temperature. Physicochemical characterization of RIG and drug loaded RIG has been done. The electrostatic and the hydrogen bonding interaction between drug and the polymer has been confirmed by nuclear magnetic resonance (NMR) spectroscopy. The loaded drug showed sustained release for 18 days at 37°C which involved initial burst release for a short time followed by further controlled release for a long time. Furthermore, internalization of the polymer has been studied by preparing RIG with the poly(acrylic acid) (PAA) conjugated 5-aminofluorescein (5-AFL), followed by its ROS scavenging activity by using 5-(and 6)-chloromethyl-2,7-dichlorodihydrofluorescein diacetate (CM-H2DCFDA) in bovine aortic endothelial cells (BAEC). Our study demonstrated that MA partially scavenges ROS and partially improves cell viability unlike RIG and MA loaded RIG which significantly scavenge ROS produced by tumor necrosis factor- α (TNF- α) and improve cell viability. Therefore, the drug loaded RIG can be a potential therapeutic arsenal.

Keywords: ROS, Mefenamic acid, drug delivery systems

Efficacy of extraction methods of natural food colours

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Abstract:

Coloring is significant factor for identifying various foods and for, deciding about their quality, and attracting people to experiences with them. Since colouring is typically the most important factor many industries are producing them. In many cases the original colours of the food must be maintained for naturally produced fruits and vegetables. They are many sources from which food colours can be extracted like plants, vegetables, fruits, chemicals microorganisms and many more. But in present many people are using only chemically extracted food colours those are artificial food colours. These artificial food colours have various adverse effects like causing cancers, destroy nutrients in foods, they can also increase hypersensitivity in children because of these effects they are to be replaced with natural food colours which are directly extracted from natural sources like plants, vegetables , fruits , flowers etc., There are various methods in extracting natural food colours like soxhlet extraction , maceration,super critical fluid extraction, microwave assisted food extraction etc. In this we are discussing about various sources of naturally extracted food colours and their extraction method and the efficiency of extraction methods for production of natural food colours from natural source.

Keywords: *Natural food colours, Soxhlet extraction, Maceration, Super critical fluid extraction*

A comparative analysis on spike proteins of different types of corona viruses prone to homo sapiens

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Abstract:

Corona viruses have been first evolved in 1965 later found gradually in different types of animals. Among those corona viruses, seven types of types of corona viruses have been discovered and validated. But as per the emerging science, there is no such cure to viruses and drug developments. So, in this article we have taken the spike proteins of SARS CoV-2(Severe Acute Respiratory syndrome), MERS (Middle East Respiratory Syndrome & Influenza viruses(H1N1,H3N2&H5N1) and compared those spike proteins namely surface glycoprotein along with its subunits. For comparison, spike proteins are noted down by reviewing articles. Comparison is performed for sequences & structural analysis of those spike proteins by phylogenetic tree &dali structural comparison server; prone to humans (homo sapiens) which has shown the differences, mutations & origin of changes taken place in spike proteins, in turn can pave a way for drug development, disease cure and control.

Keywords: *Corona viruses, Spike proteins, SARS COV-2,MERS, Influenza (H1N1,H3N2 & H5N1 subtypes), dali, drug development & disease control.*

Dinoxin B Withanolide as a Staphylococcal Accessory Regulator Inhibitor

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Abstract:

Introduction: Withanolides are well known for their therapeutic applications ranging from antitumor, anti-inflammatory, antioxidant, anticancer, immunoregulatory and so forth. However, their poor pharmacokinetic and safety properties create significant hurdles in the formulation of the antibacterial drug.

Objective: This study is to enhance the potential and to explore the antibacterial efficacy of Dinoxin B, a natural withanolide.

Methodology: A comprehensive analysis of Dinoxin B withanolide to evaluate its drug-likeness properties including the Lipinski rule of five, absorption, distribution, metabolism, excretion, drug likeliness, and toxicity were conducted using PreADMET. To study its efficacy as an antibacterial drug candidate, evaluated its binding potentialities to different resistant proteins (retrieved from Protein Data Bank) of *Staphylococcus aureus* such as Sar A protein(2FNP), AgrA Protein(4G4K), Multi-Drug Efflux pump Protein(4LLL), Penicillin-binding Protein(3HUM), Topoisomers(4PLB) and DNA gyrase(2XCT) through docking studies, using Maestro 12.4 Schrodinger software. The highest affinity was observed with Sar A protein, therefore, its docking performance was compared to that of vancomycin, a commercial SarA inhibitor. Virtual screening analysis was conducted to target the active molecule involved in the interaction. Pharmacokinetic properties such as human intestinal absorption (HIA), cellular permeability (P_{CaCO_2}), cell permeability of Maden Darby Canine Kidney (P_{MDCK}), skin permeability (P_{Skin}), plasma protein binding (PPB), penetration of the blood-brain barrier ($C_{Brain/Blood}$), toxicological mutagenicity and carcinogenicity also evaluated.

Result: Dinoxin B showed good pharmacokinetic properties and drug-likeness. It showed a high docking score(-7.52) with Sar A protein. SarA a known master controller of biofilm formation by regulating Quorum-signaling is an attractive target for drug development. Virtual screening results proved that amino acids involved in the interaction between 2FNP and Dinoxin B Withanolide and that of 2FNP and Vancomycin are the same such as ASP:120, GLU B:135, LYSB:127. It is an indication of Dinoxin B Withanolide's mechanism of action to that of Vancomycin.

Conclusion: Dinoxin B Withanolide can be considered as an effective phytocompound due to its pharmacological properties and significant antibacterial efficiency against *S.aureus*. In silico results showed its good binding potentiality against Sar A protein(biofilm regulator) which threatens the modern era as they promote Methicillin Drug Resistance.

Keywords: SarA inhibitor, Dinoxin B withanolide, Pharmacokinetics.