



MANIPAL INSTITUTE OF TECHNOLOGY  
MANIPAL  
(A constituent unit of MAHE, Manipal)

INSTITUTION OF  
**EMINENCE**



MANIPAL  
ACADEMY OF HIGHER EDUCATION  
*Institution of Eminence Deemed to be University*



PRATHAM  
TRADERS



SDGs



The Institution of Engineers - Biotechnology, Manipal Chapter (IE-Bt)  
and  
Department of Biotechnology, MIT Manipal

INTERNATIONAL CONFERENCE

# SYMBIOT'24

*(Symphony of Medicine, Biological sciences & Omics Technologies)*

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# MAHE

MAHE has branch campuses in Bangalore, Malaysia, Dubai and Antigua in the Caribbean Island. There is also a campus in Mangalore with a medical college, a dental college and a nursing college with attached teaching hospitals. MAHE has an international academic collaboration for twinning programmes in engineering with universities in the US, UK, Australia and other countries. Manipal Group institutions are located on scenic campuses, which provide a high-quality lifestyle and ideal environment for study. All campuses have excellent infrastructure for academic activities, sports and other extracurricular activities. The infrastructure includes air-conditioned lecture halls, a skills lab, air-conditioned hostels, and a multi-cuisine food court. The state-of-the-art health sciences library is fully air-conditioned, accommodates 1300 learners and has over 62,000 books and over 600 journals. The library facilities include Medline, Proquest medical library of online databases, audio-visual, Cochrane library, e-learning, computer and Internet services. The Skills Lab and Anatomy Museum are considered amongst the best in the world. The latest addition to the facilities, a Simulation Lab with computer-driven mannequins, is an achievement, which the university is proud of. It is of considerable help to students in the field of health care.

MAHE believes in providing the finest in infrastructure and facilities to its students when it comes to learning and research. In fact, some of the facilities, like the Innovation Centre, have served as a valuable 'incubation centre' for industry and research. The state-of-the-art innovation centre bridges the gap between universities and industries for industrial-academic research.

Other facilities on the campus include a gym, swimming pools, and football and cricket grounds.

The new indoor sports complex is perhaps one of its kind in Asia. The complex has five badminton courts, four squash courts, three tennis courts, a basketball court, gymnasiums and a walking track. Besides being an ISO 9001:2008 and ISO 14001:2004 certified University, it is home to many top 10 ranked institutions of India. MAHE has won the prestigious IMC Ramkrishna Bajaj National Quality Award and International Asia Pacific Quality Award during 2007- 2008. MAHE attained the Institute of Eminence by MHRD in 2018.

# MANIPAL INSTITUTE OF TECHNOLOGY

Manipal Institute of Technology (MIT), one of the Premier Engineering Institutes in India, was among the first self – financed engineering colleges in the country. It was started in 1957 by Padmashree late Dr.T.M.A Pai, as Manipal Engineering College with an undergraduate course in Civil Engineering. In 1965, the institute got affiliated to the University of Mysore from Karnataka University. In 1974, it was renamed as Manipal Institute of Technology (MIT). In 1980 it got affiliated to the University of Mangalore. After the creation of the Visveswaraiah Technological University (VTU), MIT along with a number of other engineering colleges in the state got affiliated to the VTU in 1998. As the Manipal Academy of Higher Education (MAHE) had acquired a Deemed University status, MIT became a constituent institution of MAHE in May 2000.

In 2003, MIT obtained full academic autonomy and adopted credit system with 10 point grading. In 2007 MAHE was renamed as Manipal University and MIT retained its status as a constituent institution of Manipal University. With total student strength of over 7500, MIT has emerged as the largest institute of University. MIT currently offers undergraduate programs (B.TECH) in 16 disciplines and postgraduate courses (M.TECH/MCA) in 24 different streams and Doctoral programs (Ph.D) in all streams of engineering, basic sciences, humanities and management. Academic programs offered by institute are approved by AICTE and have been accredited by the National Board of Accreditation (NBA). The institution plays a vital role in producing world – class engineers tuned to the demands of a fast changing global village.

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## SYMBIOT'24

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# DEPARTMENT OF BIOTECHNOLOGY

The Department of Biotechnology, MIT, Manipal was founded in the year 2005. The department has state-of-the-art infrastructure, well defined and updated curriculum, and wide range of electives to encourage interdisciplinary research. The faculty are highly qualified and experienced with research interests in diverse and emerging areas of biotechnology. The department has received up to 5 crores in research grants from various funding agencies.

The vision of the department: Excellence in the teaching-learning process and research.

The mission of the department: To impart and disseminate knowledge, develop competencies and to produce industry-ready and academically enriched engineers for the emerging areas of applied biotechnology.

## IE-BT

The Institution of Engineers-Biotechnology, Manipal Chapter (IE-Bt) is a premier society of Indian engineers from MIT, Manipal, which organizes technical and non-technical activities relating to different aspects of biotechnology. SymBiot is a national level symposium conducted annually by IE-Bt, Manipal with the aim of providing participants an exposure to a real-life work environment. Every year more than 200 students from all over the country take part in the event.

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# BioAI-Based FemTech Healthcare Platform

**Dr. Junhyung Park**

**CEO and Co-Founder of 3BIGS Co. Ltd., South Korea**

FemTech, a burgeoning field dedicated to technology-based solutions for women's health, encompasses services addressing various stages of a woman's life, including menstruation, pregnancy, childbirth, and menopause. The integration of BioAI, which combines artificial intelligence (AI) with biotechnology, is gaining prominence in healthcare and shows significant potential in FemTech applications. The primary objective of this research is to develop a BioAI-based FemTech healthcare platform that provides personalized health management services tailored to the various stages of a woman's life. This platform aims to enable women to monitor their health in real-time and receive customized healthcare solutions. The BioAI-based FemTech healthcare platform has the potential to revolutionize women's health management. By providing innovative and personalized health solutions, it supports women in leading healthier and happier lives. This platform represents a significant advancement in the FemTech field and sets the stage for future research aimed at expanding its functionalities and addressing a broader range of women's health issues.

# Biotechnological approaches for caffeine degradation: environmental and food applications

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Caffeine is a purine alkaloid which is a major constituent of coffee, tea and other beverages. Caffeine acts as a central nervous system stimulant but it also has negative withdrawal effects. Decaffeinated beverages are being used to overcome its negative effects. In addition, effluents from coffee and tea processing plants have high concentrations of caffeine at ranging between 1 g/l, which will affect the microbial community in soil and water. Hence from both food and environmental point of view, caffeine degradation is necessary. Conventional decaffeination processes are expensive and uses toxic solvents. Hence development of a process involving an enzymatic (specific) degradation of caffeine to non-toxic compound is necessary. Identification of enzymes specific to caffeine degradation will solve the problem of chemical extraction of caffeine in food products and as well as treating the wastes containing caffeine. *Pseudomonas* sp. was isolated from coffee plantation area capable of utilizing the caffeine as sole carbon and nitrogen source. The rate of caffeine degradation was enhanced in the presence of sucrose. The isolate was characterized as *Pseudomonas putida* based on 16S rRNA analysis. The effect of different nutrients, physical parameters affecting caffeine degradation was studied and optimized using statistical experimental design. Kinetics of caffeine degradation by whole cells and immobilized cells were performed. Localization studies revealed that caffeine degrading enzymes are located in cytoplasm and they are inducible in nature. Purification and biochemical characterization of the enzyme was performed. Optimization of conditions for maximum production of caffeine degrading enzymes is studied in bioreactors. Induced cells were used as biocatalyst to degrade caffeine in commercial tea samples and effluent samples. In addition, whole cell biotransformation of caffeine to theobromine was optimized.

# Hepatitis and Hepatoprotective Plants of the Western Ghats

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The liver is the basic organ that regulates homeostasis in the body and is involved with almost all the biochemical pathways associated with growth, against diseases, nutrient supply, energy provision, and reproduction. The liver is also expected to protect the hazards of harmful drugs and chemicals. In spite of tremendous scientific advancement in the field of hematology in recent years, liver related problems are on the rise. Hepatitis is the major hepatic disorders that account for a high death rate caused due to the infection of infective hepatitis and serum hepatitis viruses, toxic effect of the chemicals and drugs. In spite of tremendous advances made in the modern medicine, there is no specific drug to jaundice only symptomatic treatment, physical rest prescribed to the patients and for which suitable drugs are yet to be investigated from the natural sources. Thus, interest and effort have shifted toward medicinal plants as new sources of hepatoprotective agents.

The herbal products today symbolize safety when compared with the synthetic drugs that are regarded as unsafe to human and are usually associated with various side effects. Although herbs had been prized for their medicinal, flavouring and aromatic qualities for centuries, the synthetic products of the modern age surpassed their importance in the past decade. However, the blind dependence on synthetic drug is coming to an end and people are turning their attention towards the natural product with hope of effective and long term therapy against alcohol induced liver diseases. Over three-quarters of the world population relies mainly on plants and plant based medicines for health care. However, due to lack of scientific clinical validation most of these herbal drugs cannot be recommended by competent medical authority for the treatment of liver diseases. Only a few herbal formulations are existing in the market as potent hepatoprotective drugs Ex. Silymarin, Liv-52, Arginine-Thiazolidine Carboxylate, Lecithin, Syllimarine + B-complex, Beta-Carotene equivalent to Vitamins etc.



Due to the Industrial Revolution and development of organic chemistry, preference has been given for synthetic products for pharmacological treatment. The reasons for this were that pure compounds were easily obtained, structural modifications to produce potentially more active and safer drugs could be easily performed and the economic power of the pharmaceutical companies was increasing. In most of the countries chemical synthesis dominates the pharmaceutical industry and 25% of the pharmaceuticals are based on plant-derived chemicals. Of the 252 drugs considered as basic and essential by the World Health Organization (WHO), nearly 11 % of them are being exclusively from plant origin and a significant number are synthetic drugs obtained from natural precursors.

Herbal based therapeutics for liver disorders has been in use in India for a long time and has been popularized worldwide over the leading pharmaceuticals. Despite the significant popularity of several herbal medicines for physiological ailments in general and for liver diseases in particular, there are still unacceptable treatment modalities for liver diseases. Popularity of herbal remedies is increasing globally and at least one quarter of the patients with liver diseases use ethno-botanicals. More efforts need to be directed towards methodological scientific evaluation of herbal medicines for their safety and efficacy by subjecting to vigorous preclinical studies followed by clinical trials to unravel the mysteries hidden in the hepatoprotective plants. This approach will help in exploring the real therapeutic value of these natural pharmacotherapeutic agents and standardized the dosage regimen on evidence based findings to become more than a fashionable trend.

Many investigators have evaluated the hepatoprotective potency of various plant based drugs or isolated compounds using CCl<sub>4</sub> as the hepatotoxic chemical in experimental animal models and it was known that the hepatotoxic effect of CCl<sub>4</sub> simulates with the human viral hepatitis condition. The metabolism of carbon tetrachloride via CYP2E1 to highly reactive free radical metabolites, trichloromethyl and trichloromethyl peroxy free radicals are mainly associated with CCl<sub>4</sub>-induced hepatic damage. These radicals are suggested to react with sulfhydryl groups of glutathione and protein thiols. The covalent binding of these radicals to sulfhydryl-containing proteins in cells will initiate a chain of events leading to membrane lipid peroxidation and cell necrosis.

The primary metabolites, are highly reactive and are capable of covalently binding locally to cellular macromolecules, with preference for fatty acids from membrane phospholipids. When these radicals attack the polyunsaturated fatty acids of the cellular membranes, the fatty acid free radicals generated initiate autocatalytic lipid peroxidation, ultimately resulting in the loss of membrane integrity and leakage of microsomal enzymes. This was evidenced by an elevation in the serum marker enzymes namely AST, ALT and ALP after CCl<sub>4</sub> administration in the experimental rats. Therefore, in this review a detailed account on the phytochemicals and hepatoprotective properties of the various medicinal plants of the Western Ghats have been investigated and discussed in detail. This study also authenticates the traditional medicinal claim of the plants as the hepatoprotective herb.

# Advancement of Surface Enhanced Raman Spectroscopy in Diagnostic Applications

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Surface-enhanced Raman scattering (SERS) has been investigated as a highly sensitive spectroscopic modality where the signal intensity of molecular vibration enhanced up to  $10^8$ – $10^{14}$  folds compared to simple Raman spectra. Multiplexing capability of Raman fingerprints, molecular specificity, high sensitivity, and capability to fish out complex biological compositions at the molecular level augmented SERS as a potential diagnostic modality in biology and medicine. While assessing all the merits of classical Raman spectroscopy, SERS provides a more sensitive and selective detection and quantification platform. Non-invasive, chemically specific, and spatially resolved analysis facilitates the exploration of SERS-based nanoprobe in diagnostic and theranostic applications with improved clinical outcomes compared to the currently available so-called state-of-the-art technologies. Adequate knowledge of the mechanism and properties of SERS-based nanoprobe is inevitable in utilizing the full potential of this modality for biomedical applications. The safety and efficiency of metal nanoparticles and Raman reporters have to be critically evaluated for the successful translation of SERS into clinics.

On the other hand, the advancement of nanotechnology holds great promise for both diagnosis and therapy in a number of communicable and non-communicable diseases including cancer, neurodegenerative disorders, and infectious diseases which is coined as nano-theranostics. Exploration of a sensitive diagnostic nanoprobe especially with the aim of point-of-care treatment is another challenging task for early and accurate detection of cancer biomarkers which facilitates efficacious therapy by reducing mortality and morbidity. Recently, we have fabrication programmable nanoparticles that feature an “on-off” switching transition between fluorescence and SERS for the multiplex detection of lung cancer biomarkers which furnished a semi-quantitative evaluation of biomarkers through both modalities. In another approach, we have developed a gold nanorod (GNR) based theranostic nanoprobe for targeting metastatic melanoma by combining PTT, PDT, and chemotherapy along with SERS imaging for better treatment and effective follow-up therapeutic response. We believe that this proof-of-concept will provide a blueprint for the diagnosis and differential staging of cancer into various histological subtypes based on the differential expression of the antigens. We have also developed a SERS based immune-sensor to evaluate the presence of Alzheimer’s Disease (AD) biomarker i.e., beta amyloid ( $A\beta_{42}$  protein). An efficient SERS based sandwich assay has been successfully demonstrated for an efficient detection of beta amyloid proteins in AD. Therefore, SERS techniques explored as an upcoming molecular diagnostic modality ranging from simple detection platforms to complicated clinical applications.

# **Molecular evolution of SARS-CoV-2 and its association with comorbidity by deciphering of multiomics and system biology data**

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Abstract:

SARS-CoV-2 has constantly been evolving into different forms throughout its spread in the population and cross species transmission. Emerging SARS-CoV-2 variants, predominantly the variants of concern (VOCs), could have an impact on the virus spread, pathogenicity, and diagnosis.

Spike protein sequences of SARS-CoV-2 genomes were analysed to assess the impact of mutational diversity. The underlying effect of the variations of mutational patterns were observed to be on their amino acid properties such as hydrophobicity. The recently emerged Omicron variant when compared to other VOCs showed a discrete amino acid usage pattern which was significantly correlated with the increased hydrophobicity of spike proteins. This selection of more hydrophobic amino acids in omicron spike proteins facilitated in effective binding with ACE2 receptors across different population. The association of comorbidity with SARS-CoV-2 infection have also been studied which could help us assess the impact of Covid on global health in the long run.

# Breath Analysis in Disease Detection

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Human exhaled breath contains a large number of different molecular species. Elevated concentrations of these molecules, or of specific isotopologues, can be markers for particular medical conditions. An appropriately devised breath analysis protocol may provide a non-invasive and rapid diagnostic method. We can develop such non-intrusive methods by combining sensitive and accurate spectroscopic detection techniques with molecular interactions. Considering that diseases alter the essential chemical reactions among biologically relevant molecules and affect outcomes, spectroscopic measurements can provide a unique pathway. This talk will provide a nuanced understanding of how exhaled breath can be used to facilitate early diagnosis for a spectrum of diseases by probing various molecular signatures of exhaled breath species.

# Applications of microorganisms from Bornean tropical ecosystems

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Microbial diversity encompassing a spectrum of various types of microorganisms (bacteria, fungi, algae etc.) is a promising natural resource. Brunei, located in the pristine island of Borneo, consisting of terrestrial, marine and forest ecosystems in addition to oil reserves, is a great reservoir of beneficial microbes. Microbes in general, have not just adapted to diverse environments on earth but can also consume metals, chemicals, pesticides, petroleum – all of which are toxic to us and can function as agents of bioremediation. Efficient waste management is imperative for ensuring sustainable communities. Microbes also drive biotechnological applications with novel biochemicals, enzymes and active ingredients useful to humans as industrial agents, food products, biopharmaceuticals, cosmetics, biofuels and more.

Furthermore, microbes from marine ecosystems have evolved unique features and metabolites like enzymes and osmolytes, to adapt to varying conditions of salinity and temperature. Such marine microbes and their biomolecules are potential sources of bioactive compounds and bioremediation agents. Recent studies in Brunei has found a diversity of culturable fungi and bacteria of biotechnological value. These microbes have found applications as biosurfactants, lignolytic enzymes, biofertilizers, biocontrol agents, inducers of agarwood among others. Finding new strains, optimizing the conditions for better performance and scale-up studies offer challenges and scope for further investigations and applications towards a sustainable future. In this paper the diversity and applications of microorganisms, newly isolated from Brunei, a tropical Bornean island will be discussed.

# **Clinical, Molecular, and Histopathological Analysis of Myotonia Congenita, a Rare Neuromuscular Disorder**

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Myotonia congenita (MC) is a rare neuromuscular disease caused by CLCN1 gene mutations, leading to delayed muscle relaxation and stiffness. This study examined MC's clinical, molecular, and histopathological aspects using electrophysiological and hematological analyses, genetic profiling through in silico methods, gene expression, epigenetic, allelic expression, and functional study using protein expression, and histopathological analyses.



# **Unveiling the pathogenesis of hypersensitivity pneumonitis: An integrated transcriptomics and metabolomics approach**

**Dr. Koel Chaudhury**

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Abstract:

Background: Hypersensitivity pneumonitis (HP) is an immune-mediated granulomatous interstitial lung disease (ILD) caused by repeated inhalation of specific antigens. Despite considerable research advancements, the pathophysiology of HP remains poorly understood.

**Methods:** The present study integrates metabolomic and transcriptomic datasets to identify alterations in HP subjects compared to healthy controls. Metabolic signatures were identified in serum, exhaled breath condensate (EBC), and bronchoalveolar lavage fluid (BALF) of HP patients using proton nuclear magnetic resonance (NMR) metabolomics. The differential diagnosis potential of these metabolites was evaluated by assessing their expression in patients with sarcoidosis, another type of granulomatous ILD. Additionally, whole blood transcriptomic gene expression data of HP patients obtained from the Gene Expression Omnibus (GEO) database were analysed. Over-representation analysis of the identified metabolites and genes was performed using IMPaLA (Integrated Molecular Pathway Level Analysis) version 12.

**Results:** Three metabolites, lactate, pyruvate, and proline were observed to be significantly altered across serum, EBC, and BALF in HP patients. These metabolites also demonstrated strong potential in distinguishing between HP and sarcoidosis, indicating their clinical significance in differential diagnosis. Transcriptomic analysis identified 59 significantly dysregulated genes in HP patients. The integrated metabolic-transcriptomic data highlighted dysregulation in the PI3K–AKT signaling and TCA cycle pathways. **Conclusion:** This study enhances the understanding of HP pathogenesis by identifying differentially expressed metabolomic and transcriptomic signatures of the disease. Furthermore, these molecules hold promise as candidate diagnostic markers for differentiating HP from other lung diseases.

**KEYWORDS:** HYPERSENSITIVITY PNEUMONITIS, METABOLOMICS, TRANSCRIPTOMICS, INTEGRATED OMICS, DIFFERENTIAL DIAGNOSIS

# **The Algae Advantage: Sustainable Solutions for Tomorrow's Challenges**

**Mr. Balaji Elangovan**

**Vice-President, Seagrass Tech Pvt Ltd., Chennai.**

Microalgae is the new sustainable solution to many of humanity's manifold problems. They have a huge array of applications in diverse domains ranging from food, supplements, cosmetics, fuels, medicine, agriculture, aquaculture to remediation of potential contaminants. However, there are challenges involved in the large-scale production, harvesting and purification of specific compounds from the algal cells. The lecture introduces the audience to the operational aspects of M/s Seagrass Tech Pvt Ltd and its scale of operations. The broad areas of application of microalgae are enlisted with real-life examples to evince interest in the minds of the audience.

# Molecular epidemiological typing methods to identify MRSA and an approach to combat antibiotic resistance with CRISPR-Cas system

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Molecular epidemiology and evolution of MRSA is an expansive topic. The burden of community-associated methicillin resistant *Staphylococcus aureus* (CA-MRSA) is on the rise in population and clinical settings on account of the adaptability and virulence traits of this pathogen. The isolates were genotyped by staphylococcal cassette chromosome *mec* (SCC*mec*) typing, staphylococcal protein A (*spa*) typing, accessory gene regulator (*agr*) typing, and multi-locus sequence typing (MLST). Four sequence types (STs) belonging to three major clonal complexes (CCs) were identified among the isolates: CC22 (ST2371 and ST22), CC1 (ST772) and CC8 (ST8). Our study also documents for the first time, the appearance of ST8-SCC*mec*IV (USA300) strains in India. Representative strains of the STs were further analyzed by pulsed field gel electrophoresis (PFGE). Inducible clindamycin-resistance was identified in 37.7% of the isolates and it was attributed to the presence of *erm*(A), *erm*(C) and a combination of *erm*(A) and *erm*(C) genes. Isolates which showed a phenotypic pattern of MR/LS (macrolide-resistance/lincosamide-sensitivity) harboured the *msr* (A) gene. In conclusion, we report a high rate of multidrug resistance among Indian strains of CA-MRSA and the emergence of the lineages ST2371 and ST8 in India. The reason for the concern is that MRSA often becomes resistant to multiple antibiotics limiting the treatment options. There is an urgent need to develop new strategies to control bacterial infections and the spread of antimicrobial resistance. CRISPR/Cas system has been developed into a new gene-editing tool for the prevention and control of bacterial drug resistance. Here CRISPR-Cas9 and CRISPR-Dcas9 have been shown to have bactericidal and attenuation property in MRSA.

# A novel anti-inflammatory structure: The nitron spin trap 5,5-dimethyl-1-pyrroline-N-oxide modulates the signaling triggered by lipopolysaccharide in macrophages

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Macrophages are innate immune and ubiquitous cells in tissues. Lipopolysaccharide (LPS)-triggered toll-like receptor (TLR) signaling and downstream nuclear factor (NF)- $\kappa$ B activation leading to inflammatory priming of macrophages and tissue damage. The nitron spin trap 5,5-dimethyl-1-pyrroline N-oxide (DMPO) traps protein-centered radicals and dampens LPS-induced inflammatory priming of macrophage, but the mechanism remains unknown. Herein, we used *in vitro* and *in-silico* models to test the mechanism by which DMPO dampens the LPS-induced priming of macrophages. Our *in silico* data indicates that DMPO binds tightly to four specific residues within the BB-loop in the TLR2-TIR domain. Our functional analysis showed that DMPO blocks zymosan-activated TLR2-mediated NF- $\kappa$ B activation using HEK cells expressing hTLR2.6. However, DMPO did not affect the overall TLR2-MyD88 protein-protein interaction. Therefore, DMPO binds to the BB loop within the TIR domain and dampens downstream signaling without affecting the overall TIRMyD88 interaction. By binding to the BB-loop, DMPO blocks TLR-downstream signaling, thus preventing the LPS-induced priming of macrophages towards an inflammatory phenotype. DMPO can serve as a structural platform for the design of novel mechanism-based anti-inflammatory drugs to prevent inflammatory activation of macrophages in acute (e.g., sepsis) and chronic (non-communicable) inflammatory diseases.

The total protein content present in LHP by Bradford assay was found to be  $409.35 \pm 0.005$   $\mu\text{g/ml}$ . The analytical techniques such as Attenuated Total Reflectance-Fourier Transform Infrared spectroscopy (ATR-FTIR), solid state carbon-13 Nuclear Magnetic Resonance (ssC13 NMR) spectroscopy, and Differential Scanning Calorimetry (DSC) revealed the secondary structure and conformational stability of LHP. X-Ray diffraction (XRD) studies showed its amorphous nature. Bioactivity assessment of LHP was performed in human keratinocytes (HaCaT) and human dermal fibroblasts (HDF) by 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) assay. The LHP was highly proliferative against skin cells and non-toxic, based on the findings of the bioactivity assay. LHP has the potential to be used as a therapeutic agent for OA, as its characterisation unveiled its physical stability, significant concentration of bioactive components that are pertinent to cartilage repair and its conformational stability.

**KEYWORDS:**

Osteoarthritis, Lyophilized human placenta, Characterization, Protein biofactors, Bioactivity

# FORMULATION AND EVALUATION OF HERBAL EXTRACT BASED NANOGEL

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## ABSTRACT:

This work aimed to create a herbal nanogel formulation that would facilitate and expedite wound healing, tissue repair, and damage remodeling by employing an ethanolic extract of *Morinda citrifolia* leaves. Microwave assisted extraction was employed using ethanol to extract the active constituents and subjected to GC-MS analysis. Carbopol 940 and HPMC were used in varying concentrations to formulate herbal nanogel. The pH, viscosity, spreadability, swelling studies, flavonoid content, and release of nanogel formulations were assessed. Since the pH ranged from 5.14 to 6.52 and the yield was 96%, it is unlikely that the nanogel will cause skin discomfort. The formulations' rheological examination, which demonstrated a decrease in viscosity with increasing RPM, supported the nanogel's shear thinning capability. In comparison to the other formulations, formulation F3 demonstrated good spreadability, with a value of 28.33 gm.cm/sec. In PBS 6.8 and 7.4, the swelling behaviour was superior in formulation F3. The flavonoid release of the formulations was found to be 90% and the percentage flavonoid content was determined to be 91.21%. The 24-hour prolonged release of flavonoids in the F3 formulation suggested that it have potential wound-healing properties. Formulation F3 showed the most promising and potential activity in terms of its ability to promote wound healing.

**KEYWORDS:** *Morinda citrifolia*, ethanolic extract, nanogel, wound healing

# The Intersection of Omics and Sepsis: Mapping the Patent Terrain

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## ABSTRACT:

Advancements in genomics, transcriptomics, proteomics, metabolomics, integrative omics and other high throughput technologies have extracted translatable insights into sepsis by analyzing genetic variants, gene expression, protein alterations, metabolic abnormalities, and microbiome composition. In addition to collaboration and integration, technical progress in sequencers, spectrometers, microarrays, bioinformatics platforms, or data visualization are driving discovery in the biomedical field of sepsis. These transformative processes and technologies enhance system science and therapeutic management of complex and challenging concerns like sepsis which have profound global health impact representing 20% of all global mortality. We analysed patent data from World Intellectual Property Organisation (WIPO) from 1990-June 2024 to explore how technological innovations in omics, catalyze knowledge generation and outcomes in sepsis. Our analysis outlines key trends in innovation, revealing geographical hotspots of patent activity, emerging technologies, clusters of related technologies and emerging areas of integration. This study identified over 6,488 omics-related patents with applications in sepsis recorded in WIPO. The five most active patent offices in terms of patent publication in this field are from the US, Europe (European Patent Office), South Africa, Canada, and India. The number of patents in these regions ranges from over 1,710 in the US to 20 in India. We categorized patents based on their International Patent Classification (IPC) as health and therapeutics, informatics, treatment of food and agriculture products, microbiology, materials or compounds, and diagnostics. Over 3,653 patents in the field have the classification A61K, which refers to preparations for medical, dental, or toilet/sterile purposes, followed by 2,260 patents with classification C07K, pertaining to peptides. Visualizations derived from this analysis not only inform research and development (R&D) strategies and investment decisions but also pinpoint gaps in integrated advancements in sepsis and omics technologies to inspire new research and development.

**KEYWORDS:** omics technologies, sepsis, patent, science and technology integration, biomedical research



# Evaluation of Antioxidant activity and Antimicrobial Activity of *Zanonia indica* L.

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## ABSTRACT:

*Zanonia indica* is a monotypic genus in the flowering plant family *Cucurbitaceae*, reported to occur in North East India, South India, Southeast Asia east and New Guinea. It is a climber with long flexible stem, usually twines around other trees for support. The fruit of *Zanonia indica* is known to cure various diseases. Water is filled inside the empty fruit and left overnight, and the same water is taken for fever, stomach-ache, urinary problems and to cure asthma. Petroleum ether, chloroform, methanol and aqueous crude extracts of fruit of *Zanonia indica* showed the presence of alkaloids, glycosides, flavonoids, terpenoids, tannins, saponins, quinones in preliminary analysis. Quantitative analysis of these extracts showed that methanol extract was rich in alkaloids, phenols and flavonoids. Antioxidant activity of fruit extracts of *Zanonia indica* using DPPH assay and ABTS radical scavenging assay revealed the presence of antioxidant property. The extract also showed Antimicrobial Activity against several pathogens like *S. hominis*, *E. coli*, *S. aureus*, *E. faecalis*, *S. typhimurium*, *B. cereus*. The methanol extract of this plant was subjected for phytochemical analysis through Gas Chromatographic Mass Spectrometry (GCMS) and the bioactive components were identified. Many bioactive constituents were identified namely Eugenol, Benzoic acid, 4-hydroxy-3-methoxy-, methyl ester, Octadecanoic acid, gamma.-Sitosterol, Trolox, Homogenol, Indole etc. The presence of these bioactive constituents in the plant extract may authenticate the scientific evidence for various pharmacological activities and therapeutic potentiality of the plant.

**KEYWORDS:** DPPH, ABTS, GCMS, antioxidant, *Zanonia indica*.

# Quantifying the Antibacterial Effects of Bacteria-Derived Silver Nanoparticles on the Growth Rates of *Escherichia coli* and *Staphylococcus aureus*

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## ABSTRACT:

The emergence of antibiotic-resistant bacteria demands the exploration of alternative antimicrobial agents. Silver nanoparticles (AgNPs), particularly those derived from biological sources, have shown promise as effective antibacterial agents. This study aims to quantify the antibacterial effects of bacteria-derived silver nanoparticles on the specific growth rates of *Escherichia coli* and *Staphylococcus aureus*. Utilizing a systematic experimental approach, we investigated the influence of varying concentrations of bacteria-derived AgNPs on the growth dynamics of these two bacterial strains. Pure cultures of *E. coli* and *S. aureus* were treated with different concentrations of AgNPs synthesized by *Klebsiella pneumoniae* NSB-2, a strain isolated from soil. Growth rates of *E. coli* and *S. aureus* were monitored by measuring the optical density at 600 nm (OD<sub>600</sub>) at regular intervals, and specific growth rate constants ( $\mu$ ) were calculated during the exponential phase of bacterial growth. The experimental design was optimized using Design Expert software to ensure robust and reliable results. Our findings demonstrated a significant reduction in the specific growth rates of both *E. coli* and *S. aureus* in response to increasing concentrations of bacteria-derived AgNPs. The statistical analysis provided by Design Expert software enabled the identification of optimal nanoparticle concentrations for maximum antibacterial efficacy. Response surface methodology (RSM) and contour plots were utilized to visualize interaction effects and optimize experimental conditions further.

This study confirms the potent antibacterial activity of bacteria-derived silver nanoparticles and highlights their potential as alternative antimicrobial agents. The optimized use of AgNPs could lead the way for new strategies in combating bacterial infections, particularly those caused by antibiotic-resistant strains. Future research should focus on the mechanisms of action, long-term effects, and potential applications of these nanoparticles in clinical settings. Our results contribute to the growing body of knowledge on the application of nanotechnology in microbiology and public health.

**KEYWORDS:** Design Expert Software, Response Surface Methodology (RSM), Nanotechnology, Antibiotic Resistance, Specific Growth Rate.

# Evaluation of phytochemical and antioxidant property of selected medicinal plants from Mizoram

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## ABSTRACT:

*Aporosa octandra* (Buch.-Ham. ex D.Don) [Euphorbiaceae] is a small tree, used by traditional healers to treat stomach ulcer, hypotension, and diarrhea, wounds, cuts and itches, curing rheumatism and bone fractured area; its stem bark juice is applied on cuts and abscess. *Mallotus roxburghianus* Müll.Arg. [Euphorbiaceae] is a deciduous shrub, the decoction of leaves is used by the tribal people of Mizoram for the treatment of diabetes. This plant has been used as a therapeutic agent for liver-related issues, diabetes, hypertension, inflammations and ulcers. *Dillenia pentagyna* Roxb. [Dilleniaceae] is a small tree with tortuous twigs, whose fruits are edible and are cooked as a dish by the tribal people of North-East and central parts of India. The plant's bark and fruits have been traditionally used for treating inflammatory diseases, chest pain, and cancer. *Callicarpa arborea* Roxb. [Lamiaceae] is a tree whose bark juice is applied on cuts and wounds as haemostatic. Decoction of the bark or of the young leaves is taken orally in abdominal colic. *Begonia inflata* by Clarke. [Begoniaceae] is a perennial flowering plants. Decoction of the plant is given orally in dysentery and for the treatment of haemorrhoids. Decoction of rhizome is given orally in malaria. The flower is used as fish poison. *Securinega virosa* (Roxb. ex.Willd.) Baill [Phyllanthaceae] is a shrub that It is used by traditional healers treat gonorrhoea, diarrhoea, dysmenorrhoea, epilepsy, chest complaints, renal calculus, rheumatism, edema gastrointestinal conditions, Malaria, liver disease, inflammation and pain and for aphrodisiacs. Its extracts are used for the expulsion of round worms and in the treatment of bilharziasis. Amongst the selected plants we performed qualitative phytochemical analysis and quantification of Phenolics and Flavonoids using methanol extracts. We also checked for antioxidant potential of the extracts using DPPH and ABTS assay, furthermore we checked for the presence of compounds such as Gallic Acid and Chrysin using High Performance Liquid Chromatography (HPLC).

# Identification of Genetic variants in Hereditary Breast & Ovarian Cancer Patient using Multi gene panel -A Single Centre Study

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**Objective:** The identification of additional genetic variants in hereditary breast and ovarian cancer by using a multigene panel and its implication on Genetic counseling and cancer risk assessment

**Methodology:** A prospective analysis was performed on 169 patients with breast and ovarian cancer. Multigene panel testing was conducted on the extracted DNA of all 169 patients using a capture kit on the Illumina sequencing platform. Variations were classified according to the guidelines of the American College of Medical Genetics.

**Result:** Out of 169, Total positive rate was 31%, Most of this mutation was detected in BRCA1(74%), BRCA 2(8%), and other pathogenic variants observed in non-BRCA high penetrance gene and variants of unknown significance were identified in 30% and no mutation was detected in 39%.

**Conclusion:** In our cohort of 169 individuals with Hereditary Breast and Ovarian Cancer (HBOC), we observed a higher proportion of pathogenic variants among patients diagnosed with ovarian cancer. These variants were found in the BRCA1 and BRCA2 genes. Additionally, mutations were identified in other non-BRCA genes, including ATM, CHEK2, TP53, PALB2, MUTYH, PMS2, BIRP1, and FNACM, which are associated with varying degrees of penetrance from high to moderate. Patients with these pathogenic mutations, including those in non-BRCA genes, are currently undergoing comprehensive monitoring and follow-up. Our findings underscore the importance of expanding genetic testing beyond BRCA1 and BRCA2, as this comprehensive approach aids in treatment, management and surveillance of the affected patients and facilitates monitoring of at-risk family members.

**KEYWORDS:** Hereditary breast and ovarian cancer, Genetic testing, multi-gene panel.

**ABBREVIATION:** HBOC-Hereditary Breast and Ovarian Cancer, VUS-Variants of unknow Significance

# Exploring the Genomic DNA: Isolation, Analysis, and Comparative Study of Algal DNA

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Abstract:

This study delves into the intricate realm of algal genomics through a comprehensive exploration encompassing isolation, qualitative and quantitative analysis, and comparative evaluation of genomic DNA from four different algal species. The genomic DNA from four different random Algal species was extracted according to the standardized protocol of the CTAB method. The concentration, yield, purity and contamination analysis was carried out for the isolated DNA through spectrophotometry. DNA fragment size and integrity was qualitatively analyzed through agarose gel electrophoresis. Our results demonstrate significant variation in both quality and quantity of isolated genomic DNA that were studied. The spectrophotometric analysis revealed variation in DNA yield, purity and concentration of different species of algae. In our study, the ratio A260/A280 was used to indicate the purity of isolated DNA; if it is less than 1.6 then it indicates the presence of RNA and other protein contaminants. The ratio A260/A230 was taken as an indicator of Salt carry over in the sample. Agarose gel electrophoresis showed varying sizes of DNA isolated among samples. Comparative analyses provided valuable insights into the similarities and distinctions among the sampled algal genomes, elucidating underlying genetic determinants governing their ecological adaptations and physiological traits. This multidimensional approach not only enhances our understanding of algal biology but also holds implications for applications ranging from biotechnology to environmental conservation.

**KEYWORDS:** Algal genomic DNA, Qualitative analysis of DNA, Quantitative analysis of DNA, Comparison of algal genomic DNA

# Optimizing 2,4-D Removal Using Rice Husk Biochar by adsorption

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## Abstract:

In both agricultural and non-crop areas, 2,4-D (2,4-Dichlorophenoxyacetic acid) is a common

herbicide used to control broadleaf weeds. Hence, we plan on removing the pesticide from the soil using an adsorptive material known as rice husk ash. A byproduct of burning rice husks, rice husk ash (RHA) is rich in silica and has a variety of industrial uses. Due to its adsorptive qualities, it is often used in environmental engineering and as an additional cementitious material in the construction industry. The project focused on finding the best parameters for the biochar to work at maximum efficiency. The project applied colorimetric method with an absorbance test @283 nm for finding concentration values. The experiment parameters were chosen as follows: pH of the 2,4-D solution (5,7,9), mixture ratio (0.5,1,2 g/20ml), activated RHA molarity (0.5,1,2 M) and time (8,16,24 hrs). The findings demonstrated that the adsorption capacity and efficacy of eliminating contaminants were greatly increased at pH of 5.62, ratio of 1.46g/20ml, molarity of 1.57M, reaction time of 24.22 hrs. The results showed that there was a percentage removal of 96.13% and adsorption capacity of 2.06mg/g. The enhanced performance of the activated RHA suggests that it has the potential to be used in more effective environmental applications.

**KEYWORDS:** 2,4-D, rice husk ash, adsorption, biochar



# Gene expression profiling predicts the development of oral cancer in KBCHR 8-5 cell lines

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## Abstract:

Oral cancer is a major devastating head and neck cancer subtype and is any cancerous tissue growth located in the oral cavity or oropharynx . There are several types of oral cancers, but around 90% of oral cancers are squamous cell carcinomas. Oral cancer is the sixth most common malignancy in humans. Its incidence and mortality have also increased over the past decades. . It ranks among the top 10 cancers in incidence, and despite advances in research and treatment, survival has not significantly improved over the past few years, which remains an ongoing challenge for biomedical sciences. The present study focuses on the measurement of cell viability and proliferation as the basis for numerous in vitro assays of a cell population's response to external factors and the gene expression of MIR5580 in oral cancer KBCHR8-5 cell lines. The MTT Cell Proliferation Assay measures the cell proliferation rate and, conversely, the reduction in cell viability when metabolic events lead to apoptosis or necrosis. The anti-cancer activity of Lomustine on KB-CHR-8.5 cells IC50 ( $\mu\text{g}$ )  $140.98 \pm 3.581$ .

Studied the cytotoxicity of drugs of Lomustine, with the oral cancer cell lines of KBCHR. Based on the cytotoxicity KBCHR cells treated with Lomustine IC50 Concentration, MIR5580 upregulated with the 995.99 folds cytotoxicity of the drugs to cells, studied further the Lomustine, for the gene expression analysis by Real-Time PCR with genes of MIR5580 and. GAPDH is used a control gene for normalization of gene expression regulated with the 64.89 folds express significantly compare to untreated control cells. Relative Gene Expression of Lomusitne treated with KBCHR Cells. Results are expressed in mean±SE (n=3) and  $p < 0.05$  considered significantly .

**KEYWORDS:** oral cancer, anti-cancer activity, gene expression .

# Chemopreventive Effects of Bioactive Compounds from Tulsi (*Ocimum sanctum*) against Ovarian Cancer: In Vitro and Natural Model Investigations

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## ABSTRACT:

Extraction and identification of bioactive molecules from natural sources with potential anticancer properties have become pivotal in cancer research. This study focuses on the chemopreventive effects of bioactive compounds derived from Tulsi (*Ocimum sanctum*) leaves against ovarian cancer, employing both in vitro cell lines and a natural animal model.

Tulsi leaves were subjected to extraction using standard protocols, and the resulting solution was assessed for cytotoxicity against ovarian cancer cells. The findings revealed a concentration-dependent reduction in cell viability, accompanied by altered cell morphology, DNA damage, and induced cell death. Anti-inflammatory activity was further investigated using a nitric oxide assay with mouse macrophage cells, demonstrating significant effects on cellular health.

In animal experiments, a laying hen model—a spontaneous model of ovarian cancer—was utilized. Laying hens, aged one-and-a-half years, were randomly divided into control and test groups. The test group received Tulsi extract in capsule form at varying doses (167, 334, and 667 mg/kg body weight) for 90 days. Surrogate endpoints were examined to identify the optimal dose for long-term studies. Results indicated a dose-dependent increase in antioxidant activity in ovarian and liver tissues, specifically in the Tulsi-treated groups. Prostaglandin E2 levels were notably reduced in ovarian tissue, suggesting a potential protective effect against inflammation.

Ovarian cancer remains a substantial cause of mortality, necessitating innovative approaches for prevention and treatment. This research proposes a nutritional intervention using Tulsi, a traditional herb, to prevent or delay ovarian cancer naturally. The utilization of a laying hen model, mirroring the spontaneous development of ovarian cancer in humans, provides valuable insights into the potential health benefits of Tulsi. If successful, this intervention holds promise for enhancing women's overall well-being in society.

**KEYWORDS:** Chemoprevention, Ovarian Cancer, Tulsi, Laying hen model.

# Unveiling Integrin Trafficking in Oral Squamous Cell Carcinoma: A Potential Target for Disease Intervention

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## ABSTRACT:

Integrins are vital for cell adhesion and are associated with cancers. However, due to inconsistent research, the primary integrin in oral cancer remains still unidentified.

Objective: To elucidate the expression pattern and cross-talks of integrin in oral cancer; and to confront them with known drugs.

Methods: The tissue transcriptomic profiles from oral cancer patients, were extracted from Omnibus database. Differential gene expression patterns of these profiles were then analysed by using LIMMA. The prevalent integrin cluster was retrieved through overlapping analysis. To validate the influence of the shortlisted integrins on the disease prognosis, overall disease survival of the patients was studied in the Head and Neck Cancer, of TCGA cohort (The Cancer Genome Atlas). The Protein-Protein interaction network of the significant DEG integrins was constructed using STRING and visualized in Cytoscape. The short-listed integrin was then docked using AutoDock Vina against the drug library, derived from literature.

Results: The GEO datasets, GSE6791, GSE13601, GSE30784, GSE31056, and GSE138206 satisfying the inclusion were retrieved. The overlapping analysis of the DEG's (adjusted p-value <0.05) revealed ITGA3, ITGA5, ITGA6 and ITGAV as shared integrins among the profiles. The identified integrins showed an upregulated expression pattern in all the profiles with a log fold change > 1, except for ITGA3 (0.76 in GSE13601) and ITGA5 (0.96 and 0.86 in GSE138206 and GSE6791, respectively). A consistent and notable, up-regulation pattern in all the profiles was observed for ITGA6. The overall survival analysis revealed significant results for ITGA3(p=0.0014), ITGA5(p=0.0029), ITGA6 (p=0.0001). The protein network constructed showcased the highest nodal degree of ITGA6. The drug library constructed on the structural similarity of Pranlukast antagonistic ligand with evident inhibitory activity against ITGA6, revealed a pool of 19 drugs. Compounds having similarity threshold greater than 0.5 such as Novobiocin in the library showcased comparable binding sites and energy.

**KEYWORDS:** Integrin, Oral Cancer, Protein-Protein interaction, Molecular docking

# Bioreactors and 3D Bioprinting: A Collaborative Approach to Advance Tissue Engineering

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## ABSTRACT:

Additive manufacturing or bioprinting is a technological process in which feasible biomaterials and bioinks comprised of natural and synthetic polymers are used to generate a 3-dimensional (3D) model of tissues, scaffolds, or organs. Conversely, bioreactors are vessels that provide a favorable environment that is feasible for the growth of organisms, animal cells, plant cells, and other biological products. Integrating bioreactors into bioprinting technology has further advanced its application in healthcare and other industries. Different bioreactor models have also emerged over the years, having specific functions and environmental conditions favorable for the construction of the 3D model. The availability of feasible polymers, composites, ceramics, and other biocompatible biomaterials has led to the establishment of 3D bioprinting of living tissues through regenerative medicine to overcome the limitations faced in organ transplantation. Biomaterials play a crucial role in facilitating the growth and organization of tissues newly constructed by providing temporary scaffolding. The inherent properties of the biomaterials intricately guide the layer-by-layer organization along the z-direction during the construction of the 3D model. 3D bioprinting in pharmaceutical and drug design has exhibited enormous advantages in better spatial control, high throughput, automation, and fabrication of structures.

**KEYWORDS:** 3D Bioprinting, Bioreactor, Biomaterials, Tissue Engineering

# **Role of Vitexin in Alleviating Cisplatin Induced Acute Hematotoxicity in Rats**

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## **Introduction:**

The hemopoietic system is well-regulated and can help assess drug toxicities. Cisplatin induced myelosuppression is an illustration of such drug toxicity. Vitexin is an apigenin flavone glycoside, and its role in acute hematotoxicity is unclear. The present study aims to investigate the influence of vitexin on cisplatin induced acute hematotoxicity in rats.

## **Methods:**

Thirty female Wistar rats were randomly divided into five groups (n = 6 per group); Group1: Normal control, Group2: Cisplatin control received a single dose of cisplatin (7mg/kg b.w; i.p.), Group3: Vitexin control received Vitexin (1.5 mg/kg b.w; orally) once daily for 7 days. Group4: Therapeutic group received single dose of cisplatin followed by daily dose of Vitexin for 7 days. Group 5: Prophylactic group received Vitexin daily for 15 days, followed by one dose of cisplatin. Peripheral blood cell counts were done on the 3rd and 6th days.



### Results:

Compared to Group1, Group2 showed significant leucocytopenia ( $p<0.01$ ) and thrombocytosis ( $p<0.05$ ) on day 3. A non-significant increase in the RBC count and Hb was observed. On 6th day, thrombocytosis, leucocytosis, and anemia were observed, although variations were insignificant. Compared to Group2, on day 3, Group4 showed a significant increase in RBC count ( $p<0.05$ ). There was no significant increase in WBC count; however, a reduction in Hb and platelet counts was observed. On day 6, only platelet count increased substantially ( $p<0.001$ ). Group-5 showed significant increase in WBC count ( $p<0.01$ ) and a decrease in RBC( $p<0.05$ ) and platelet( $p<0.05$ ) counts on day 3 without any alteration in Hb concentration. On day 6, there was significant ( $p<0.001$ ) decrease in platelet and RBC counts, with a non-significant decline in WBC counts & Hb concentration.

### Conclusion:

Based on these results, the therapeutic dose of vitexin improved the cisplatin-induced anemia, whereas the prophylactic dose improved the immune response by leucocytosis.

**KEYWORDS:** Cisplatin, Hematotoxicity, Wistar rats, Vitexin

# Anaerobic digestion of food waste using selective microbial consortia and its optimization studies

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## ABSTRACT:

The amount of food waste (FW) generated worldwide is expected to exceed 2.2 billion metric tonnes per year, with developing nations seeing the fastest growth in FW creation. The high moisture content (>80%) and high total organic carbon content (40–50%) of food waste make it highly biodegradable. Management of this FW incorrectly can result in groundwater contamination by leachate, reproduction of pathogenic organisms, greenhouse gas (GHG) emissions, and landfill life-shortening. For this, the anaerobic digestion of FW treats it and provides energy from methane. Anaerobic digestion (AD) of FW follows a complex process that involves a four-stage sequential bioconversion of organic matter into biogas, catalyzed by a group of microorganisms at every stage. Due to the complexity of FW arising from the presence of carbohydrates, proteins and lipids, there is a need for microbial consortia that degrade FW completely, having the capability of solubilisation all three polymers like carbohydrates and protein lipids. For this, three different mixed consortiums were considered: cow dung (R1), sewage sludge (R2), and a mixture of cow dung and sewage sludge (R3). It was observed that the mixed consortia (R3) produced maximum biogas (310 mL) along with remarkable volatile fatty acids (VFA, 2445 mg/L) due to a higher soluble chemical oxygen demand (sCOD) R3 (62%), R2 (61%), and R1 (54%), as well as efficient removal of sCOD in R3 (66%), R1 (34%). Metagenomics analysis of R3 showed better microbial diversity than individual ones (R1 and R2), and the experimental results were corroborated with the potential metabolic mechanisms involved in the AD of the FW process. A study of the performance of developed consortia for stable AD operation optimization was done using The stable operation of AD with FW requires optimization using two widely used optimization methods: Response Surface Methodology with Box-Behnken Design (RSM-BBD) and Taguchi orthogonal array L9. The optimized condition shows improvement in biogas production: 906±20 mL, and VSr (volatile solid removal) was 44±1%

**KEYWORDS:** bioenergy; hydrolysis; methane; renewable energy; solid waste management; valorization

# Obesity associated differential molecular alteration in Breast Carcinoma

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## ABSTRACT:

Obesity is a significant risk factor for various cancers, including breast carcinoma, profoundly influencing its molecular landscape. This research is planned to explore the obesity-associated differential molecular alterations in breast cancer, aiming to uncover the specific signaling pathway alteration linked to obesity. By examining these alterations, the study seeks to enhance the understanding of how obesity accelerates the breast cancer progression and affects treatment outcomes.

In the present study, we leveraged transcriptomics data obtained from The Cancer Genome Atlas (TCGA) database and conducted comprehensive analyses using the TCGA R package. This allowed us to identify gene expression patterns and molecular alterations associated with obesity in breast carcinoma. Additionally, we carried out RNA profiling utilizing microarray technology to obtain high-resolution data on gene expression. To further understand the metabolic changes, we performed detailed metabolic profiling on breast cancer cell lines MCF-7 and MDA-MB-231, which were cultured in adipocyte-conditioned media.

We found that the presence of adipocyte-conditioned media significantly increased breast cancer cell proliferation and migration. Our analysis revealed that fatty acid and glucose metabolic pathways were notably altered due to adipocyte secretions. Interestingly, different metabolic pathways were affected in triple-negative (TNBC) and estrogen receptor-positive (ER-positive) breast cancer cells.

This suggests that obesity-related factors distinctly influence the metabolic landscape of various breast cancer subtypes, potentially contributing to their differential progression and treatment responses. The findings could pave the way for more tailored therapeutic strategies, ultimately improving prognosis and patient care for obese individuals diagnosed with breast carcinoma.

**KEYWORDS:** adipocyte-conditioned media, triple-negative breast cancer, Obesity

## ***An invitro and insilico screening***

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Acanthaceae is the least exploited family comprising a large number of medicinal plants and are the major sources of Chinese medicines. A compound named 1-[(3,3-dimethyl-4H-isoquinolin-1-yl)methyl]-3,3-dimethyl-4H-isoquinoline(DI) is a quinolone derivative from *A.gangetica* was collected after ethyl acetate fractionation with silica gel column (60-120,200-400,400-700) and TLC. Phytoconstituents were identified by LC-MS analysis and they were screened for their antioxidant properties by ABTS scavenging assay. The *in-silico* studies evidenced that the major phytoconstituents of the plants are the reason behind their antioxidant properties so that we could exploit plant species much more to reveal their drug candidature.

**KEYWORDS:** Acanthaceae, TLC, LC-MS, ABTS, *INSILICO*

# Computational Mass Spectrometry-based data analysis with the metabolomics approach for the Non-Invasive detection of COVID-19

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Abstract:

Background: The identification of volatile organic compounds (VOCs) emitted from human skin has gained interest for non-invasive medical diagnostics. The VOCs, low-molecular-weight chemicals, reflect physiological and pathological states. The skin emits a series of various compounds, indicating health status. The COVID-19 pandemic highlights the need for rapid, reliable diagnostic tools. Current methods like RT-PCR and antigen tests, while effective, require specialized equipment and lengthy sample preparation.

Objective/Aims: The study aimed to develop an alternative non-invasive diagnosis method for distinguishing COVID-19 disease from healthy control subjects by monitoring the skin-emitted metabolic profile using a mass spectrometer-compatible, with highly sensitive Thin-Film Solid Phase Microextraction (TF-SPME) patch.

**Methods:** We monitored the skin-emitted metabolic profile using TF-SPME patches coated with Divinylbenzene/Polydimethylsiloxane (DVB/PDMS). The patches were wrapped on human skin for 30 minutes to capture skin-emitted metabolites. To avoid saturation of the patch due to sebum from the skin, we customized a pocket-shaped porous scaffold to hold the membrane inside before placing the patches on the forearm of the subjects. After sampling, the patches were desorbed in a Gas Chromatography-Mass Spectrometer (GC-MS) for profiling of skin-emitted metabolites. GC-MS data was analyzed using Agilent Mass Hunter software and to visualise and identify the pattern in the obtained data we are using machine learning technique.

**Results:** Our study showed that a few skin-emitted VOCs, including tetradecane, 1-bromoeicosane, 1-nonanal, nonadecane, benzyl alcohol, dodecanal, toluene, were associated with distinguishing between COVID-19 and healthy controls.

**Conclusion:** This study demonstrated the feasibility of the utilization of a disposable, easy-to-handle microsorbent patch integrated with GC-MS for non-invasive distinguishing COVID-19 from healthy control subjects. This method may aid in the development of non-invasive diagnostic technique, contributing to better disease management and control in the future.

**KEYWORDS:** Thin-Film Solid Phase Microextraction, Volatile Organic Compounds, COVID-19, Non-invasive Diagnostics, Mass Spectrometry.

# Isolation and Identification of Antibacterial compounds from *Rheum emodi* extract against ESKAPE pathogens

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## ABSTRACT:

The increasing incidence of drug resistant pathogens raises due to extensive and irregular use of antibiotics and a crucial need to new drugs. Natural products have been recognized and utilized by humans in management of disease, infections and health problems from ancient days. Medicinal plants are prospective source of antimicrobial agents for the treatment of human infectious diseases. This study was conducted to evaluate antibacterial properties and phytochemical constituents from *Rheum emodi* extract. Antibacterial activity of extract was tested against ESKAPE pathogens using zone of inhibition assay (ZOI) and determination of Minimum inhibition concentration (MIC) using broth dilution method. Phytochemical constitution estimated by chemical analysis and number of compounds determined using thin layer chromatography (TLC), purified antibacterial was isolated by column chromatography and confirmed by TLC bioautography. The active fractions were subjected to spectral analysis by LC-MS and NMR. On the basis of molecular weight and molecular formula the compound were identified as emodin of anthraquinone derivatives from the active fraction of *R. emodi* extract. In conclusion, the analyzed compounds revealed *R. emodi* extract is potentially effective and can be used as alternative natural drug to control bacterial infections especially for multi-drug resistance. The result of antibacterial study showed that ethyl acetate extract of *R. emodi* exhibited antibacterial activity and number of compounds in TLC. Although the mechanism of action of these herbal extract in most cases is still needed to be validated scientifically. In conclusion, these findings indicated that *R. emodi* extract may become interesting candidate for treatment of bacterial infections and diseases.

**KEYWORDS:** *Rheum emodi*, phytochemical screening, antibacterial activity, Thin Layer Chromatography (TLC), TLC-bioautography, Liquid Chromatography Mass Spectrometry (LCMS) and Nuclear Magnetic Resonance (NMR).



# Creation of Toxicophore Database of Natural Compounds and their Analysis

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## Abstract:

**Background:** Natural products contain numerous bioactive compounds that exhibit therapeutic potential but can also be toxic. Toxicophores, the structural fragments that cause toxicity, are valuable for toxic risk assessment and management in drug development. However, the present toxicophore databases mainly deal with synthetic derivatives and have insufficient information on natural substances.

**Objective:** This study aims to create a toxicophore database of natural compounds and help determine the toxicity of natural products that can be used in drug development.

**Methods:** A wide range of natural compounds was obtained from databases and literature. The toxicological data were summarized, and approximately 60 toxicophores were identified and analyzed using substructure search analysis. Data mining, cheminformatics, and machine learning were used for data processing, analysis, and toxicophore prediction. The generated information was saved into the PostgreSQL database and combined with the RDKit cheminformatics platform. A web-based user interface was designed and developed using HTML, CSS, JavaScript, and PHP for user interaction with the database.

**Results:** The study used 20,000 natural compounds to identify six toxicophores with different structural features and biological functionalities. Of these, 18,933 compounds were successfully mapped to the database with further chemical information. The most frequently observed toxicophore, aromatic nitro, was identified in 7,161 compounds. The web interface allows data input, compound browsing, substructure search, and data analysis in the form of graphs and statistics.

**Conclusions:** The generated toxicophore database of natural compounds can be considered a valuable tool for assessing potential toxicity in the early stages of drug development and improving the safety of natural product-derived drugs. It enhances computational toxicology because it provides a molecular basis for toxicity in natural products, and it can be combined with current toxicology tools to enhance its predictive accuracy.

**KEYWORDS:** Toxicophores, Natural Products, Database, Computational Toxicology, Drug Discovery.

# Evaluation of *in-vitro* and *in-vivo* Wound Healing Efficacy of Plant Extract Loaded Biopolymer

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Abstract - The creation of wound healing dressings intended to treat various wound types (such as burns and chronic wounds) and the customization of therapies for various stages of the wound healing process are the current developments in wound care research. The creation of cutting-edge nanotherapeutic materials is emphasized in this context as a viable tactic to effectively regulate particular stages of the wound healing process. In this study the *in vitro* and *in vivo* wound healing of the plant extract loaded biopolymer was fabricated using solvent casting technique. Wounds were closed within 7 days. Histopathological studies were carried out for the wound tissue. Th *in-vitro* wound healing was carried out with human fibroblast. *In-vivo* wound healing was done with mice models, which showed complete wound healing within 7 days.

**KEYWORDS-** Wound healing, *In-vitro*, *In-vivo*, histopathology

# **Biomaterialization, Antifungal, Antibacterial and Cytotoxicity Investigation of Larnite/Nano Titania Composite**

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## **Abstract:**

Biomaterials dalliance is an immanent vocation in the modern healthcare sector. Multidisciplinary attribute of biomaterials requires scientists to contrive and concoct the material, engineers to design and fabricate the prosthesis and physicians to swot the response of natural tissues on artificial biomaterials implanted in the body. Globally, it has been appraised that about 60% of artificial bone substitutes are mustered for bioceramics. Thus, much enthrallment has been rapted towards use of different bioceramics for bioactive fixation of artificial implants. Most important acmes in the field of biomedical materials for hard tissue engineering applications are biocompatibility and mechanical stability.

The arch factual of this work was to synthesize and characterize Larnite/nano titania ( $\text{Ca}_3\text{SiO}_4/\text{TiO}_2$ ) through a facile sol-gel assisted combustion route using l-alanine as fuel for the very first time. Various relevant analytical techniques such as powder X-ray diffraction, FT-IR spectroscopy and scanning electron microscopy were employed to study the characteristic behaviour of the newly synthesized ceramic/metal composite. FEI-Tecnai G2 20S-TWIN, 200 kV SAED (selected area electron diffraction) and the nature of the particles were examined using a high-resolution transmission electron microscope. In-vitro biomaterialization of the synthesized bioceramic was examined on the surface of the scaffold for 9 days of immersion in SBF.

Using the well diffusion technique, four samples of larnite- nano titania composites were tested for their antibacterial properties against four infectious microbial species, including *Staphylococcus aureus*, *E. coli*, *Klebsiella pneumonia*, and *Bacillus subtilis*; and against *Candida albicans* for their antifungal properties. The MTT [3-(4, 5-dimethylthiazolyl-2)- 2, 5-diphenyltetrazolium bromide] test was used to investigate the in vitro cytotoxicity of Larnite/nano titania composite.

**KEYWORDS:** Larnite/nano titania composite, l-alanine, biomineralization, cytotoxicity, antibacterial and antifungal

# **Development of a Disposable Paper substrate based Thin Film- Solid Phase Microextraction (TF-SPME) patch for detection of Carbofuran from Fruit matrix**

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## **Abstract:**

Ensuring the safety and quality of food is of paramount importance for safeguarding human health, facilitating trade and enabling effective official control measures. As a result, there is an urgent necessity to develop an effective and reliable detection tool for monitoring pesticide

residues in fruits and vegetables. The current study utilises the application of a disposable paper based Thin Film- Solid Phase Microextraction (SPME) patch for extracting carbofuran from mango matrix. The use of nanomaterial coated paper patch has significantly identified and quantified the carbofuran residue present in the fruit matrices at trace level.

The coating for the disposable paper based Thin Film- Solid Phase Microextraction (SPME) patch was prepared using the mixture of DVB (divinylbenzene), PDMS (polydimethylsiloxane) and MWCNT (multi-walled Carbon nanotubes) along with hexane as they can significantly impact the surface area of the material. The mixture was uniformly spread to the paper surface for extracting carbofuran efficiently and effectively. Besides its cost-effective nature, this paper membrane can be conveniently disposed due to its eco- friendliness and further helps in preventing the risk of contamination among the samples. To verify the efficiency of our patch, we spiked a frequently used pesticide i.e, carbofuran in mango matrix at different concentrations. The obtained result was satisfactory as due to the use of nanocomposite (DVB/PDMS/MWCNT) mixture. Furthermore, the developed paper membrane has eliminated the lengthy time required for extraction procedure, making it easier and sustainable replacement for the regulatory agencies and agricultural industries.

The findings signify the implications of the patch as a promising tool for the easy, sensitive and highly efficient quantification of multi-pesticide residues from different food matrices at trace level making it an efficient tool for ensuring food safety and meeting regulatory compliance in agricultural products.

# **In silico analysis of telomerase inhibiting phytochemicals isolated from *Blumea eriantha* for cancer treatment**

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**Abstract –** One potential treatment target for cancer cells is telomerase, an essential enzyme involved in the longevity of cancer cells. Current cancer treatments targeting telomerase often involve synthetic drugs with significant side effects, necessitating alternative approaches such as plant-based therapeutics. This study investigates the anti-telomerase activity of several phytochemicals derived from *Blumea eriantha* for use in cancer treatment. We examined the binding relationships between telomerase and several phytochemicals by performing molecular docking using CB-Dock2 and Achilles Blind Docking. Among the phytochemicals screened, Tyrphostin AG494 was shown to have the highest binding affinity, making it the most optimum alternative. These results were supported by a comprehensive pharmacokinetic and pharmacodynamic analysis done using SwissADME and pkCSM, which showed the drug-like qualities of these phytochemicals.

The study further went on to identify synergistic treatment combinations using the Handy Recommendation Algorithm for Cancer Synergy (HRACS), where certain pairs of phytochemicals demonstrated enhanced anticancer efficacy against the A549 cancer cell line, suggesting that combinatorial therapy techniques may have potential. These results warrant for further wet lab experimentation which include MTT, wound scratch and colony formation assays to validate these compounds' full therapeutic potential.

**KEYWORDS**— Molecular docking, phytochemicals, pharmacokinetics, telomerase



# Microextraction Patch for Non-Invasive Detection of Lung Cancer

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## Abstract:

**Background:** Lung cancer remains a leading cause of cancer-related deaths worldwide, often diagnosed at advanced stages, significantly reducing survival rates. Early detection is important but challenging due to the non-specific nature of initial symptoms. Therefore, there is a precise need for the development of a potential technique for fast diagnosis of lung cancer, as early detection can dramatically improve survival rates of patients.

**Objective/Aims:** This study aimed to develop a non-invasive technique through human skin- emitted scent profile analysis for discriminating between lung cancer and healthy control subjects.

**Methods:** We utilized a mass-spectrometer compatible with highly sensitive thin film solid phase microextraction (TF-SPME) to capture and analyze skin-emitted metabolites. A Divinylbenzene/polydimethylsiloxane (DVB/PDMS) patch was placed on the skin surface of lung cancer patients and healthy control subjects for 30 minutes. A specially designed pocket- shaped porous envelope was utilized to hold the membrane to prevent the patch from fast saturation due to oil secretion from the skin of the patients. Following skin sampling, the patches were desorbed into a gas chromatograph-mass spectrometer (GC-MS), and the data were analyzed using Agilent Mass Hunter software to identify the compounds from the chromatogram.

Results: We identified a few skin-emitted metabolites for distinguishing lung cancer and healthy control subjects. These compounds included Benzoic Acid, Phenol, Benzene, 1- Octanol, 1-Nonanol, 2-Dodecenal, Tridecane, Tetracontane, and Dodecyl Acrylate. The study also demonstrated that 30 min skin sampling by solid phase microextraction patch was sufficient for distinguishing the lung cancer subjects.

Conclusion: This study demonstrates the potential of using skin volatile analysis to distinguish between lung cancer patients and healthy subjects. The identified volatile compounds may serve as biomarkers for non-invasive lung cancer diagnosis, paving the way for novel screening methods that could improve early detection and patient outcomes in lung cancer management.

**KEYWORDS:** Lung cancer, Thin-Film Solid Phase Microextraction (TF-SPME), Gas Chromatograph-Mass Spectrometer (GC-MS), Volatile Organic Compounds (VOCs)

# Development of Paper-based Microextraction Patch for the Non-Invasive Detection of Ketone Body for Diabetes Ketoacidosis

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## Abstract:

**Background:** Diabetes ketoacidosis (DKA) is a life-threatening condition that produces high levels of ketone bodies (3- $\beta$ -hydroxybutyrate, acetoacetate and acetone) and is mainly associated with type 1 diabetes. Increased amounts of ketone bodies in the blood and urine reduce the pH, which leads to DKA and, disturbs normal metabolic functions of the body and causes serious complications. As most of the symptoms are primarily unnoticeable, the need for a rapid, practical and non-invasive diagnostic approach is essential for continuous monitoring, better management, and avoiding medical emergencies.

**Objective/Aims:** To develop a paper-based patch operating on the thin film solid-phase microextraction (TF-SPME) principle and coupled it with gas chromatography-mass spectrometry (GC-MS) for rapid quantification of ketone body (3- $\beta$ -hydroxybutyrate) from the urine.

**Methods:** To fabricate paper-based TF-SPME patches, regular A4-sized papers were coated with nanocomposite blended polymer solution, including multiwalled carbon nanotubes (MWCNT), polydimethylsiloxane (PDMS) and divinyl benzene (DVB) with the help of an automatic film applicator to get a uniform coating, and finally, the coated sheet was trimmed into multiple 4 cm length patches. We performed a direct immersion technique from phosphate buffer saline (PBS) matrix for the quantification of 3- $\beta$ -hydroxybutyrate (BHB). To check the efficiency of CNT for the fabrication of TF-SPME, we performed the calibration curve with and without CNT at 500ng/ml-20000ng/ml BHB solution.

Results: Our study showed that DVB/PDMS extracted more ketone bodies than the DVB/PDMS/CNT coated patch. We also derived the fittings equation the linearity around  $R^2 = 0.99$  for quantification of BHB from PBS matrix.

Conclusion: Utilization of these cost-effective paper-based disposal patches can help in the rapid detection and determination of ketone bodies and can facilitate the early diagnosis of DKA.

Keywords: Diabetes Ketoacidosis, Solid-phase microextraction, Ketone bodies, Non-invasive diagnosis

# Planar Chiral [2.2]Paracyclophanes: Pioneering Green Catalysis

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## ABSTRACT:

Catalysts are integral to green chemistry, enabling more sustainable chemical processes by enhancing efficiency, selectivity, and the use of renewable resources. Green chemistry aims to reduce both the environmental impact and the potential negative health effects of chemicals and chemical synthesis. Out of the twelve principles that govern green chemistry, the use of catalysts can enable reactions with higher atom economies. Catalysts can be easily recycled over many times and are not used up by chemical processes making no contribution to can allow for the utilization of reactions which would not proceed under normal conditions, but which also produce less waste. My research is based on developing new green chemistry to make planar chiral compounds based on [2.2]paracyclophane that can be employed as enantiopure representative catalysts to facilitate the selective transformation of prochiral or racemic substrates into enantiopure products and the insights gained will permit the rational design of asymmetric processes.



Herein, we report a one-pot strategy that provides easy access to [2.2]paracyclophane-oxazolines that have great potential as planar chiral ligands in catalysis. Further, these oxazolines could be readily hydrolyzed to furnish enantiomerically enriched carboxylic acids that could have wider use in catalysts, bioactive compounds, and materials.

KEYWORDS: Green Chemistry, Asymmetric Synthesis, Catalysis, [2.2]Paracyclophanes

# IDENTIFICATION OF KRASG12D INHIBITORS AGAINST PANCREATIC CANCER USING COMPUTATIONAL TOOLS

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Abstract:

In this study, we report KRAS G12D inhibitors against pancreatic cancer using computational tools. Pancreatic cancer is the seventh most common cancer globally. Surgery, radiation therapy, targeted therapy, and chemotherapy are the current treatment methods for pancreatic cancer. However, the current treatment methods show some adverse side effects like fatigue, vomiting, loss of appetite, and blood clotting. Also, the overall survival rate is 6%. A new target identified for Pancreatic Cancer is KRAS G12D. Therefore, in our attempt, we have screened the NCI (National Cancer Institute) natural library with around 230 compounds. The compounds were prepared using the lig-prep tool of Maestro 11.8 Schrodinger software at pH 7.4. KRAS G12D protein with PDB ID 7RPZ was retrieved from the protein data bank and was minimized with the protein preparation wizard at 7.4 pH. Prepared protein and ligands were docked using the ligand docking tool with the HTVS, SP, and XP features. The selected potent compounds from the docking were further subjected to Molecular Dynamic Simulations for 200ns. Two potent compounds Curcumin and Plathymenin showed good docking scores of -9.395 and -9.097 respectively with KRASG12D retaining all the crucial interactions with amino acids when compared with the standard drug, MRTX1133. As these two naturally available compounds showed good docking scores indicating inhibition for the KRASG12D target, they can be considered further for carrying out the in-vitro activity against pancreatic cancer cell lines.

Keywords: KRAS, Pancreatic cancer, Curcumin, Plathymenin.

# Combined effect of pretreatment on improving liquefaction of sago waste for biofuel generation

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**ABSTRACT:** For centuries, people have considered sago as a major staple food in the world. As a result, the sago processing sector promotes economic expansion. Nonetheless, this study addresses the environmental issue of this industry's waste disposal. The global energy crisis is growing nowadays due to the rapid depletion of fossil fuels. This energy crisis can be reduced by introducing the bioenergy production concept, where the waste such as from sago industry can be used as a feedstock. A solid sago waste is a starchy-rich substrate that is underutilized but has more potential towards bioenergy production. The goal of the current study was to improve the hydrolytic efficiency of sago waste biomass during anaerobic digestion by implementing a combination of microwave and bacterial pretreatment methods. At a microwave power of 720 watts and an 11 min of time duration, the liquefaction reaches 11%. Adding bacterial pretreatment enhances the liquefaction from 11.6 to 31.6 %. In comparison to the control sample (44 mL/gCOD) and microwave (106 mL/gCOD) sample, the combined pretreatment of sago biomass results in biomethane generation of 223 mL/gCOD. Thus, this study proves that the pretreatment of biomass results in improved hydrolysis and biomethane generation.

**KEYWORDS:** liquefaction; sago waste; pretreatment; energy; microwave

# **Profiling the host cytokine markers in patients with melioidosis and tuberculosis in South west coastal regions in India**

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Background: Melioidosis is an emerging infectious disease posing a significant threat to public-health globally, with rising incidence observed in southern India. The mortality varied across the endemic regions, ranging from 19% to 54% of the reported cases. Cytokines are crucial mediators in regulation of immune as well as inflammatory responses through complex cellular interactions and communications. Quantifying cytokines provides valuable insights into disease pathophysiology and contributes to the development of upcoming diagnostic methods, therapeutic strategies and monitoring of patients. Therefore, current study investigated the modulations in the cytokine secretion among Melioidosis cases comparing to pulmonary tuberculosis cases and healthy individuals.

Methods: Multiple cohorts of individuals were recruited from tertiary care hospital, Kasturba Medical College, Manipal between 2021 and 2024.



A total of 64 subjects were enrolled into three cohorts including melioidosis patients (n= 16), pulmonary tuberculosis (PTB) (n= 16) and healthy controls (n= 32). Samples were analysed using Luminex platform to quantify levels of 10 analytes involving inflammatory cytokines (IFN $\gamma$ , TNF and NGF $\beta$ , IL-6), Gal-3, growth and cellular cytokines (IL2, IL7), chemokine (IL8), growth factor (HGF), LIF. Results: Among the 10 analytes, Gal-3, HGF, IL-6 and IL-8 levels were notably upregulated in plasma samples of Melioidosis cases. Gal-3, HGF, IL-6 and IL-8 demonstrated strong discriminatory performance in diagnosing Melioidosis with AUC values of 0.9, 0.83, 0.97, and 0.81 respectively. Whereas, IL-6 and IL-8 effectively could discriminate between TB and Melioidosis with AUC values of 0.85 and 0.80 respectively.

Conclusion: The present study showed that plasma levels of Gal-3, HGF, IL-6 and IL-8 were significantly elevated during melioidosis. Our study provides preliminary evidence suggesting that these cytokines could be a potential host biomarker for the differential diagnosis of melioidosis and may pave way to the targeted therapeutic approaches. Further studies with a larger population are required to validate our findings.

Keywords: melioidosis; tuberculosis; cytokines; Galectin-3 (Gal-3); Hepatocyte growth factor (HGF); interleukins; India.

# Development of microsorbent analytical tool for the determination of water pollutants

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**Abstract** – Water pollution is a global issue affecting human health and the ecosystem. Monitoring water pollutants is crucial for maintaining water quality. Traditional techniques like Solid phase extraction (SPE) and liquid-liquid extraction (LLE) use large amounts of harmful solvents. An eco-friendly alternative is Solid phase microextraction (SPME). Our study introduces a novel paper-based thin film microextraction (TFME) technique. This technique uses a coating of Divinyl benzene (DVB), polydimethylsiloxane (PDMS), and Carbon nanotube (CNT) to effectively extract three pesticides (Atrazine, Simazine, and 4-chlorophenol) from water samples at various concentrations.

**Objective** – This research aims to develop and validate a new paper-based TFME patch coated with DVB/PDMS/CNT, for extracting and monitoring various water pollutants.

**Methods**- We developed a novel paper-based TFME patch using a mixture of DVB, PDMS, CNT as a coating material. We spiked different concentrations of the pollutants (Atrazine, Simazine, and 4-chlorophenol) to the water sample and used four replicates for each concentration. The patches were immersed in the water samples for effective extraction. After adsorption, the patches were desorbed using acetonitrile and analyzed using Gas chromatography- Mass spectrometry (GC-MS). The peak areas corresponding to the adsorbed pollutants were measured.

**Results** – the paper-based TFME patches successfully extracted atrazine, simazine, and 4- chlorophenol. GC-MS analysis revealed distinct peaks for each pollutant, with good peak areas, indicating effective adsorption. The DVB/PDMS/CNT coating exhibited high affinity and sensitivity for targeted pollutants.

Conclusion- We have developed an innovative paper-based TFME patch that effectively absorbs a variety of water pollutants. The combination of DVB, PDMS, and CNT as coating materials significantly enhances the ability of the patch to capture both volatile and semi-volatile compounds. This new tool provides an efficient method for detecting and monitoring water pollutants, with promising applications in environmental analysis and water quality management.

Keywords - solid phase microextraction (SPME), Gas chromatography- Mass spectrometry (GC-MS), DVB/PDMS/CNT

# **In Silico Identification of Anticancer peptide against Epithelial Ovarian Cancer**

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**ABSTRACT:** Anticancer peptides (ACPs) are small peptides containing amino acid sequences which are selective and toxic to cancer cells. Epithelial ovarian cancer, which arises from the surface of the ovary (the epithelium), is the most common ovarian cancer. The peptide-based anticancer therapy has gained a tremendous interest in the last decade due to the need of more efficient, easy to produce and anti-chemoresistance therapy solutions. ACPs are collected from databases (CancerPPD, AntiCP etc) as well as bioassay and ligand databases. Various physiochemical features [number of amino acids, theoretical pI (isoelectric point), instability index, aliphatic index, and grand average of hydropathicity (GRAVY)] of peptide were analysed using ExPASy-ProtParam tool. The ACPs, as screened above, will be subjected molecular docking against targeted receptors by using HDOCK Server. This study helps in understanding ACPs and their role as alternative treatment approach as anticancer drug for Epithelial Ovarian Cancer.

**KEYWORDS:** ACPs, GRAVY, Epithelial Ovarian Cancer, Hydropathicity, Molecular Docking, Anticancer Drug

# Leveraging GXP for Target Identification and Virtual Screening for GEM Antagonists in Rheumatoid arthritis

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## Abstract:

Rheumatoid arthritis (RA) is a prevalent autoimmune disorder causing chronic inflammation of joint tissues, if left untreated, will lead to joint deformation and functional limitations, involving vital organs. According to the Global burden report- 2021, the incidence of RA has increased over the past decades and will continue to increase in the coming years, and therefore much more attention should be given to early diagnosis and treatment to reduce the burden of RA. To explore the differentially regulated genes (DEGs) in RA, we analysed the gene expression profile (GXP) of GSE10500 GEO dataset and identified 1163 significant DEGs between control and RA samples. Functional enrichment analysis revealed that these DEGs are mainly involved in peptidyl tyrosine phosphorylation, Ras protein signal transduction, tyrosine kinase activity, and other processes. We constructed a protein-protein interaction (PPI) network for the DEGs using the STRING database, which was visualized and analysed with Cytoscape and its plugins. This analysis identified 15 hub genes, including GAPDH, ACTB, TNF, and JUN. Of the 1163 DEGs, 325 were upregulated and 212 were downregulated. Notably, the GEM protein was the most upregulated gene, with a log fold change of 6.6 and a significance value of  $P=0.0003$ . Considering the GEM's role in immune cell recruitment and trafficking and its elevated expression, we targeted the GEM protein in our study. Docking studies with bridged heterocyclic compounds synthesized through three different schemes showed that most compounds had a strong affinity for GEM. Specifically, compound 1e, 2c, 3 had the best binding scores of -21.18, -16.66, and -14.37 respectively.

These findings suggest that GEM protein could be a promising novel target for RA treatment, though further in-vitro and in-vivo evidences are required. Also, the hub genes and the pathways thus identified may assist further exploration of the molecular basis of RA holistically and may therefore offer therapeutic and diagnostic hints.

Keywords: Rheumatoid arthritis, GEO2R, DEGs, GEM, SeeSAR

# *In Silico* Lipoxygenase inhibitory potential of Compounds from *Aconitum* species

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## Abstract:

Inflammation is a normal body response against infection or injury. But prolonged inflammations are frequently associated with harmful side effects on health. Presently used common drugs for inflammatory conditions are mostly non-steroidal. Considering safety reasons, especially the increased side effects of such non-steroidal drugs, plant-based compounds are more sought-after drugs. Lipoxygenase (LOX) is a key pro-inflammatory enzyme involved in the biosynthesis of leukotrienes, postulated to play an important role in the pathophysiology of inflammation associated diseases. Search for selective LOX inhibitors has led to the finding of several classes of natural products with good inhibitory potential. Such inhibitors of LOX include alkaloids, flavonoids, arachidonic acid analogues, and certain phenolics. *Aconitum* species are rich sources of diterpenoid alkaloids and flavonoids, with important medicinal properties including anticancer, antimicrobial, analgesic and anti-inflammatory activities.

In the present study, compounds reported from species of Genus *Aconitum* were subjected to in silico screening using LOX as the target. Structural information of LOX was retrieved from PDB. Molecular docking studies were performed on 131 compounds to check their LOX inhibition activity using Schrodinger program. Out of 131 compounds, 2 lead compounds were selected based on their glide score and ADMET analysis was performed. Molecular dynamic studies on the lead compounds showed strong inhibitory potential towards LOX. Some other compounds out of the 131 compounds mentioned also showed LOX inhibitory potential. The results of the above analyses are reported.

**Keywords:** Genus *Aconitum*, inflammatory diseases, lipoxygenase, molecular docking.

# Morpho-physiological and Biochemical Responses of *Stevia rebaudiana* to Drought Stress

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**Abstract:** *Stevia rebaudiana*, a natural sweetener, is an important source of sweetening compounds, Stevioside and rebaudioside A. This plant has become important in recent years due to the rise in diabetes and other health issues worldwide and is now growing globally. Drought stress, a major factor adversely affecting plant growth and yield, necessitates a thorough understanding of plant morpho-physiological and biochemical responses. This study focuses on the impact of drought stress on *Stevia rebaudiana*, analyzing various morpho-physiological parameters such as plant growth, relative water content (RWC) alongside biochemical markers like Malondialdehyde (MDA) content, chlorophyll content and antioxidant enzyme activity. Additionally, histochemical detection of H<sub>2</sub>O<sub>2</sub> (hydrogen peroxide) and O<sub>2</sub><sup>-</sup> (superoxide) provides visual insight into the production and distribution of reactive oxygen species (ROS) under stress conditions. Observations reveal a reduction in leaf disc size alongside a decrease in RWC with increasing polyethylene glycol (PEG) concentrations, indicating drought-induced physiological responses. Biochemical analyses showed increased MDA content, peaking at 5.1 μmoles g<sup>-1</sup> FW under 12% PEG. Furthermore, soluble sugar content increased to 77.2 mg GE g<sup>-1</sup> DW at 11% PEG but sharply declined under 12% PEG treatment. Additionally, an elevation in Superoxide Dismutase (SOD) activity in response to drought stress was observed. These findings underscore *Stevia's* adaptive mechanisms at the physiological and biochemical levels to mitigate drought stress. Future research may explore molecular changes and gene expression profiles associated with drought stress to deepen our understanding and facilitate the development of drought-resistant varieties using genomic and molecular techniques. Such insights are pivotal for advancing sustainable agriculture and ensuring food security amidst changing environmental conditions.

**Keywords:** *Stevia rebaudiana*, Drought stress, Polyethylene glycol (PEG), Biochemical responses, Sustainable agriculture



# Isolation of Isoflavones from *Lepidagathis Keralensis*

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Abstract:

*Lepidagathis keralensis* is a perennial herb endemic to the laterite hillocks of the Western Ghats. Ethnic herbal practices use it as a nutrient supplement because it contains isoflavones, one of the largest groups of polyphenols with bioactive properties. It contains various bioactive compounds with anti-oxidant and antimicrobial activities. In addition, the plant is also supposed to have estrogen receptor modulators (ERMs) that bind to estrogen receptors and mediate various cellular responses. These ERMs can be utilized for the treatment of female-related cancers. This study includes the collection of plant material, isolation and analysis of the bioactive compounds. The plant has been collected from laterite rocks in northern Kerala, cleaned and shade-dried. The dried plant was ground to fine powder. Solvent extraction was carried out using various solvents such as hexane, chloroform, and methanol using a Soxhlet apparatus. The solvents were evaporated using a rotary evaporator. Isolation of isoflavones is done by a specific method. Separated fractions were subjected to GC-MS analysis, and the presence of isoflavones was confirmed. In-silico protein ligand docking studies of identified isoflavone was done on estrogen receptor alpha using maestro Schrodinger software.

# Studying Microbiome of Collagen Induced Arthritis in Resistant mice C57BL/6

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Abstract:

Rheumatoid arthritis (RA) is a chronic autoimmune disease that causes inflammation in the joints and surrounding tissues, leading to pain and swelling. RA is associated with the production of inflammatory cytokines such as TNF- $\alpha$  and IL-1 $\beta$  play a major role in the inflammatory process, and contribute to joint destruction. The human gut microbiota, a complex ecology of microbes that live in the digestive tract plays a vital role in human health and well-being. The objective of this study was to identify the microbiome of resistant mice (C57BL/6) injected with collagen type II obtained from the bovine nasal septum to induce arthritis. Stool samples were collected from the control group and diseased group mice and analysed by 16S rRNA sequencing to study the microbiome on all levels. Taxonomically, 11, 16, 22, 33, 63, and 10 different bacteria were identified at levels of phylum, class, order, family, genera, and species, respectively, with no significant difference between the control and diseased groups ( $P < 0.05$ ). Pathways such as TLR2 and CD4 $^+$  T cells were studied by flow cytometry and showed a mild increase in the disease group up to (58.7%) and (56%), respectively. Pathways such as NF- $\kappa$ B and Pro and anti-inflammatory markers such as IL-1 $\beta$ , TNF- $\alpha$ , and IL-10 were studied by ELISA, and the results showed a mild increase in the disease group but no statistical difference compared with the control group ( $p < 0.05$ ). An X-ray was conducted for the affected joints. Our results suggest that collagen type II from the bovine nasal septum, under the conditions tested, does not significantly affect the primary disease markers in C57BL/6 mice, which are resistant to rheumatoid arthritis.

Keywords: Rheumatoid Arthritis, Collagen Type II, Microbiome

# Evaluation of antihypertensive activity of *Padina boergesenii* extract

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## ABSTRACT:

Natural products have historically been the foundation of pharmaceuticals. They provide us lead for new drug development because to their unique attributes as a source for therapeutic phytochemicals. Hypertension is a potentially dangerous condition that requires attention and action in order to prevent its serious health consequences. The hunt for bioactive molecules as a novel medicine, has focused on marine resources like seaweeds. Seaweeds are a valuable source of bioactive compounds, and this study aims to identify the phytoconstituents present in brown seaweed-*Padina boergesenii*. Five different solvents were used to prepare extracts and their antihypertensive activity was evaluated. Among them, 70% ethanolic extract exhibited significant and concentration dependent Angiotensin Converting Enzyme (ACE) inhibition activity. Phytoconstituents were identified using LC-MS/MS, and subjected to molecular interaction against ACE enzyme. Identified bioactive compounds with known mode of actions have been considered in molecular docking study. Findings of this study will continue to be a cornerstone of antihypertensive drug discovery from *Padina boergesenii*.

**KEYWORDS:** Seaweed, ACE inhibition, LC-MS/MS, Molecular Docking

# Determination of GC/MS-based characterisation, the antimicrobial effect and anticancer activity of *Saussurea lappa* extracts by Mitochondrial Cytochrome C Release on HepG2 and K-562 cell lines.

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## ABSTRACT:

Background with objectives:

According to the World Health Organization (WHO), the number of cancer deaths is projected to reach more than 11 million annually by 2030. Also, the development of new antimicrobial agents is declining for present antibiotic-resistant microbes. Several plant screenings have been performed as potential antimicrobial and anticancer drug candidates; *Saussurea lappa* (*S. lappa*) is an example. Therefore, this study was done a) to determine GC/MS analysis of *S. lappa* root using different solvents and b) To evaluate the antimicrobial effect and anticancer activity of extracts against the K-562 and HepG2 cell lines.

Methods:

*S. lappa* roots were powdered and then extracted successively using soxhlet apparatus with chloroform, ethyl acetate, and n-butanol at 40°C and water using a hot extraction method at 80°C for six hr, followed by GC/MS analysis. The antimicrobial and anticancer activity of the best appropriate extract using the agar well diffusion method and MTT assay against the K-562 and HepG2 cell line, respectively.

#### Results:

GC/MS analysis of chloroform, n-butanol, and ethyl acetate solvent extracts recorded 54 compounds like dehydrocostus lactone, costunolide, etc. The ethyl acetate extract exhibited moderate antimicrobial activity against pathogens such as *Staphylococcus aureus*, *Pseudomonas aeruginosa*, *Shigella flexeneri* and *Klebsiella pneumoniae*. The cell cytotoxicity study showed significant cytotoxic potential properties against K-562 and HepG2 cells, as confirmed with dual staining of acridine orange (AO)-ethidium bromide (EB) under a fluorescent microscope. Apoptosis, as the mode of cell death, was also confirmed by the higher release of cytochrome C from mitochondria, increased caspase-3 and bax, and down-regulation of Bcl-2.

#### Conclusion:

These findings suggest *S. lappa* root extract depicts a potential antimicrobial effect and has anti-oncogenic properties against the CML and HCC for further research.

Keywords: *Saussurea lappa*; anticancer; apoptosis; cytochrome C release; Bcl-2

# Paper-based solid phase microextraction patch for characterization of bacterial pneumonia

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## ABSTRACT:

**Background:** Pneumonia caused by bacterial pathogens and antibiotic resistance is a major cause of morbidity and death in India, particularly in immunocompromised patients. There is a precise need for rapid characterization of bacterial pathogens.

**Objective/Aims:** The study aimed to develop polymer-coated paper-based thin film microextraction patches and couple it to gas chromatography-mass spectrometer (GC-MS) for identification of pneumonia-causing *Staphylococcus aureus* bacterial species.

**Methods:** We fabricated paper-based microextraction patches by coating them with materials including divinylbenzene, carbon nanotube, and polydimethylsiloxane. The coating was performed by commercial film applicator technique. We exposed the patches to the culture medium of bacterial species through headspace and direct immersion methods. The pathogen-emitted metabolites were captured by the patches and desorbed in GC-MS. We used the NIST library for the identification of the compounds.

**Results:** Our study showed that the *Staphylococcus aureus* bacterial pathogen produced Cyclopropane, Hexadecenal oxime, Proline 1-isopropyl ester, Butyric acid 2-phenyl- 2-ethylhexyl ester, Heptadecane and Benzamide 3-bromo-Nbenzyl-N-tetradecyl metabolites during direct immersion of patches in culture media, whereas the headspace immersion yielded Glutaric acid, Acetamide, Dichloroacetic acid, 2-methyloct-5-yn-4-yl ester, Benzoic acid, Benzoic acid, 4-(3-oxo-3-phenyl-1-propenyl)- metabolites.

Conclusion: Our study demonstrated that the disposable, cost-effective paper-based microextraction patches integrated with GC-MS may be a viable tool for monitoring the *Staphylococcus aureus* pathogen. This study may be helpful for the future diagnosis of *Staphylococcus aureus* infection without the need for traditional culture tests. It may be helpful for clinical diagnosis of respiratory infection.

KEYWORDS: Solid Phase Microextraction, Sample preparation, Infectious diseases

# The Molecular Mechanism of Dicofol as an Endocrine Disruptor by Interacting With Estrogen Receptor: Insights From Molecular Docking, and MM GBSA Studies.

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Abstract: The organochlorine pesticide dicofol (DCF), a persistent organic pollutant, is used as acaricide worldwide. Considering its large consumption in the agriculture sector and potential toxic effects such as endocrine disruption and environmental persistence are detrimental to human health. To take an extensive evaluation of its potential toxicity, the current study was aimed to explore the binding mechanism of DCF on human Estrogen Receptor (ER). ER is a member of the steroid hormone receptor family, plays an important role in the physiology and pathology of diverse tissues. The estrogenic activity of a vast number of chemicals has been studied for their potential adverse effects on the hormone regulation of the endocrine system. Herein, Docking studies and Molecular Mechanics Generalized Born and surface area continuum solvation (MM GBSA) method were performed to explore the detailed interaction mechanism between DCF with the ER. The Docking, and calculated binding free energies indicate that dicofol could efficiently bind to the ER. The present work provided the structural evidence to recognize dicofol as an endocrine disruptor and would be important guidance for seeking safer substitutions of dicofol.

Keywords: Dicofol, Estrogen receptor, Molecular docking, MM GBSA



# NEUROPROTECTIVE POTENTIAL OF CITRUS MAXIMA BURM. F MERR FRUIT PEEL EXTRACT AGAINST BILATERAL CAROTID ARTERY OCCLUSION-REPERFUSION INDUCED CEREBRAL ISCHEMIA MODEL IN RATS

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Abstract:

**Introduction:** A stroke occurs when blood supply is compromised to the brain which damages the brain tissue and eventually leads to neuronal death/neurodegeneration. Bilateral carotid artery occlusion model is well documented to induce cerebral ischemia in Wistar rats. And *Citrus maxima* Burm. F Merr belongs to the family Rutaceae, its peels are rich in bioflavonoids which has been bestowed with anti-oxidant, anti-inflammatory potential to treat an array of medical conditions.

**Aim:** To investigate the neuroprotective potential of *Citrus maxima* Burm. F Merr fruit peel extract (PRECM) against bilateral carotid artery occlusion induced cerebral ischemia in Wistar rats.

**Methods:** The study comprises five groups (n=6) of six rats. Group I served as Sham control received normal saline (10 ml/kg), group II as disease control, group III and IV received PRECM (100 mg/kg and 200 mg/kg p.o. respectively), group V served as standard control received Vitamin-E (10 mg/kg p.o.). Animals were pre-treated for 10 days, except group I remaining groups were subjected to ischemia for 30min and 24hr reperfusion whereas for group I small incision was made and sutured back on the 10th day of study duration. On 11th day rats were assessed for behavioral alterations and later animals were euthanized for assessing the biochemical, enzymatic levels in brain homogenate, TTC staining to examine infarct size and histopathological alterations.

Results: The results revealed the protective effect of PRECM by attenuating the BCAAO-I/R induced behavioral alterations, oxidative stress markers such as GSH, LPO, SOD, CAT in addition infarct area and histopathological changes when compared to the inducer control group.

Conclusion: Our investigation revealed the neuroprotective potential of PRECM against Bilateral Carotid artery occlusion induced cerebral ischemia which could be owing to its potential anti-oxidant and anti-inflammatory activity.

Keywords: Neuroprotective, BCAAO-reperfusion, Vitamin E, Ischemia, Stroke.

# DEVELOPMENT AND EVALUATION OF GUAIPHENESIN DRUG LOADED SOLID LIPID NANOPARTICLES

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## Abstract:

**Introduction:** Recently, solid lipid nanoparticles (SLNs) have garnered significant attention from researchers due to their biodegradability, biocompatibility, and versatile drug delivery capabilities. This study focused on developing and evaluating Guaifenesin-loaded SLNs. The nanoparticles were created using the hot homogenization technique with Tristearin as the lipid, soy lecithin as a stabilizer, and Tween 80 as a surfactant.

**Aim:** To develop and evaluate guaiphenesin loaded solid lipid nanoparticles.

**Methods:** The solid lipid nano-particles of guaiphenesin were prepared by hot homogenization method and they were evaluated for its particle size & PDI, zeta potential, entrapment efficiency, SEM and *in vitro* drug diffusion studies.

**Results:** The particle size of the guaiphenesin solid lipid nanoparticles ranged from 61.97 to 160 nm. All formulations had a good PDI, falling between 0.119 and 0.411. The zeta potential varied from -6.26 to -20.1 mV, and the entrapment efficiency ranged from 78 to 96.30%. The cumulative release of guaifenesin SLN obtained from the 2<sup>3</sup> full-factorial design which was optimized reached 95.65% at the 12th hour. Release kinetic studies indicated that the release followed the Higuchi model, and the n values from the Korsmeyer-Peppas model suggested a non-Fickian release mechanism, with an n-value of 0.6325.

**Discussion:** Solid lipid nanoparticles (SLNs) were developed, achieving optimal particle size and entrapment efficiency, and sustained drug release for 12 hours using high-shear hot homogenization and ultrasonication, the optimized lipid and surfactant amounts, minimizing raw materials and time was found to be successful. SLNs provide controlled drug release and enhance bioavailability, making them effective drug carriers.

**Keywords:** Guaiphenesin, solid lipid Nano-particles, FTIR, *in vitro* drug release.

# Optimizing Parkinson's disease treatment: A novel intranasal co-delivery system for levodopa and amantadine

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## Abstract:

**Introduction:** Parkinson's Disease (PD) is a progressive neurodegenerative disorder with motor and non-motor symptoms. Amantadine, an antiviral with dopaminergic and neuroprotective properties, and Levodopa used to replenish brain dopamine, are effective but limited by oral bioavailability and side effects. This study explores using polymeric nanoparticles for intranasal co-delivery of amantadine and levodopa to enhance therapeutic efficacy and neuroprotective effects in PD.

**Methodology:** Polymeric nanoparticles were synthesized and characterized for size, morphology, and drug encapsulation efficiency using SEM. In vitro studies evaluated the release kinetics of amantadine and levodopa. The brain-targeting efficiency, biodistribution, and therapeutic efficacy of intranasally administered nanoparticles will be assessed in a PD mouse model. Behavioral tests (Rotarod and open field) evaluated motor function, while biochemical assays will measure oxidative stress markers and neuroinflammatory cytokines in brain tissues.

**Result:** The synthesized polymeric nanoparticles containing levodopa had a mean diameter ranging from 201-217 nm, a negative zeta potential of -6.09 mV, and an encapsulation efficiency of 60.2%. In vitro studies indicated a sustained release of levodopa, achieving 96.01% over 12 hours. Similarly, polymeric nanoparticles of amantadine exhibited a mean diameter between 171-180 nm, a negative zeta potential of -28 mV, and a high encapsulation efficiency of 95%. In vitro studies showed that amantadine was released in a sustained manner, reaching 88% over 12 hours.

Conclusion- Intranasal delivery of levodopa and amantadine via polymeric nanoparticles significantly enhances brain targeting and therapeutic efficacy, showing potential neuroprotective effects in Parkinson's Disease. We propose that the co-delivery of these two drugs will offer superior therapeutic outcomes compared to their individual administration. This novel delivery system could represent a promising strategy for improving PD management and slowing its progression.

Keywords: Parkinson's disease, Amantadine, Neuroprotection, Polymeric nanoparticles, Intranasal delivery.

# Nanoguardians Against Leishmaniasis: Formulation and Evaluation of Optimized Polymeric Nanoparticles in Biocompatible Hydrogel

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## ABSTRACT:

### Background:

Leishmaniasis, a neglected tropical disease caused by the protozoan parasite *Leishmania*, is a massive global health concern. Traditional treatments include disadvantages such as medication resistance and toxicity. The potential of polymeric nanoparticles (PNPs) as a viable approach to resolving these issues and enhancing leishmaniasis treatment outcomes is examined in this research. The research focuses on the potency of PVA and PLGA-based PNPs when employed singly and in combination to provide an optimal formulation against leishmaniasis.

The research aims to design and develop an Amphotericin B loaded optimized PNPs using PLGA and PVA loaded in Hydrogel for a sustained release effect.

### Methods:

The PNPs were prepared using nanoprecipitation technique. The formed nanoparticles were characterized by its size, shape, surface charge, drug content and the compatibility studies between drug and polymers were conducted through FTIR and NMR. The hydrogels were made by swelling Carbopol in water for 24 hours and then dispersed in the prepared PNPs suspension with a constant stirring. The thickening of gel is achieved by optimizing the pH. The prepared hydrogel were evaluated for its thickening property, spreadability, skin permeation and drug release studies.

### Results:

The fabricated AmB PNPs were spherical in shape, with an optimized particle size, PDI and zeta potential. The hydrogel loaded with AmB PNPs was homogeneous and compatible with the skin. The hydrogel had optimum viscosity and spreadability. The encapsulation efficiency was  $97.25 \pm 0.02\%$ . Furthermore, about 89% of AmB was released within 24 hours, while in the ex vivo permeation study, 69.19% of AmB passed through the skin after 24 hours.

Conclusions:

Hydrogels loaded with AmB PNPs provide a hopeful step in the search for more efficient, safer, and more affordable therapies. The study shows that AmB was successfully formulated into sustained-release PNPs and has significant drug release for up to 24 hours, showing good efficacy in accelerating the treatment against leishmaniasis.

Keywords: Leishmaniasis; Amphotericin B; Polymeric Nanoparticles; Nano Drug Delivery System; Drug Release.

# Pharmacokinetic and Network Pharmacological Studies of Cucurbitacin Analogues in Association with CVDs

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## ABSTRACT:

Cardiovascular diseases (CVDs) are the leading cause of mortality globally. According to WHO, every year 17.9 million deaths are estimated due to CVDs. Cucurbitacin, a phytochemical present in the Cucurbitaceae plant family is reported to control CVDs. Cucurbitacin analogues includes CuA, CuB, CuC, CuD, CuE, CuF, CuH, CuI, CuJ, CuL, CuO, CuP, CuQ, CuR and CuS. The aim of the present study was to hypothesize the mode of drug action of various analogues of cucurbitacin through computational docking studies, for which the target proteins ACE (Angiotensin Converting Enzyme) and REN (Renin enzyme) that play a significant role in CVD progression were considered for the study, their crystallographic structures were collected from PDB database with the PDB-ID 1UZF and 2VOZ respectively. The domain analysis and secondary structure analysis of the target proteins were carried out. Further, the *in-silico* pharmacokinetics analysis of the cucurbitacin analogues was carried out using SwissADME, ADMETSAR and PreADMET, which indicated that all the molecules possessed drug likeness. Computational docking studies using Autodock 4 showed that all the analogues of cucurbitacin exhibited potential interaction with the target proteins. Among all the analogues, CuE showed higher affinity towards ACE with binding energy (-11.36 kJ/mol) and CuS towards REN with binding energy (-11.54 kJ/mol). Furthermore, 15 analogues of cucurbitacin were analysed for network pharmacology, which revealed that 06 genes viz., ITGAL, HIF1A, PAX8, STAT3, EcR and USP were identified as key genes in the network. Among these genes, ITGAL gene is highly interacting gene in the network of all the 15 analogues.



Additionally, ITGAL is involved in 3 pathways viz. integrin signalling pathway, blood coagulation and viral myocarditis pathways, whereas HIF1A is involved in angiogenesis pathway. STAT3 is involved in angiogenesis, interleukin signalling pathway, PDGF signalling pathway. EcR involved in vascular smooth muscle contraction, arrhythmogenic right ventricular cardiomyopathy pathways and USP is involved in MAPK signaling pathway. In correlation, ACE and REN proteins used in the study are the potential targets appear to involve in the above mentioned pathways. Importantly these pathways play a crucial role in cardiovascular diseases mainly in the pathogenesis of cardiac hypertrophy and pulmonary hypertension. The results of this investigation revealed that CuE and CuS can be considered as potential molecules for the development of treatment against cardiovascular diseases.

Keywords: Cardiovascular diseases, Pharmacokinetics, Molecular docking, network pharmacology, Angiotensin Converting Enzyme, Renin enzyme

# NOVEL ASENAPINE NANOCRYSTAL-LOADED ORODISPERSIBLE FILMS: A POTENTIAL STRATEGY FOR ENHANCED BIOAVAILABILITY IN SCHIZOPHRENIA TREATMENT

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**Background:** Asenapine, an antipsychotic medication for schizophrenia, suffers from limited oral bioavailability, hindering its therapeutic efficacy. This study investigates a novel drug delivery system – asenapine nanocrystals incorporated into orodispersible films – to improve drug dissolution and potentially enhance bioavailability.

**Methods:** A central composite design was employed to optimize asenapine nanocrystals with a desired particle size using the antisolvent precipitation method. The nanocrystals were subsequently embedded within orodispersible films formulated with hydroxypropyl methylcellulose E15 (HPMC E15) and polyethylene glycol 400 (PEG 400) for optimal film properties. Physicochemical characterization like thickness, folding endurance along with in-vitro disintegration and dissolution testing using phosphate buffer of pH 6.8 was conducted.

**Results:** The developed films successfully encapsulated the asenapine nanocrystals, achieving a mean particle size of 175.1 nm and a narrow polydispersity index (PDI) of 0.114, indicative of uniform particle distribution. The films exhibited rapid disintegration in the simulated oral fluid, suggesting rapid drug release upon administration. In-vitro dissolution studies demonstrated sustained release of asenapine over 36 hours, potentially offering a prolonged therapeutic effect.

**Conclusions:** This study reports the successful development of novel asenapine nanocrystal-loaded orodispersible films. These films demonstrate promising potential as a novel drug delivery strategy for enhanced asenapine bioavailability, potentially leading to improved treatment outcomes in schizophrenia patients. Further in-vivo investigations are warranted to confirm these findings and assess the in vivo performance of the formulation.

**Keywords:** Asenapine; nanocrystals; orodispersible films; schizophrenia; bioavailability; drug delivery

# **Estimation of CD34 for prognostication of patients with Oral Squamous Cell Carcinoma**

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## ABSTRACT:

Oral squamous cell carcinoma is the most commonly diagnosed cancer affecting the oral cavity where the overall survival rate of patients is limited to 60 % with a poor prognosis. Angiogenesis is believed to be one of the important key hallmark feature in carcinogenesis. CD34 antibody, a highly sensitive marker for endothelial cell differentiation has been used to study the vascularity in tumors.

AIM : To determine the reliability of the immunohistochemical expression of CD34 for

prognostication of patients with oral squamous cell carcinoma.

## OBJECTIVES :

- To evaluate the immunohistochemical expression of CD34 across histological grades of oral squamous cell carcinoma.
- To correlate the immunohistochemical expression of CD34 in the tumors with clinic-pathological parameters and follow up status of patients with oral squamous cell carcinoma.

## MATERIALS & METHODS:

Group I : Well differentiated oral squamous cell carcinoma (n= 17)

Group II : Moderate & Poorly differentiated oral squamous cell carcinoma (17)

Tissue sections cut from formalin fixed paraffin embedded tissue blocks of 34 oral squamous cell carcinoma cases were immunohistochemically stained for CD 34 antibody.

## SCORING CRITERIA:

The mean microvessel numbers in five high power fields of each hot spot will be taken as microvessel density for each case being examined.

## RESULTS:

The expression of marker was found to be positive. The mean value and standard deviation for the microvessel density as evidenced by CD 34 staining were higher in the Group 1 ( $189 \pm 122.9$ ) compared to Group 2 ( $140 \pm 68.1$ ). Chi square test to explain the relationship between different clinicopathologic parameters. Kaplan Meir survival analysis to predict the prognosis.

CONCLUSION: CD34 acts as a critical prognostic factor in predicting the clinical aggressiveness of the tumor.

KEYWORDS: Oral squamous cell carcinoma, angiogenesis, carcinogenesis

# Deciphering Gene-TF-miRNA regulatory mechanism in breast cancer through systems biology approaches

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Cancer is a disease that has implications all over the world, including in developing countries. It is known for its notorious ways of adapting and gaining resistance to the therapies available. Breast cancer (BC) majorly affects women and leading cause of death in women worldwide. Despite studying BC for many decades, we are not yet certain about a definitive therapy that can cure it with confidence. One of the challenges associated of treating BC is its metastasis and resistance to available therapies. Non-cancerous cells exhibit a tightly regulated transcription profile. Altered transcription profile is considered one of the main causes of origin of cancers and their progression including resistance, metastasis. Tumor suppressor genes are associated with mitigating any oncogenic signals induced by either external factors or from internal dysregulation in oncogenic genes. Changes in the expression profiles of tumor suppressor and oncogenic genes is associated with BC progression and metastasis. Transcription factors (TFs) play a major role in maintaining the tight regulation of transcription. In this study we have analyzed Genes(N=1057), TFs (N =233) and miRNAs (N = 246) that are promoting BC from literature and publicly available data bases, we have analyzed regulation of Gene-Gene, miRNA-miRNA, TF-TF, miRNA-Gene, miRNA-TF, TF-Gene, TF-miRNA as a network of three node Feed Forward Loops (FFLs). Upon constructing 3, 4,5 and 6 node FFLs, we have Identified that the miRNA130a is promoting BC by inhibiting crucial Tumor suppressor genes like TGFBR1, TGFBR2, SOD2, PTEN, SMAD4, RUNX3 etc.

**Key words: miRNAs, Breast Cancer, Systems biology, Transcription Regulation**

# Fabrication and Evaluation of Tamoxifen Citrate Loaded MWCNTs for Breast Cancer Management

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**Introduction:** Breast cancer is the 2nd most common cancer among female worldwide. According to GLOBOCAN estimates of cancer incidence and mortality, burden of breast cancer is expected to rise more than 3 million new cases per year. Targeted drug delivery with the help of nanotechnology has improved and maximised therapeutic activity and minimized undesirable side effects and toxicities. Carbon nanotubes are one of the promising platforms showing efficient cellular internalization and high target specificity for cancer cells.

**Aim:** The aim is to develop & evaluate tamoxifen citrate loaded functionalized multiwalled CNT's for breast cancer treatment.

**Methods:** c-MWCNTs were initially loaded with estrogen receptor modulator Tamoxifen citrate by sonication and centrifugation method. Afterwards targeting ligands bio-chi were conjugated to synthesize bio/chi/TAM/MWCNT for achieving dual targeting. Pre formulation studies revealed the compatibility of targeting ligands by FTIR, DSC and solubility studies. Characterization of the synthesised product was done by Encapsulation Efficiency with help of STD calibration curve of Drug(TAM), SEM & in vitro studies was done to check the drug release from formulation at 2 different pH medium.

**Results:** FTIR and DSC graphs revealed that all components TAM, c-MWCNTs, Bio-chi were found to be compatible. Solubility studies revealed that drug TAM was completely soluble in ethanol & insoluble in other organic solvents. The drug loading efficiency was found to be 88.3%. with the help of calibration curve of pure TAM and by using extrapolation method. SEM revealed the microstructure study of formulation c-MWCNT with presence of chitosan coating. XRD demonstrated that the synthesised product is amorphous. In-Vitro drug release showed a pH dependent drug release of TAM from formulation with a higher drug release at pH-4.0 i.e. under acidic pH conditions.

**Conclusion:** c-MWCNT loaded with TAM was successfully formulated for targeting breast cancer.

**Keywords:** Carbon nanotubes, Breast Cancer, Targeted Drug Delivery, TAM.

# **Fabrication of antibiotics loaded and DNase/ Surfactants adsorbed solid lipid nanoparticles for combating *Staphylococcus aureus* biofilm resistance**

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## **ABSTRACT:**

Antimicrobial resistance is an immediate threat to global health because it reduces the effectiveness of current medications and makes addressing previously attainable diseases more challenging. This research paper explores to evaluating the potential of Tween-80 and DNase I. The biofilm destabilization was studied by crystal violet staining, bright field microscopy, and scanning electron microscopy. During the study, *Staphylococcus aureus* biofilm was exposed with Tween-80 or DNase I. Same Tween-80 and DNase I was adsorbed onto the surface of gentamicin-loaded solid lipid nanoparticles to disrupt *S. aureus* biofilms in vitro. It was observed that Tween-80 and DNase I potentially destabilized the biofilm. After SLNs formation, the maximum disruption was reported in the drug-loaded SLNs and DNase I was adsorbed on the SLNs, which further needs to explore in an in-vivo animal model to access the actual potential of biofilm disruption in natural conditions.

This study could play a pivotal role to overcome the problem of antibiotic resistance imposed due to biofilm formation to combat antibiotic resistance imposed by bacteria. This approach could be help to develop an efficient therapy to combat against biofilm-mediated diseases.

Keywords: Antimicrobial Resistance, Biofilm, Solid-Lipid Nanoparticles, Tween-80.

# Development and Characterization of Novel $\beta$ -TCP Reinforced Nanocomposite Scaffold from Human Placental Chorionic Membrane for Guided Tissue and Bone Regeneration

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Abstract:

Introduction: The human placental membranes are acclaimed for their high bioavailability and excellent regenerative capacity, making them a fine source of natural biomaterial for tissue regeneration since the 1900's. They have been widely used in various fields of regenerative medicine from treating corneal ulcerations to wound closures and even periodontal Guided Tissue Regeneration (GTR) and Guided Bone Regeneration (GBR). Despite having high bioactivity and regenerative capacity, these biomaterials suffer the limitations of having low mechanical properties which can be modified by reinforcing them with fillers, including nanoparticles because of their size-dependent properties. Beta-Tricalcium Phosphate ( $\beta$ -TCP) is a bioceramic known for its bioactivity in terms of osteoconductivity and high resorbability, thereby enabling a faster turnaround time during regeneration process. The present work involves the development of a novel nanocomposite membrane with enhanced properties from the chorionic membrane of the human placenta as the organic phase and the  $\beta$ -TCP nanoparticles ( $\beta$ -TCP NP) as the inorganic phase.

Aims and Objectives: The present study aims to develop and characterize a novel nanocomposite barrier membrane scaffold with superior properties from human placental chorionic membrane reinforced with  $\beta$ -TCP NP.



**Methodology:** Human placental membranes were collected from pre-screened consented donors who were posted for elective caesarean. The chorionic membrane was separated from the amniotic membrane and was processed separately. The membranes were subjected to the process of decellularization using 0.5% and 0.1% Sodium Dodecyl Sulphate (SDS), 1.5% Triton X 100 and DNase I enzyme. Following decellularization the membranes were subjected to lyophilization, pulverization and solubilization. Scaffolds were fabricated with the solubilized matrices through casting and lyophilization at 10mg/ml, 20mg/ml, 30mg/ml and 40mg/ml concentrations and cross-linked. Characterization of the scaffolds was done (morphological, physicochemical and mechanical) and the best concentration of 30mg/ml was selected as the control chorion (CC) for the incorporation of  $\beta$ -TCP nanoparticles at concentrations of 2.5 wt%, 5 wt%, 10wt% and 15wt%. The newly fabricated nanocomposite scaffolds were then subjected to SEM, EDS, XRD, FTIR, Tensile testing and biocompatibility assays.

**Results and Conclusions:** The study is ongoing, and the results are awaited.

**Keywords:** Placental membranes, Periodontal, Regeneration, Guided Tissue Regeneration, Guided Bone Regeneration, Nanoparticles,  $\beta$ -TCP

# Application of Next-Generation Sequencing in Cancer Genomics

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Next-Generation Sequencing (NGS) has revolutionized cancer genomics, providing unprecedented insights into the molecular underpinnings of cancer. This technology allows for comprehensive and high-throughput sequencing of entire genomes, exomes, and transcriptomes, facilitating the identification of genetic mutations, structural variations, and gene expression changes associated with cancer. NGS has enabled the discovery of novel oncogenes, tumor suppressor genes, and driver mutations, significantly advancing our understanding of cancer biology.

One of the critical applications of NGS in cancer genomics is the identification of somatic mutations that drive tumorigenesis. By comparing tumor DNA to normal DNA from the same patient, NGS can pinpoint mutations unique to the cancer cells. This information is crucial for developing targeted therapies tailored to the genetic profile of individual tumors, a cornerstone of precision medicine. Additionally, NGS aids in the detection of rare and sub clonal mutations, providing a more detailed landscape of tumor heterogeneity and evolution.

NGS also plays a vital role in identifying genetic alterations that confer resistance to therapy. By sequencing tumors before and after treatment, researchers can uncover mechanisms of resistance, enabling the development of strategies to overcome or prevent resistance. Furthermore, NGS-based liquid biopsy techniques allow for the non-invasive monitoring of tumor dynamics and response to treatment through the analysis of circulating tumor DNA (ctDNA) in blood samples.

Despite its transformative potential, the implementation of NGS in clinical practice faces several challenges, including data interpretation, standardization of workflows, and ethical considerations related to genetic information. Nonetheless, ongoing advancements in NGS technology and bioinformatics are continually enhancing its accuracy, affordability, and clinical utility.

In conclusion, NGS has become an indispensable tool in cancer genomics, driving forward precision oncology by enabling comprehensive genetic profiling of tumors. Its applications in identifying mutations, understanding tumor heterogeneity, and monitoring treatment response hold significant promise for improving cancer diagnosis, prognosis, and therapy. As technology continues to evolve, NGS will undoubtedly play an increasingly central role in the fight against cancer.

Keywords: Next-Generation Sequencing, Cancer Genomics, Somatic Mutations, Tumor Heterogeneity, Precision Medicine, Liquid Biopsy, Tumor Suppressor Genes.

# **Molecular Identification and Biochemical composition of Cladocera – Diaphnasoma excism**

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## **Abstract:**

Zooplankton, the ecological indicator of ecosystem was identified in Banapureeshwar temple pond at Kumbakonam, Thanjavur District, Tamil Nadu, India from March 2018 to February 2019 to assess the morphological observations. The present study was employed molecular techniques for the quick detection and Identification of Zooplankton species.

Species identification is crucial for studying biography of plankton and applying laboratory culture results. Traditionally morphological traits were used but recent molecular methods have not been incorporated into species descriptions. Currently, a total evidence approach is recommended, combining molecular and morphological information. This will help and solve the mystery of cryptic species and ensure correct identification of species when DNA sequences are published. The identified species were then cultured and subjected to biochemical analysis.

**Keywords:** Zooplankton, Ecosystem, Molecular methods, Biochemical analysis

# SCREENING OF HIGH-YIELDING BACTERIAL CELLULOSE MUTANTS

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## ABSTRACT:

*Acetobacter xylinum* is a Gram-negative, aerobic bacteria and model microorganism for the synthesis of Bacterial Cellulose, it secretes cellulose fibrils as a part of its normal metabolic activity. Bacterial Cellulose, known for its unique properties such as high-water holding capacity, high crystallinity index (CI) and it is devoid of impurities such as lignin and pectin, which increases its demand in numerous industrial applications such as food industry, medical, pharmaceutical, paper industry, etc. In this study, bacterial cellulose was synthesized using mutated *Acetobacter xylinum* NCIM 2526 by UV irradiation and then cultivated in different media at  $30 \pm 2$  oC for 7 days under static condition. Mutation studies were carried out in three different ways by exposing the bacterial culture to UV irradiation for 0, 10, 20, 30, 60, 90, 120 seconds to select the best mutated culture. 30 seconds mutant of *Acetobacter xylinum* resulted in highest Bacterial Cellulose production. Maximum yield of BC was obtained at 37°C with 15% inoculum size. Later the obtained BC was represented as BCM (BC obtained from Maltose), and was characterized by FTIR that indicated functional group of cellulose obtained by mutated bacterial culture were similar to that of commercial standard microcrystalline cellulose. The fibril structure of cellulose was characterized in Scanning Electron Microscope. Thus, Bacterial Cellulose obtained from the optimized semi-synthetic medium was characterized for both structural and chemical properties.

**KEYWORDS:** FTIR, Cellulose, Mutation, *Acetobacter xylinum*, Scanning Electron Microscope.

# **In silico identification of crucial miRNAs involved in Diabetic Cardiomyopathy**

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Diabetic cardiomyopathy is a chronic disorder that affects cardiac muscles and their ability to contract, thereby affecting blood pumping. It occurs solely or majorly as a complication of diabetes and related pathophysiological changes in the myocardium. The clinical presentations are left ventricular dysfunction, hypertrophy, perivascular and interstitial fibrosis, cardiac remodeling, and eventually, heart failure. Being a lifestyle disorder, epigenetic regulations play a prominent role in the pathogenesis. This study comprehensively analyzed the differentially regulated genes (411), microRNAs (383), and their targets related to Diabetic Cardiomyopathy and other relevant pathways. 383 miRNAs associated with Diabetic Cardiomyopathy were obtained from the Gene Expression Omnibus (GEO) database, Human MicroRNA Disease Database (HMDD), and Literature. The miRNA- targets were obtained from MirWalk and MirTarBase databases. Genes related to DCMY were curated from the KEGG database and DisGeNET. These genes were then compared with the miRNA targets. This gave a total of 411 common targets. The protein-protein interactions were constructed using the STRING platform. The miRNAs associated with these common targets were identified. Finally, we narrowed it down to 17433 gene-miRNA interactions. The data was used to create an interaction network using Cytoscape software. The topological features were studied to identify the hub genes and miRNAs. The miRNA-gene network showed the signature miRNAs regulating the highly-ranked hub genes. Further analysis will be done to validate the microRNAs in regulating Diabetic cardiomyopathy through in vitro approaches.

Keywords: Diabetic Cardiomyopathy, microRNAs, network analysis

# In-silico Molecular Docking and ADME/Pharmacokinetic Prediction Studies of curcumin and curcuminoids as human histone deacetylase (HDAC) inhibitors

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Chemotherapy is one of the most well-established and effective cancer treatments available. However, non-tumour-associated damage restrict the treatment's effectiveness and safety. Our growing understanding of cancer epigenetics has resulted in new therapeutic options and the potential of better patient outcomes in recent decades. In cancer, epigenetic changes are widespread, particularly increased expression and activity of histone deacetylases (HDACs). Epi-drugs are chemical agents that modify the structure of DNA and chromatin facilitating disruption of transcriptional and post-transcriptional changes. First generation epi-drugs include HDAC inhibitors (HDACi) (approved to treat haematological malignancies) harbour various adverse effects demanding the discovery and development of potential natural HDACi that might benefit cancer treatment especially in haematological malignancies. Curcumin (diferuloylmethane), a polyphenolic, component of *Curcuma longa*, is a well-known anti-inflammatory, anti-oxidative, and anti-lipidemic agent and has recently been shown to be a pan HDACi. Yet the potential of other curcuminoids in *Curcuma longa* as pan HDACi remains unexplored. (i) *To virtually screen curcumin and curcuminoids (Desmethoxycurcumin [DMC] & Bisdemethoxycurcumin [BDMC]) against human Histone deacetylase (HDAC) class I, II and IV enzymes in comparison to their pan HDAC inhibition activity with FDA approved human HDACis available in market and also (ii) to predict the drug likeness property and ADME/ toxicity of curcumin, curcuminoids and approved HDACis via computational approach. Homology modelling followed by docking was performed for human HDAC class I, II and IV enzymes with curcumin, Desmethoxycurcumin, Bisdemethoxycurcumin and with 5 reference HDACi compounds Vorinostat (SAHA), Trichostatin A (TSA), Chidamide, Romidepsin, and Panobinostat to understand the protein -ligand interactions and binding efficiencies.*

Further, the study ligands with low binding energy were predicted for pharmacokinetic properties and Lipinski's rule of 5. Our study revealed that BDMC followed by DMC and curcumin had high inhibitory effect by interacting at the active site of Zn<sup>+</sup> HDACs similar to that of the standard HDACi (curcumin, DMC, BDMC, Belinostat, Chidamide, Romidepsin, Panobinostat, Trichostatin A and Vorinostat). Likewise, all of the chosen ligand molecules, with the exception of Romidepsin (refractive index >130 m<sup>3</sup> mol<sup>-1</sup>), adhered to Lipinski's rule of five and none of the natural compounds (curcumin, DMC, BDMC) did report any toxicity and mutagenic property also, the lethal doses (LD<sub>50</sub>) of all the natural compounds were higher when compared to chemical drugs. BDMC could be a potential pan HDACi than curcumin and DMC owing to high binding affinity among human Zn<sup>+</sup> HDACs. The results of our present study can be useful for the design and development of novel compounds having better HDAC inhibitory activity against several types of cancers. Moreover, these findings could be validated with invitro investigations and by clinical trials to evaluate the survival outcomes in cancer patients when treated with the natural HDACi along with standard chemo regimen.

Keywords: Curcuminoids, HDAC, Epidrugs, cancer.



# Production, Purification and Characterization of tannase from *Aspergillus aculeatus* KUSR2

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Abstract:

Microbial enzymes, with their diverse catalytic properties, have revolutionized various industries by providing more sustainable and economically competitive production processes as well as offering solutions to several challenges faced by traditional chemical synthesis methods. Tannase also known as tannin acyl hydrolase is a microbial enzyme that has gained significant attention in industries such as the food and beverage industry, pharmaceuticals, textile processing, and animal feed production. Its main function is to hydrolyze tannins, which are a type of plant polyphenol found in various fruits, vegetables, and beverages. The use of tannase in these industries offers several benefits, including the removal of bitterness from food and beverages, improvement of product quality and stability, enhancement of flavour and aroma, and reduction of tannin related health risks.

In this study, a promising tannase producing fungi was isolated after screening. Isolated fungal strain was identified as *Aspergillus aculeatus* KUSR2. Optimization of production media by traditional one factor at a time and statistical methods lead to enhanced production in tannase from  $5.38 \pm 0.12$  to  $50.57 \pm 3.73$  U/mL, which is tenfold increase over the initial production stage. Tannase enzyme from *Aspergillus aculeatus* was purified by 20-60% ammonium sulphate, dialysis and gel filtration chromatography. Purification resulted in an increase in specific activity of 27.91 U/mg with a recovery of 7.45%. The molecular weight of purified enzyme was found to be approximately 97.2 KDa, and shows a significant potential of tannin degradation by showing clear zone of hydrolysis in tannic acid containing media.

Keywords: Microbial enzyme, Tannin acyl hydrolase, *Aspergillus aculeatus*

# **Irrefutable Impact of Nanoparticles Instigated Nanomedicine for the Prevention of Invasive Disease and Nasal Colonization Persuaded**

**Streptococcus pneumoniae**

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## **ABSTRACT:**

Transmittable diseases are a foremost chauffeur of sickness and impermanence universally. Treatment of pneumonia, tuberculosis, malaria and AIDS contagion are predominantly challenging, as specified by the continuing transmission and high death related with these diseases. The formulation of new-fangled and present drugs in nano-sized carters aptitudes to overawed numerous challenges associated with the treatment of these diseases. Moreover, nanoparticles can be castoff for articulating nanomedicines, which epitomize a key armament in bout against infectious diseases. At this point, we highlight how nanotechnology can support in enlightening prevailing treatment modes. Diverse subdivisions of medicine and treatment have also focused on the use of nanoproducts. Current developments in the turf of nanotechnology, predominantly the capability to formulate extremely tidy nanoparticles to a confident size and shape, have led to the progress of new medicinal agents. Nanoparticles are used to develop nano medicine. Antibiotics killing feasibly a 140 diverse disease producing organisms but nanomedicine can killing around 600 type of pathogenic organisms. Metal nanoparticles based nanomedicine have been studied widely for the reason that of their exclusive antimicrobial, anticancer, and wound therapeutic chattels . Among the metal nanoparticles, silver, copper, gold, titanium, plain, zinc, magnesium, and alginate nanoparticles are interesting, because it has vast applications in various areas including medical applications. At present, plant interceded bio synthesis of nanoparticles are acquisition of importance owing to its uncomplicatedness, eco-approachability and all-embracing antimicrobial activity.

In our present work, we swotted the application and development of phyto nanomedicine in the prevention of invasive disease and nasal colonization persuaded by *Streptococcus pneumoniae*. The magnesium oxide nanoparticles (MgONPs) were fortified using *Avicennia marina* leaf extracts. The MgONPs invigorated phytomaterial used and tested as a novel nanomedicine to kill the *Streptococcus pneumoniae* bacterial species. The decidedly crystalline phase of MgO nanoparticles were inveterate by XRD, UV-Vis spectroscopy, SEM, TEM and FTIR studies. Further, the antibacterial medicinal activity of MgONP-PNM was plaid against harmful invasive pathogens such as *Streptococcus pneumoniae* and a perceptible zone of inhibition was observed at 150 and 200 µg/mL. Accordingly, MgONP-PNM nanomedicine can be considered as a possible novel nanomedicine to eradicate the *Streptococcus pneumoniae* infection and also an effective antibacterial agent against all types of antibacterial invasions.

**KEYWORDS:** Antibacterial activity, nanoparticle, nanomedicine, phytomaterial, biosynthesis

# Evaluation of cardio-protective activity of isolated Telmisartan from *Elaeagnus conferta* Roxb. leaf ethanol extract

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## Abstract:

Cardiac disorders are the major threat affected majority of population in the world and the etiology of the disease varies from the physiology of the person and environmental condition. In traditional medicines many herbal formulations were used to cure cardiac but scientific validation is lacking. This study evaluates the cytotoxicity and cardioprotective effect of telmisartan isolated from the leaf ethanol extract of *E. conferta* using H9C2 cardio myocyte cell model. The result of this investigation showed that telmisartan at the concentration of 25 µg/ml, demonstrated noncytotoxic effects in maintaining cell viability significantly at 79.40% and exhibited cardioprotective property in reduced damage induced by H<sub>2</sub>O<sub>2</sub> at the range of 68.07%. Higher concentrations exhibited moderate toxicity, indicating a dose-dependent cytotoxic response. The result was also evidenced with increased levels of antioxidant enzymes such as SOD, CAT, GSH, and GPx. These findings suggest that telmisartan not only mitigates oxidative stress but also enhances cellular antioxidant defenses, thereby protecting cardio myocytes from damage. The outcome of this investigation revealed a novel cardio protective drug.

**Keywords:** *Elaeagnus conferta* Roxb., Telmisartan, Cardioprotective.

# Nutritional and in vitro antioxidant activities of the Indian Coral tree (*Erythrina stricta* Roxb.) seeds

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## **Abstract:**

The underutilized Indian Coral tree (*Erythrina stricta* Roxb.), a legume plant indigenous to the Indian subcontinent, has long been used for a variety of therapeutic purposes. With an emphasis on describing the seed oil, this study methodically investigates the nutritional quality of Indian Coral tree seeds, including their proximate and mineral composition. The seeds have an excellent proximate composition, containing 18.71% fiber and 26.81% protein. 5.0 mg/g DW of calcium and 787.0, 32.7, 36.8, and 497.0 µg/g of iron, copper, boron, and zinc, respectively, are noteworthy mineral elements. The seeds yield 13.43% oil, with the main fatty acids being oleic, palmitic, linoleic, and stearic, which make up 48.82%, 20.63%, 20.27%, and 6.47% of the oil, respectively. The 2,2-Diphenyl-1-picrylhydrazyl (DPPH) radical scavenging activity, total antioxidant activity, and ferric reducing antioxidant power (FRAP) assay all show that the water extract of seeds has a higher antioxidant capacity. These findings highlight the Indian coral tree's seeds as a reliable supply of nutrients and oil, indicating the need for more research and thought about possible uses.

**KEYWORDS:** *ERYTHRINA STRICTA*; UNDERUTILIZED LEGUME; SEED OIL; PHYTOCHEMICAL ANALYSIS

# PROTEOMIC CHARACTERIZATION OF HUMAN PLACENTA: INSIGHTS INTO POTENTIAL THERAPEUTIC APPLICATIONS FOR OSTEOARTHRITIS

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## ABSTRACT:

Biologics have become increasingly prominent as therapeutics in recent years due to their innate immune-privileged nature, biocompatibility, and high levels of protein biofactors. The aim of the study is to characterise the biologic, lyophilized human placenta (LHP) and explore its therapeutic potential for osteoarthritis (OA). The presence of six bioactive constituents that regulate cell-extracellular matrix interaction was identified by liquid chromatography coupled to electrospray ionization and quadrupole time-of-flight mass spectrometry (LC-ESI-QTOF/MS). Metalloproteinase inhibitor 3 (TIMP3), alpha-1 anti-trypsin (a1AT), basic fibroblast growth factor (bFGF), and transforming growth factor  $\beta$ 1 (TGF $\beta$ 1) were detected and quantified using ELISA.

# HR-LCMS phytochemical profiling and Antioxidant potentialities of antiaging formulation of *Morinda citrifolia* (Noni) based composition

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Abstract:

Noni (*Morinda citrifolia* L.) is a traditional polynesian medicinal plant which has a large range of therapeutics claims including antiaging, antitumor, analgesic, hypotensive, anti-inflammatory and immune enhancing effects due to the biosynthesis of key secondary metabolite molecules. These molecules help mitigate oxidative stress by scavenging reactive oxygen species (ROS) and preventing lipid peroxidation. This study aimed to evaluate the HR-LCMS profiling of phytochemicals and antioxidant potentials of noni based antiaging formulation. The aqueous extract of the formulation subjected to qualitative and quantitative phytochemical analysis and then analyzed for phytochemical profiling using HR-LCMS. *In vitro* antioxidant assays, including DPPH, ABTS, Fe<sup>2+</sup> metal chelating and total antioxidant activities, were performed.

The investigation revealed significant antioxidant potential with IC<sub>50</sub> values of 766.453 µg/ml for DPPH, 169.52 µg/ml for ABTS, 50.192 µg/ml for Fe<sup>2+</sup> metal chelating and 670.1 µg equivalent to standard ascorbic acid for total antioxidant activities. HR-LCMS analysis identified several strong antioxidants in the formulation of aqueous extract. The cation spectra revealed the presence of the Picolinic acid, which exhibits potent neuroprotective, immunological, and anti-proliferative activity. Agmatine a compound which has cardioprotection, antidiabetes, decreased kidney function and neuroprotection activity. The anion spectra identified strong antioxidants such as Quinic acid, Gallic acid, Azelaic acid, and Suberic acid. The findings suggest that antiaging formulation of noni can serve as a potent asset in the pharmaceutical industries to develop various range of products.

Keywords: *Morinda citrifolia*.L, Antiaging, HR-LCMS profiling, Antioxidant potentials.

# Antioxidant potentialities and HR-LCMS phytochemical profiling of *Arachis hypogaea* L. root methanol extract

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Abstract:

Groundnut (*Arachis hypogaea* L.) is a vital oilseed and cash crop grown in semiarid zones, known for its resilience to drought due to the secondary metabolite molecules. These molecules mitigate oxidative stress by scavenging reactive oxygen species (ROS) and preventing lipid peroxidation. Nutritional properties of groundnut pods are well-studied however, there is a limited literature on phytochemical profiling and medicinal properties of its roots. This study aimed to evaluate the antioxidant potential and HR-LCMS profiling of phytochemicals in *Arachis hypogaea* L. root methanol extract. The sequential Soxhlet extraction method was followed for the preparation of root extract, and then subjected to qualitative and quantitative analysis. The root methanol extract was further analyzed using HR-LCMS. In vitro antioxidant assays, including DPPH, ABTS, Fe<sup>2+</sup> metal chelating, nitric oxide radical scavenging, and total antioxidant activities, were performed. The investigation revealed significant antioxidant potential with IC<sub>50</sub> values of 822 µg/ml for DPPH, 43.823 µg/ml for ABTS, 225.976 µg/ml for Fe<sup>2+</sup> metal chelating, 362.5 µg/ml for nitric oxide radical scavenging, and 670.1 µg equivalent to standard ascorbic acid for total antioxidant activities. HR-LCMS analysis identified several strong antioxidants in the root methanol extract. The cation spectra revealed the presence of the N-containing iminosugar fagomine, which exhibits potent antihyperglycemic activity, and 2-amino-3-methylhexanoic acid, a plant inducer with high heat stress resistance. The anion spectra identified strong antioxidants such as quinic acid, rutin, astragaloside 7-rhamnoside, and azukisaponin IV, which significantly reduce serum triglycerides, total cholesterol, low-density lipoprotein-cholesterol, and liver lipid levels. The findings suggest that groundnut roots, beyond their pod yield, could serve as raw materials for pharmaceutical industries to isolate potential bioactive compounds, and this would be the additional source of income for the farmers.

Keywords: Ground nut, Root methanol extract, HR-LCMS profiling, Antioxidant potentials



# HRLCMS analysis and molecular docking studies of root ethanol phytochemicals of *Hibiscus lobatus* Kuntze against bacterial DNA gyrase

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## Abstract:

*Hibiscus lobatus* Kuntze, commonly referred to as Lobed Leaf Mallow or Kaadu daasavala, is traditionally utilized for its medicinal properties in managing diabetes, debility, aphrodisiac effects, spermatorrhea, inflammation, bacterial and fungal infections, hair loss, anti-aging, and gastric ulcers. This study aims to investigate the HRLCMS chemical profiling and Molecular docking study of HR-LCMS identified compounds against bacterial target. The root ethanol extract (HREE) was prepared using the sequential soxhlet extraction method and subsequently analyzed via HR-LCMS then Molecular docking study of HR-LCMS identified compounds was performed by docking with bacterial enzyme DNA gyrase. HR-LCMS analysis reveals that the compounds Naringin 6''-rhamnoside, Kaempferol 3-rhamnoside 7-xyloside, Feruloylputrescine, Obtusin, Pseudoecgonine, Valganciclovir are the major constituents. Naringin 6''-rhamnoside, Pseudoecgonine, Obtusin, have shown drug likeliness of 0.826, 1.815 and -0.97 the molecular docking of Naringin 6''-rhamnoside, and Feruloylputrescine against the bacterial enzyme DNA gyrase exhibited good binding affinity of -4.8, -5 and -3.7 kcal/mol. Naringin 6''-rhamnoside has 5 hydrogen bonds and hydrophobic interaction with 3 amino acid residues, so that Naringin 6''-rhamnoside processes good inhibitor as compared to other 5 compounds. *Hibiscus lobatus* root ethanol extract showed significant inhibitory activity against bacterial enzyme DNA gyrase. This investigation supported traditional claim of HREE as potential antibacterial drug.

**Key words:** *Hibiscus lobatus*, HRLCMS, ADMET, DNA Gyrase, Molecular docking.

# Ischemia-Modified Albumin and Thiol/Disulfide Homeostasis as a Markers of Oxidative Stress in Metabolic Syndrome

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Abstract:

Background: A constellation of risk factors for cardiovascular disease (CVD) is called metabolic syndrome (MetS), and oxidative stress is considered a contributing factor to it. In recent years, ischemia-modified albumin (IMA) and thiol-disulfide homeostasis (TDH) have been used as a potential marker of oxidative stress in various disease conditions. In this study, we evaluated IMA and TDH in MetS by a newly developed spectrophotometric method.

Methods: This study includes 162 participants, 54 each in healthy control, MetS, and MetS with Type 2 diabetes mellitus (T2DM). In this study, IMA and TDH parameters were evaluated in the control and MetS groups and compared among the groups. Correlation analysis was performed to find out the relationship between oxidative markers and components of MetS.

Results: When comparing demographics, lipid parameters and fasting blood sugar (FBS) across the group show significant differences. In contrast to the healthy control group, the MetS groups showed higher IMA levels; however, the total and native thiol levels were significantly reduced in control groups ( $P < 0.001$ ). With blood pressure and FBS but not with triglycerides, IMA has shown a significant correlation. There was a strong positive relationship ( $P < 0.001$ ) between total and native thiol with high-density lipoprotein cholesterol. However, FBS, waist circumference (WC), and triglyceride showed a significant negative correlation ( $P < 0.001$ ).

Conclusion: Evaluation of these parameters could help to monitor the future complications of MetS.

# Preparation and characterization of agrowastes based natural polymers for dye degradation applications

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## ABSTRACT

**Objective:** The present study was aimed to synthesize and characterize the corn waste based carboxy methyl cellulose membranes for dye degradation.

**Materials and Methods:** The corn husk waste material was collected and subjected for washing with distilled water and dried. With the help of solvent extraction the crude cellulose was extracted and used for the membrane preparation. For Membrane CMC was used in defined percentage with conjugation with the extracted crude cellulose. Further, synthesized membranes were characterize during physical techniques such as SEM-EDX, XRD analysis and also for physical properties such as water holding, moisture retention. In-vitro dye degradation was studied using methylene blue.

**Results:** The crude cellulose was extracted and confirmed through biochemical tests. Further membranes were prepared using gel casting techniques. SEM results revealed porous morphology on the crude cellulose conjugated CMC which might be enhances the dye degradation studies. EDX analysis showed the presence of different elements such as carbon, oxygen, hydrogen as major constituents. XRD analysis showed the presence of crystalline nature of synthesized membranes. Based on photo degradation studies on methylene blue results showed that as compared to plane CMC membrane cellulose conjugated membranes has shown the better dye degradation with colour change and higher percentage of degradation.

**Conclusion:** the prepared membranes were well characterized and it has shown promising results in the dye degradation studies which was proven by morphological and spectral observation. Further in future these membranes can be employed for the dye industry for the treatment process.

**Key words:** Corn husk waste; SEM-EDX, XRD and Dye degradation.

# Extraction and characterization of crude Betalain pigment from beetroot peel and its therapeutic applications

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## ABSTRACT

**Objective:** The present study was planned to extract and characterize Betalain from the peel waste of beet root for therapeutic applications.

**Materials and Methods:** using the beet root peel the crude Betalain pigment was extracted with the help of citric acid ethanol. The crude Betalain extract was subjected for the characterization such as UV, XRD and FTIR analysis. The crude pigment was subjected for the antibacterial, anti-diabetic and antioxidant studies using standard procedures.

**Results:** The crude red Betalain pigment was analyzed through UV studies which showed sharp peak at 535nm. FTIR analysis results revealed the presence of -OH group for band at 3359  $\text{cm}^{-1}$  was attributed to the stretching vibration of the -OH phenol, the next band at 1378  $\text{cm}^{-1}$  was assigned to the extension stretching vibration of the C-H bond, while the band centered at 1243  $\text{cm}^{-1}$  correspond to the stretching vibration of the C-O bond of the carboxylic acid. XRD analysis confirmed the crystalline nature of the extracted crude Betalain. Further the crude dye was screened for the antibacterial activity against E. coli and it has shown significant activity with higher zone of inhibition. Anti-diabetic activity has shown appreciable results with higher percentage of inhibition with the alpha-amylase. The DPPH assay of antioxidant activity was shown significant activity with the increase in the concentration.

**Conclusion:** the extracted Betalain crude dye was successively screened for the therapeutic applications. In all performed assays it has shown significant results. Further future studies can be planned for the purification and structural elucidation with approach to the anticancer studies.

**Keywords:** Betalain, XRD, FTIR, DPPH assay and Antidiabetic.



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Category	Name	Institute	Designation	Mode
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<b>Best Thesis</b>	Ankita Das	Manipal Institute of Technology	Research Scholar	Offline
<b>Best Thesis</b>	Nikitha Surendran O	Kannur University	Research Scholar	Online
<b>Outstanding Researcher</b>	Aparna Tripathy	Department of Basic Medical Science, MAHE	Faculty	Online
<b>Oral Presentation</b>				
<b>Best Oral</b>	Sudharsh S	Central University, Tamiinlnadu	UG/PG	Offline
<b>Best Oral</b>	Rohit Manikantan	Manipal Institute of Technology	UG/PG	Online
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