

## PAPER



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## Antiobesity drug-likeness properties and pancreatic lipase inhibition of a novel low molecular weight lutein oxidized product, LOP6

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Elevated expression of peroxisome proliferator-activated receptor-gamma (PPAR- $\gamma$ ), a key regulator of adipogenesis, leads to lipid accumulation and obesity. Although orlistat is effective for obesity, flatulence with discharge, faecal urgency, oily evacuation and other allied side effects limit its usage. Thus, natural product-based drug intervention is the future of research and development of novel treatment. We synthesized and characterized total lutein oxidized products (LOPs) by exposing lutein to direct sunlight with a solar intensity of  $5.89 \text{ kW h m}^{-2} \text{ day}^{-1}$  and at  $31 \pm 2 \text{ }^\circ\text{C}$  for 1–10 days. Total LOPs were analyzed on  $\text{C}_{18}$  and structural elucidation was carried on LCMS/MS-TOF. The pancreatic lipase inhibition kinetics was estimated. The binding effects of LOP6 (fragmented peak 6) on PPAR- $\gamma$ , pancreatic lipase, pharmacokinetic properties and inhibition studies were analysed. Histological evaluation of liver and adipose tissues was performed to confirm the antiobesity effect of total LOPs. The yield of extracted lutein purified from shade-dried marigold flower petals was 6%. Total LOPs were formed on the 10th day upon exposure of lutein to direct sunlight. Total LOPs on the  $\text{C}_{18}$  column fragmented into eight oxidized products (LOP1 to LOP8). The total LOPs showed significant inhibition of pancreatic lipase activity with an  $\text{IC}_{50}$  of  $1.6953 \mu\text{g ml}^{-1}$ , and  $K_m$  and  $V_{\text{max}}$  of  $3.05 \mu\text{g}$  and  $1.19 \mu\text{g s}^{-1}$  respectively following mixed type of inhibition. The LOP6 [4-((1E,3E,5E)-3,7-dimethylocta-1,3,5,7-tetraen-1-yl)-3,5,5-trimethylcyclohex-3-enol] with an approximate molecular mass of 274.25 showed a binding energy of  $-5.40 \text{ kcal mol}^{-1}$  with a  $K_i$  of  $109.43 \mu\text{M}$  for PPAR- $\gamma$  and a docking score of  $-5.35 \text{ kcal mol}^{-1}$  with a  $K_i$  of  $119.4 \mu\text{M}$  for pancreatic lipase. The  $\text{IC}_{50}$  of LOP6 was  $11.8420 \mu\text{g ml}^{-1}$ , and  $K_m$  and  $V_{\text{max}}$  were  $2.519 \mu\text{g}$  and  $1.294 \mu\text{g s}^{-1}$ . The pharmacokinetic properties such as solubility, permeability, bioavailability, and topological polar surface area when tested with LOP6 were significantly better than those of lutein alone. The histological examination of the liver and adipose tissue revealed that all three doses of total LOPs were effective in alleviating the ballooning and vesicular degeneration of hepatocytes and invasion of inflammatory cells in the adipose tissue. Total LOPs and LOP6 inhibited pancreatic lipase activity *in vitro*. LOP6 showed a better docking score for PPAR- $\gamma$  and pancreatic lipase in comparison to orlistat. Histological data showed that the total LOPs exerted antiobesity activity. Thus, LOPs might provide a novel treatment approach for obesity.

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### 1. Introduction

Obesity is defined as an excessive accumulation of fat in the body that impairs human health, and the root cause is the energy imbalance between consumed calories and expended calories. The common health problems associated with obesity, especially in adults, include hypertension, type 2 diabetes, cardio vascular disease, coronary heart disease, stroke,

gastrointestinal complications, gall bladder disease, cancer, respiratory and oesophageal complications, obstructive sleep apnea, asthma and osteoarthritis.<sup>1</sup> According to the factsheet of the World Health Organization, obese people have globally tripled since 1975. According to the report, in 2016, around 39% of adults aged 18 years and above were overweight and 13% were found to be obese. In 2020, nearly 39 million children under the age of five were overweight or obese.<sup>2</sup> Obesity is a growing epidemic with India and China having the highest number of obese children, which needs to be halted for a healthy future.<sup>3</sup> Obesity is preventable by thorough monitoring and promoting research to formulate and implement an effective strategy combining diet and physical activities.<sup>4</sup>

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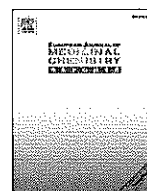
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## Structure, function and mechanistic aspects of scorpion venom peptides - A boon for the development of novel therapeutics

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## ABSTRACT

Venom of scorpions is very expensive and lethal, yet with innumerable and exciting potential as a source for the development of biotherapeutics. One of the chief components of scorpion venom is the 'peptides' which have shown diverse array of biological activities, promising site specificity and are also involved in the regulation of biological mechanisms. These peptides have especially gained more attention in the development of cardiovascular and other immune disorders due to the structural and functional specificity. This review is the compilation of the recent developments of therapeutic applications of scorpion peptides including the latest inventions (till 2020). In most of the cases, primary sequence of the peptides as well as the mechanism of action have been given and hence finds suitable in search of lead molecules for further development. Thus, the relevant findings presented here would serve as a valuable source either for improving the pharmacological profile or for new drugs development.

## 1. Introduction

The field of peptides as therapeutics saw a beginning in the year 1922 with the first ever use of insulin for the treatment of type I diabetes. Nearly after four decades, chemically produced peptide hormones like oxytocin and vasopressin made way to the clinic. During this time, solution-phase peptide synthesis was in place which was highly time consuming and this drawback led to the invention of solid-phase peptide synthesis (SPPS) [1] along with the purification methods like HPLC which attracted remarkable attention of the pharma companies.

## 2. Peptides as therapeutics

After the successful invention of the above techniques, peptides gained significant importance as key biological mediators along with the demonstration of their potency, selectivity and low toxicity. Meanwhile, limitations of peptides like low oral bioavailability, low plasma stability and short circulation time were noticed. This along with the expensive large scale manufacturing resulted in less interest in peptides from the pharmaceutical industry and thus peptide drug development was almost stagnated [2]. Nevertheless, in the late 1980s a second wave of peptide drug development began with the use of peptide as subtype-selective

probes for receptor studies and also peptides as lead compounds in various biological applications. The increased interest in peptide drugs was seen after the approval of human insulin produced using recombinant technology and synthetic gonadotropin-releasing hormones like leuprolide (1985) and goserelin (1989). As a result, the number of peptides entering the clinical trials from 2000 to 2010 almost was twice than in the 1990s [2].

Recently, the field of peptide based drug discovery has seen a renaissance wherein tens and hundreds of academic research groups as well as big pharma companies are constantly working on it. During 2015–2019, 208 new drugs, of which 150 are new chemical entities and 58 are biologics have been approved by US FDA [3]. Amongst this big number, 15 are peptide or peptide-bearing compounds (Table 1) which account for nearly 7% of the total approved number of drugs in this period. In fact, this number is quite impressive from the point of view of efforts that the pharmaceutical industries are putting in compared to small molecule drugs [3].

At present, we have around 80 peptide drugs in the market, 150 are in clinical development and nearly 400–600 peptides are in preclinical studies [4,5]. This trend shows that peptide as therapeutics will continue to grow and expand its arsenal in the years to come (Fig. 1).

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## ORIGINAL ARTICLE

# Identification and characterization of metal-chelating bioenhancer peptide derived from fermented *Citrullus lanatus* seed milk

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**Abstract**

In the present investigation, a metal-chelating bioactive peptide was derived from *Citrullus lanatus* seed milk fermented with *Lactococcus lactis*. The cationic fermented milk peptide (FMP) thus obtained was purified using the HiTrap-chelating column followed by rpHPLC. The FMP possessed the ability to chelate multiple divalent cations like  $\text{Cu}^{2+}$ ,  $\text{Ca}^{2+}$ , and  $\text{Fe}^{2+}$  with 86.81%, 61.04%, and 24.32% of chelation respectively and further it exhibited 78.03% of DPPH free radical scavenging activity. Interaction of FMP with metal ions was assessed by change in the absorption spectra and was analyzed by ultraviolet-visible and fluorescence spectroscopy. The FMP-metal complexes were found stable at simulated gastric conditions. In vitro analysis using intestinal Caco-2 cell lines revealed that there was an increase in metal bioavailability in the presence of the FMP and was least influenced by the addition of a dietary inhibitor, phytic acid. By LC-MS analysis the molecular mass of FMP was found to be 11.6 kD and it contains oxygen-rich and nitrogen-rich amino acids that favor the metal chelation. In our study, we have found that the fermented *C. lanatus* seed milk can serve as a potential functional food with bioenhancer peptides that increase metal bioavailability and enhance human health.

**Practical applications**

Chelated metals are preferred over non-chelated ones by most nutritionists for their better absorption rate. Chelation protects the minerals from the digestive process and increases their bioavailability. Fermentation with lactic acid bacteria produces bioactive peptides with metal-chelating and antioxidant ability which provides additional health benefits beyond supplying basic nutrients. *Lactococcus lactis* fermented milk acts as a probiotic product with bioenhancer peptide that increases mineral bioavailability. Consumption of metals in chelated form can reduce excess intake of metal. Fermented watermelon seed milk can be a promising probiotic drink rich in bioenhancer peptides and can enhance the bioavailability of divalent cations of a high therapeutic index.

**KEYWORDS**

antioxidant, bioactive peptides, *Citrullus lanatus*, fermented milk, *Lactococcus lactis*, metal chelation



## Experimental and DFT explorations of *tert*-butyl(1-(2-(4-nitrobenzylidene)hydrazinyl)-1-oxopropan-2yl)-carbamate on CRCA metal in 1M HCl solution

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### ABSTRACT

The performance of a novel corrosion inhibitor *tert*-butyl(1-(2-(4-nitrobenzylidene)hydrazinyl)-1-oxopropan-2yl)carbamate (AAD) has been accounted here along with physicochemical characterization studies like Fourier Transform Infrared Spectroscopy (FTIR), Scanning Electron Microscopy (SEM), <sup>1</sup>H NMR and Density function theory (DFT). Additionally, thermodynamic parameters such as weight loss, Langmuir adsorption, and the effect of temperature are investigated and are incorporated to show the enhancement of inhibition effectiveness with increasing dosages of synthesized inhibitor. A decreasing order of corrosion efficiency has been observed at elevated temperatures. Currently, AAD is examined using electrochemical methods including Potentiodynamic polarization (PDP) and Electrochemical Impedance Spectroscopy (EIS) to see how effective it is in inhibiting corrosion on cold-rolled close-annealed material (CRCA). According to the examination, the corrosion inhibitor showed anodic type of inhibition activity on CRCA metals with high corrosion efficiency.

### 1. Introduction

It is known, metals and alloys more easily corrode when exposed to acidic conditions. As structural elements, automobile peripherals, and so on, these metals have many applications in the automobile/engineering industries. Moreover, they are inexpensive and easy to fabricate because these metals being superior and having good mechanical, physical and chemical properties. The destructive nature of corrosion makes it a topic of interest throughout the world. The array of application practices makes the steel come in contact with varied destructive environments, Callister (1991) and Clayton (1987) at lower pH solutions all along the course of processes like acid pickling, etching, acid cleaning, acid descaling and oil well acidification. Most corrosion inhibition studies of mild steel have been conducted in an acidic and salt medium (Verma et al., 2016; Qiang et al., 2021; Khadiri et al., 2016; Khadom et al., 2009; Musa et al., 2010; Qiang et al., 2020).

In light of this, there is a crucial need for some outstanding corrosion prevention methods. One of the feasible methods to minimize corrosion is by the addition of organic inhibitors or by the addition of natural plant extracts (Khadom et al., 2010; Noor and Al-Moubaraki, 2008). The effectiveness of organic inhibitors is much better in comparison to natural extracts is determined by their capacity to get adsorbed and protect the metal surfaces. According to sources, the adsorption

of inhibitors on metal/solution interfaces is also affected by the type of metal surface, surface charge, and corrosive electrolyte (Sudheer M.A. Quraishi, 2014; Bhrara et al., 2008). Thus, the use of synthetic organic inhibitors which contain exclusively nitrogen is considered to lessen the corrosion attack on steel (Qiang et al., 2018). In spite of this, organic compounds containing heteroatoms, like S, O, and P have been validated as effective in a variety of acidic solutions (Bentiss et al., 2005; Khadom et al., 2018b; Qiang et al., 2017a, 2016). It is due to the influence of lone pairs and p electrons that an electron transfers from an inhibitor to the metal forming a bond. The inhibitors are known to have specific physicochemical properties that contribute to adsorption. The strength of physisorption/chemisorption is governed primarily by electron density and polarizability. An inhibitor's effectiveness is subsequently determined by its ability to get adsorb on the surface of the metal, which involves a substitution of water molecules at the interface. A decrease in the electron density may explain the decline in the cathodic or anodic reactions (Prakash et al., 2006; Oguzie et al., 2007). Hence, this paper reports on the synthesis and inhibition behavior of AAD on CRCA metal sheets in 1M HCl solution by employing weight loss and electrochemical techniques (EIS and PDP). FTIR and NMR techniques are used to confirm the structure of the synthesized compound. Here, thermodynamic parameters (activation and adsorption) are evaluated and presented. In SEM analysis, a protective

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## RESEARCH ARTICLE

# Plant seed extract assisted, eco-synthesized C-ZnO nanoparticles: Characterization, chromium(VI) ion adsorption and kinetic studies

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## Abstract

This report attempts to elucidate the potential of plant seed extract assisted synthesis of graphite-based zinc oxide nanoparticles (C-ZnO NPs) towards removal of chromium(VI) ions from water samples. The graphite-based zinc oxide (C-ZnO) composites were characterized using thermogravimetric analysis (TGA), X-ray diffraction (XRD), Fourier-transform infrared (FTIR) spectroscopy and scanning electron microscopy (SEM). The C-ZnO nanocomposites have found to remove chromium from the sample through an adsorption process. The sensitivity of chromium removal through adsorption is found to be in the range of 40 to 240 mg. The adsorption behaviour was found to be fitting with Langmuir isotherm model and the adsorption reaction follows pseudo second-order kinetics.

## KEYWORDS

adsorption, Cr(VI) removal, kinetics studies, Langmuir model, Lantana camera flowers

## 1 | INTRODUCTION

Heavy metal ions in water is a potential threat to causing adverse reactions in the biological systems.<sup>[1]</sup> The most notable heavy metals are lead (Pb), zinc (Zn), mercury (Hg), nickel (Ni), cadmium (Cd), copper (Cu), chromium (Cr), and arsenic (As). Metals even present in trace amounts can be hazardous to living beings. These heavy metal ions have a strong tendency to bind to biological molecules such as proteins, nucleic acids present in the living systems.<sup>[2,3]</sup> The heavy metal complexed biomolecules automatically lose their functions causing damage to the organism. Heavy metal ion removal from water samples involves four types of methods that are chemical precipitation, solvent extraction, ion exchange and membrane separation.<sup>[4,5]</sup> Adsorption has been identified as a simple, cost-effective strategy in the removal of heavy metal ions. Activated carbon, carbon nanotubes (CNT), organic porous frameworks, inorganic minerals, and modified polymers are the diverse class of adsorbents reported for their

potency in the removal of heavy metal ions. In nature, the element Cr appears as stable trivalent oxide chromite.<sup>[6]</sup> Chromium (Greek Chroma, meaning colour) is widely used in different industries such as electroplating, tanning, mining, and fertilizer that discharge untreated wastewater to different water sources.<sup>[7,8]</sup> Chromium exists in two oxidation states: trivalent (+3) and hexavalent (+6). Trivalent (+3) forms are biologically essential, whereas hexavalent (+6) forms are mutagenic. In aqueous medium, Cr<sup>3+</sup> exists in neutral [Cr<sup>3</sup>(OH)<sub>4</sub>]<sup>0</sup>, mononuclear [Cr(OH)<sup>2+</sup>, Cr(OH)<sub>2</sub>] and polynuclear forms [Cr<sub>2</sub>(OH)<sub>2</sub>], while Cr<sup>6+</sup> predominately remains in anionic form (CrO<sub>4</sub><sup>2-</sup>, HCrO<sub>4</sub><sup>2-</sup>, Cr<sub>2</sub>O<sub>7</sub><sup>2-</sup>). In aqueous media, Cr<sup>6+</sup> is toxic and has a higher solubility and mobility than Cr<sup>3+</sup>. In most cases, it contains some suspended particles, chemical substances, and some microorganisms. Consequently, water becomes toxic due to the high concentration of these substances. As a result of this toxicity, heavy metals and inorganic substances may pose a risk to the environment<sup>[9]</sup> and threaten human health through the nutrition chain. So, it is very important to



## Development of enhanced electrochemical sensor and antimicrobial studies of ZnO NPs synthesized using green plant extract

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### ABSTRACT

The present investigation envisages for plant mediated synthesis of ZnO NPs (ZPNs) by green combustion route using eco-friendly LCL (Lantana Camara Leaf) Extract. The optical and structural characterizations of ZPNs was studied by spectral techniques; PXRD (Powder X-ray diffraction) study confirms the phase formation and crystalline nature of NPs with its average particle size found to be 35 nm. The internal morphology of synthesized NPs comprises noticeable pores, voids and agglomeration obtained by SEM (Scanning Electron Microscopy) technique. TGA-DTA (Thermogravimetric-Differential Thermal Analysis) analysis reveals the changes in physico-chemical properties of ZPNs by the effect of temperature. The electrochemical reaction measurements of ZPNs-graphite paste electrode in a 3-electrode system using 1 M HCl solution was conducted by CV (Cyclic Voltametric) and EIS (Electrochemical Impedance Spectroscopy) techniques in the different scan rates 0.01–0.05 V/s. Further, the corrosion inhibition activities of ZPNs were examined on mild steel (MS) in 1 M HCl solution by electrochemical spectral studies (CV & EIS) and potentiodynamic polarization (PDP) measurements. The antimicrobial potential of ZPNs was discussed in detail in contrast to gram positive (*Micrococcus luteus*) and gram negative (*P. aeruginosa*) bacterial strains by the zone of inhibition concept using disc diffusion technique.

### 1. Introduction

Nowadays, the significant improvement towards nanotechnology field is employed to engineer novel, cost effective and lethal antimicrobials. Several metal oxide nanomaterials have great interest for researchers and focused towards biological and physico-chemical applications [1–5]. The nanomaterials have gained more significance for researcher in substitute and effective towards the ecological issues. Therefore, ZPNs are potential and efficient semiconductor material show significant features of biomedical systems, charge carrier recombination, electronics devices and potential activities of corrosion studies [6,7]. The different methods are existing for the preparation of ZPNs [8–12] and

hence the green mediated synthesis ZPNs is considered as suitable green route technology due to the excessive need and reduction in the hazardous substances to human health and ecological issues.

The photocatalytic process of ZPNs is governed by several parameters specifically purity of phases, optimum crystallite size, agglomeration of particles and method of preparation [13]. In order to apply the photocatalysis for contaminated water containing dye, many semiconductors have been employed. Among these semiconductors, ZPNs acts as a very good photocatalyst, specifically as heterogeneous photocatalysis for several years. Environmental pollution caused by harmful organisms and pollutants has escalated the health dangers to human and animal life over decades. Thus, heterogeneous photocatalysis using metal oxides showed

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## Original Article

# Plant-mediated synthesis of NiO(II) from *Lantana camara* flowers: a study of photo-catalytic, electrochemical, and biological activities



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## ABSTRACT

In this study, nickel oxide nanoparticles (NiO NPs) were synthesized using *Lantana camara* flower extracts. Electrochemical (EIS and PDP) are conducted on the synthesized NiO NPs nanoparticles to show the corrosion inhibition efficiency. An XRD analysis showed that NiO-NPs generated a FCC structure that exhibited single-crystalline properties. SEM images showed particle size to be between 40 and 50 nm, which matched the average size determined from the XRD pattern. As compared to the reported spectrum, Fourier-transform infrared spectroscopy confirms the formation of NiO-NPs. A degradation study of Methylene blue (MB dye) photocatalytically showed up to 96–98%. Furthermore, the study reveals NiO-NPs possess antimicrobial activity against *Escherichia coli*, *Staphylococcus aureus*, and *Micrococcus luteus*. These nanoparticles were made in a sustainable and cost-efficient manner. The research paves the way for future developments in the fields of biomedical applications.

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## A Study on Knowledge, Skills and Attitude Among Under Graduate Students of Government Colleges Regarding E-learning in Dakshina Kannada District, Karnataka, India

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### Abstract

*The development in Information Communication Technology has resulted in changing trend in learning. The digital learning platform has shifted the momentum of information-gathering than in traditional learning methods and plays a vital role in transforming Information/Knowledge in the most efficient way with effective audiovisuals. In India, the COVID-19 pandemic has opened the way to rise the use of digital platforms for learning in higher education. During the pandemic, the digital learning method helped the students a lot to keep consistency and continuity in learning. These experiences have even more increased the intensity of implementing digital learning methods in higher education for improved performance, skilling and mastery in the field of study of students. The objective of the study is to know the level of knowledge, skills, and attitude of the students of under graduation regarding E-learning. The aim of this study is understanding and analyzing the knowledge, skills, and attitude of undergraduate students regarding digital learning so as to identify the barriers and necessary actions to be taken for implementing digital learning in higher education as aspired in NEP 2020. The online survey method was used through Google form for the collection of primary data and a simple mathematical method of percentage calculation is used to analyze the data.*

**Keywords:** E-learning, knowledge, skills, attitude, under graduate

### INTRODUCTION

The educational system has been undergoing various changes of its development. At every phase, the change is significant. Indian educational system has been putting off its age-old traditional method of education and putting on the new one with expeditiously changing times. Earlier, it was a traditional and classroom-based constricted one. Presently, it has become a more modernized and digitalized one. E-learning is part of the education system in developed nations for decades but developing nations started adopting online learning after the COVID-19 pandemic which disrupted education all over the world for almost 3 years from 2019 to 2021. Learning through Online became as an alternative to face-to-face education during COVID-19 pandemic. Internet and education have been integrated to provide students with the necessary skills in the future [1].

A learning system based on formalized teaching but with the help of electronic resources is known

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## The Enhanced Oral Bioavailability Of Total Lutein Oxidized Products (Lops) Extracted From *Tagetes Erecta* Flower Petals In C57BL/6 Mice

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### ABSTRACT

The lutein extracted from shade-dried *Tagetes erecta* flower petal powder by simultaneous solvent extraction and saponification was exposed to sunlight ( $31\pm 2^\circ\text{C}$ ) for 10 days. Bioavailability and absorption kinetics of total lutein oxidised products in comparison with lutein (parent molecule) were analysed on C57BL/6 mice. Time course plasma kinetics was studied by collecting blood, liver, intestine and eyes after the 1<sup>st</sup>, 2<sup>nd</sup>, 3<sup>rd</sup>, 6<sup>th</sup> and 9<sup>th</sup> hour of intubation. The oral bioavailability of total lutein oxidized products was enhanced in contrast to lutein in plasma by 25% (2<sup>nd</sup> hr), liver by 11% and eyes by 55%. The plasma kinetic properties like area under concentration and area under moment concentration of total lutein oxidized products were 1139.418 pg/h/ml and 17750.69pg/h<sup>2</sup>/ml respectively with a half-life of 11.353h. The mean residence time of total lutein oxidized products was 15.573h with a volume of distribution of 2.874 and clearance of 0.175. The concentration of total lutein oxidized products in eyes at the 9<sup>th</sup> hour was 59.80pg/ml. Whereas, the mean lutein concentration in plasma, liver, and eye was significantly less in lutein in comparison with total lutein oxidized products. Thus, the above data suggest that total lutein oxidized products reach target tissue unaltered and enhance the absorption rate in comparison to the parental compound lutein.

**Keywords:** Lutein, *Tagetes erecta* flower, total Lutein oxidised products (LOPs), C57BL/6 mice, Bioavailability.

### INTRODUCTION

Lutein is a dietary fat-soluble pigment which is accumulated in various tissues /organs of the human body like blood, skin, liver, intestine, breast (lactating women), brain and the majority in the macular region of the eye.<sup>[1]</sup> Various pre-clinical and clinical studies suggest health beneficial aspects of lutein. Some of them include neuroprotective effects<sup>[2]</sup>, ophthalmological effects<sup>[3]</sup>, antibacterial effects<sup>[4]</sup>, photoprotection<sup>[5]</sup>, wound healing<sup>[6]</sup>, anti-inflammatory<sup>[7]</sup> and anticancerous effects<sup>[8]</sup>. Having known the mechanism of lutein in curing life-threatening diseases, yet finding it difficult to formulate into a drug. One of the reasons may be the poor bioavailability and bioaccessibility of lutein.<sup>[9]</sup>

## In-Silico Evaluation Of Anti-Acne Property Of *Syzygium (S.) Aromaticum*

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### ABSTRACT

Acne vulgaris is a common inflammatory skin diseases seen in all age types, caused by the bacteria *Propionibacterium acnes*. *Syzygium (S.) aromaticum* (clove) is an aromatic plant with rich volatile compounds and antioxidants showing high antimicrobial properties mainly anti-acne property. In recent years, computational databases and methods have been shown to be an invaluable resource for research in the field of dermatology and skin health. The structural diversity of plant-derived phytochemicals with antiacne properties against receptor bacterial proteins involved in acne signaling pathways is facilitated by molecular docking studies. The present study reports the protein-ligand interaction of *P. acnes* bacterial protein and several phytochemicals present in *S. aromaticum* which acts as ligands. Thus the authors have made an effort to evaluate the anti-acne properties various phytochemicals against the

## Computational Approach In Search Of Therapeutic For Colorectal Cancer

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### ABSTRACT

Colorectal cancer (CRC) is the second most lethal cancer in the world. Due to late discovery, a high recurrence rate, and multi-drug resistance, CRC care is difficult. Herbs and spices used in cooking have been demonstrated to include CRC protective effectors and can even be utilised as an anti-CRC adjuvant treatment when taken in large dosages. Herbs and spices include several bioactive chemicals that have numerous health benefits. These herbs and spices' chemopreventive activities are primarily mediated by multiple routes, including caspase activation, the extrinsic apoptotic pathway, and the modulation of ER-stress-induced apoptosis. As a result, Ginger (*Zingiber officinale*) was chosen for this study and studied for

ORIGINAL ARTICLE

Effects of Untreated Industrial Waste Water on Vegetative Growth and Pigmentation of Oil Yielding Crops

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ABSTRACT

Water plays an essential role in industrial facilities. Industrial waste water has to be purified before discharging into the sewer or natural water bodies. Industrial waste water contains organic and inorganic matter which affects the different types of ecosystems and crop production. India is the fourth largest producer of oil seeds accounting for about 20% of the global area and 10% of the global production. *Helianthus annuus*, *Arachis hypogaea* and *Brassica napus* are economically important crops in India. The aim of the present study is to assess the possibility whether untreated wastewater from textile, pharmaceutical and granite industry may affect the crop plants and also how it affects the plants in both aspects that is morphologically and physiologically. The soil, seeds and the different industrial waste water samples are collected from the Hyderabad city. The data includes results of physicochemical parameters of water and soil samples. The data of seed growth response to different water samples of various concentrations (25%, 50%, 100%), test results of variations in biochemical compounds among different samples. Various parameters like seed germination, vigour index, imbibition test and physical purity analysis were calculated in seven days old plants. In the present investigation it was observed, the industrial waste water samples collected from different industries have shown high amount of toxic chemical components and unfit for irrigation. It is also effects on seed growth, germination and imbibition, low chlorophyll content, low carotenoids. Low yield etc.

**KEYWORDS:** *Helianthus annuus*, *Arachis hypogaea*, *Brassica napus*, Industrial waste water, Physico-chemical parameters

INTRODUCTION

Industrial wastewater is a by-product of industrial or commercial activities. Whether it is the food wheat, the beverages we drink, the clothes we wear, or the paper and chemical products we use, water is required for nearly every step of production across a multitude of different industries. The resulting waste water must be carefully managed. Regardless of how waste water is treated, the "End Product" is called effluent. To comply with environmental protection laws, certain things must be removed from the waste water. This includes organic matter, inorganics (sodium, potassium, calcium, magnesium, copper, lead, nickel, and zinc), pathogens, and nutrients (most notably nitrogen and phosphorus). The treated waste water can then be safely discharged into water bodies, applied to land, or even reused in plant operations. One option is to discharge untreated waste water to the local municipal treatment plant, but with that comes considerable costs. The other often more favorable option is to treat wastewater at the manufacturing facility itself. This can be accomplished with the right waste water treatment technology (1, 2). The extent to which remobilization takes place, however, also differs between nutrients and this is reasonably well reflected in the distribution of visible deficiency symptoms in plants. Deficiency symptoms which predominantly occur in young leaves and apical meristems reflect insufficient remobilization. In the latter case, either phloem mobility is insufficient or only a relatively small fraction of the nutrients can be transformed into a mobile form in the fully

## FTIR SPECTROSCOPIC ANALYSIS OF *CANTHIUM PARVIFLORUM*- COMPARATIVE ANALYSIS OF FUNCTIONAL GROUP BEFORE AND AFTER EXTRACTION

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### ABSTRACT

Fourier Transform Infrared spectra of *Canthium parviflorum* Lam leaf powder before and after extraction with ethanol were determined. The frequency range and their intensities were obtained from absorption spectra using ATR-FTIR. Comparison of the functional groups present before and after extraction process was done. The results revealed that additional functional groups to be present in the sample after extraction process with ethanol. This showed the presence of alkene compounds, primary alcohol group, secondary alcohol group etc. The analysis revealed the importance of extraction process in solubilizing the phytoconstituents which was indicated through the occurrence of functional groups. Also the study showed the presence of different types of biomolecules to be present in both the samples before and after extraction.

**Keywords:** *Canthium parviflorum* Lam, Powdered leaf, Ethanol extraction, FTIR spectra, Functional groups, Phytoconstituents.

### INTRODUCTION

Alternative systems of medicines are receiving a renewed interest in present days, due to the adverse effects of synthetic medicines. Numerous medicinal plants and their purified components have been reported to possess various beneficial therapeutic potential, such as antioxidant, anticarcinogenic, antihypertensive and antimicrobial activities, etc. These properties of medicinal plants is due to presence of various secondary metabolites such as flavonoids, terpenoids, alkaloids, steroids, phenols etc<sup>1-3</sup>. As such to promote the utilization of medicinal plants and their purified compounds it is crucial to investigate their constituents (phytoconstituents) and therapeutic properties<sup>4</sup>.

Various analytical techniques have been developed for identifying phytoconstituents and these includes Liquid chromatographic Mass Spectroscopy (LCMS), Gas

Spectroscopy (FTIR) is one of such technique. It is based upon the vibrations of the atoms of a molecule. It is a nondestructive method, requires relatively a little amount of sample, is fast, and is accurate. FTIR is used for the identifying the presence of various functional groups in the chemical constituents of plants. Thus aids in structure elucidation with the help of other techniques and have gained importance to identify medicines in pharmacopoeia of many countries<sup>5</sup>.

FTIR has been utilized by numerous researchers in elucidating the structure of isolated compounds. The presence of alkanes, alcohol, phenols, carboxyl acid, alkyl halides and aromatic compounds in ethanol extracts of *Hybanthus emaxperinus* was reported by FTIR spectroscopy method. Identification and comparison of biomolecules of *Cleome gynandra* was reported to be evaluated using FTIR<sup>6</sup>. FTIR analysis of root extracts of *Canthium parviflorum* Lam, showed the presence of the

# Evaluation of antifungal effect of medicinal plants against Panama wilt of Banana caused by *Fusarium oxysporum* f. sp. *cubense*

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Banana,  
Panama disease,  
Plant extracts,  
*Fusarium oxysporum* f. sp. *cubense*,  
Antifungal.

## ABSTRACT

Panama wilt stands first among all the major fungal diseases affecting banana, by which farmers are facing huge economic losses globally, which is caused by one of the deadly fungus, *Fusarium oxysporum* formal species *cubense* (Foc). *Nanjangud rasabale*, which has been given indication tag, is devastated by this fusarium wilt. In the present study, we investigated the *in vitro* biological control of Foc using some locally available medicinal plants such as *Prasopis juliflora*, *Piper kellei*, *Garcinia indica*, *Cordia alliodora*, *Acadirachia indica*, *Decalepis hamiltonii*, and *Combretum indicum*. Soxhlet extraction of selected plants was done using methanol and antifungal activity was determined by poisoned food technique, agar well diffusion, and disk diffusion method. All the botanicals employed in the study reduced the mycelial growth of fungus in different concentrations at various levels. Among them, *G. indica* exhibited highest rank of antifungal activity against the tested plant pathogen Foc. Thereafter by *P. kellei*. Results revealed that *G. indica* is a potential source of antifungal botanicals; therefore, substantial research is required to take out their active phytochemicals, thus providing a replacement to chemical fungicides and a possible alternative approach to contemporary management practices for Panama wilt of banana.

## 1. INTRODUCTION

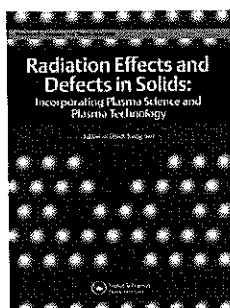
Among the different production risks affecting Banana farming, *Fusarium* wilt is considered as the most important disease globally, particularly in the tropical and subtropical regions [1, 2]. This disease is caused by *Fusarium oxysporum* f. sp. *cubense* (Foc). It was first noticed in Australia in 1874. The disease, now, has been reported from the most Banana growing regions [3]. In India, except Nendran and Red Banana, the disease is causing extensive damage in entire Banana cultivation areas particularly affecting nearly all commercial varieties [2, 4].

Karnataka is well known for the production of prime quality Bananas specially "Nanjangud rasabale" (NRB) which has its origin from a place called "Nanjangud" in the Mysuru district. Due to its high nutritional content, good fibrous texture, excellent taste, color, and aroma, NRB is most popular and pricey fruit in Karnataka and also

in other states. However, the Banana wilt is a big limitation for the profitable production of this elite variety [5].

Foc is a soil-residing filamentous fungus that mainly produces asexual reproductive structures called chlamydospores, micro and macroconidia which are produced on branched or unbranched monophthalides [Figure 1]. This enables the fungus to survive for additional 30 years in the soil, even without related host [6].

Through the roots, fungus infects Banana plants and enters xylem (vascular tissue). Then, it blocks the transportation of water and minerals causing certain visible external symptoms such as progressive wilting, gradual yellowing of leaves which spread from outer leaf margins and extend to the middle and from older leaves to younger parts and finally collapsing at the petiole region and splitting of outer leaf tissues takes place longitudinally in the pseudostem of Banana plant [7, 8]. The disease shows internal symptoms such as quiescent discoloration ranging from light yellow to dark brown color. It affects vascular tissue



## Radiation Effects and Defects in Solids Incorporating Plasma Science and Plasma Technology

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# The influence of radiation on the electrical characteristics of MOSFET and its revival by different annealing techniques

N. Pushpa & A. P. Gnana Prakash

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# Consumer perception towards electric two wheeler vehicles in Southern Karnataka

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**Abstract** - Growing population in developing countries, around the globe facing the “energy challenge” especially in context to fuel. This laid a new foundation for the raise of certain incredible technologies which has now been offering significant opportunities to kick start the phase of the automobile business. India owns 17.69 percent of the global population and reserves huge market potential for automobile manufacturers around the world. Being the majority market providers, it is a major concern to evaluate the consumer’s acceptability towards electrified vehicles. Our present research investigation aims towards evaluating the consumer’s satisfaction towards acceptance of electrified vehicles and the barriers within in context to their selection, economical affordability, acceptance, societal status, brand loyalty, and so on. This study amid to evaluate the consumer’s opinion around the selected districts of Karnataka. The outcome of this present investigation is through the limelight on understanding the willingness and dissatisfaction in consumers to develop the business and consumer’s friendly policies in encouraging the public participation in transforming the carbon-emitting INDIA to zero-emission INDIA.

**Keywords:** EV Electrical vehicle ;IEA, International energy agency

## I. INTRODUCTION

Reliance of country’s development and economic health on the infrastructure is inevitable of any country. Designing and development of sustainable technology which ease the travel between the two destinations has always offers new boost to the economy. In the late eighties for the journey of 3366.7 kilometers between the east and west coast of USA it took six months using road transportation system. this founds astonished, to cover the same distance within six days toady [1], thanks for innovation. India stands on global standers in context to the land and road development [2], this led to increased connectivity between the urban, suburban and metropolitan cities in India [3] [4][5] thus, on the transportation especially on persona-l vehicles. In addition, the covid 19 pandemic increased the concern on the personnel safety that intensifies the interest of global population on personnel vehicles than ever before.[6] IEA (International Energy Agency) statistics, over 1 million electric vehicles were sold in 2017, representing a 54 percent increase over 2016. Furthermore, after exceeding 1 million in 2015 and 2 million in 2016, the global stock of electric vehicles in 2017 exceeded 300 million, representing a 56 percent growth from 2016, Figure 1 [7]. The challenge entails increasing global ownership of electric vehicles, developing related battery production technology and material requirements, deploying electric vehicle charging stations, energy and fuel conservation, greenhouse gas

emissions reduction, and other measures that are beneficial to sustainability.

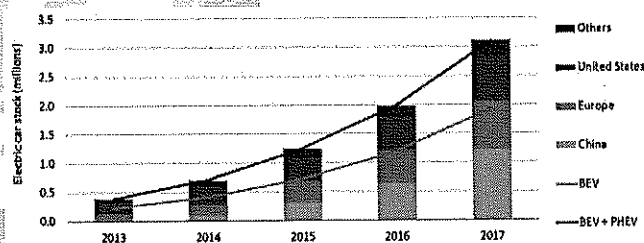


Figure:1. Evolution of global electric vehicle stock, 2013–2017 (IEA, 2018).

In light of this, more governments are setting development targets for electric vehicles, delivering clearer signals to vehicle manufacturers and other stakeholders and boosting their confidence in the future policy framework. In addition, as shown in Figure 2 [8], several nations have stated plans to ban internal combustion engine vehicles, which is a significant step forward in the development of electric vehicles.

Country	2025	2030	2032	2040	2045
France				●	
Ireland		●			
Netherlands		●			
Norway	●				
Slovenia		●			
Sri Lanka				●	
Sweden					●
Scotland			●		
United Kingdom				●	

● ICE sales ban or 100% ZEV sales target    ● Fleet without ICEs

Figure:2. Announced sales bans for internal combustion engine (ICE) vehicles (Source: [7]).





# **A CONCEPTUAL STUDY ON QUALITY OF WORK-LIFE AND IT'S DIMENSIONS**

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## **ABSTRACT:**

This study serves as an introduction and provides the necessary theoretical framework for developing perspectives on the subject. quality of work life is a relatively new concept that is defined as the overall quality of an individual's working life quality of work-life includes factors such as income, health, social relationships, and other factors such as happiness and fulfillment. Quality of work life is the main subject of the present study, meaning the definition and scope of work-life quality have been discussed in this study.

**Keywords: Quality of Work-life, Health, Social relationship, Employee satisfaction.**

## **1 INTRODUCTION**

Ever since the concept of Quality of Working Life (QWL) was first used over 30 years ago, ranges of definitions and theoretical constructions have succeeded, mitigating the many problems facing this concept (Martel and Dupuis, 2006).

QWL has several interpretations, passing from the focus of medical diagnoses to the requirement of building structural elements for the development of productive activity. Although it is a concern of very remote humans and the idea was always geared to facilitate or bring satisfaction and well-being to the employees in the execution of their tasks.

## Subclasses of Analytic Functions Associated with $q$ -Derivative

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**Abstract:** In this paper, we define the classes  $\mathcal{T}_q(A, B, \lambda)$  and  $\mathcal{C}_q(A, B, \lambda)$  using Janowski class and  $q$ -derivative also we study coefficient estimates, extreme points and many more properties.

**Key Words:** Janowski class, extreme points, convex linear combination,  $q$ -derivative.

**AMS(2010):** 30C45.

### §1. Introduction

Let  $\mathcal{A}$  denote the family of analytic functions defined in the open unit disc

$$\mathcal{U} = \{z : |z| < 1\},$$

which are of the form

$$f(z) = z + \sum_{n=2}^{\infty} a_n z^n. \quad (1.1)$$

Let  $\mathcal{T}$  denote the subclass of  $\mathcal{A}$  in  $\mathcal{U}$ , consisting of analytic functions whose non-zero coefficients from the second term onwards are negative. That is, an analytic function  $f \in \mathcal{T}$  if it has a Taylor expansion of the form

$$f(z) = z - \sum_{n=2}^{\infty} |a_n| z^n \quad (1.2)$$

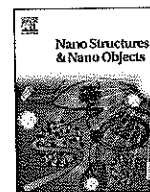
which are univalent in the open unit disc  $\mathcal{U}$ .

The  $q$ -shifted factorial is defined for  $\alpha, q \in \mathbb{C}$  as a product of  $n$  factors by

$$(\alpha, q)_n = \begin{cases} 1, & n=0; \\ (1-\alpha)(1-\alpha q) \cdots (1-\alpha q^{n-1}), & n \in \mathbb{N}, \end{cases} \quad (1.3)$$

---

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# Facile combustion derived synthesis of copper oxide nanoparticles: Application towards photocatalytic, electrochemical and DNA cleavage studies

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DNA cleavage studies

## ABSTRACT

Due of the enormous number of textile businesses, environmental contamination from dyes has been steadily expanding, posing a threat to living systems. One of the most effective methods for removing organic dyes from wastewater is photocatalytic degradation (PCD). In this regard, the major difficulty is to create photocatalytic nanoparticles that can destroy organic dyes in a simple and cost-effective manner. Methylene blue, a carcinogenic dye, is used in this study because it introduces highly poisonous organisms into the ecosystem and causes serious health issues, such as cancer, skin and kidney disorders, and so on. Copper oxide nanoparticles (NPs) were synthesized using a simple, low-cost and quick combustion technique at 500 °C for 15 min using low-cost, readily accessible sucrose as a fuel. X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), Raman spectroscopy, scanning electron microscopy (SEM), high-resolution transmission electron microscopy (HR-TEM), UV-Vis spectroscopy and photoluminescence spectroscopy have all been used to analyse the obtained CuO NPs. The XRD pattern shows the CuO NPs exhibit a monoclinic crystal structure. The presence of a Cu-O stretching bond can be noticed in the FT-IR spectrum at around 422 cm<sup>-1</sup>. Electrochemical measurement of dopamine (DA) revealed a good sensing activity with a detection limit of 9 μM in acidic media. UV-Visible, fluorescence spectroscopy was used to investigate the binding of the nanoparticles with DNA. A strong intercalating interaction of CT-DNA with the CuO NPs was investigated. After binding to DNA, the CuO NPs induce several changes in the DNA conformation. It demonstrates that the CuO NPs cleave the harmful organism's genome, preventing it from proliferating. The presented green approach provides a novel and new door for environmental, industrial and biomedical applications.

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## 1. Introduction

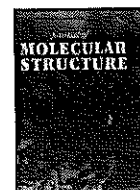
Metal oxide NPs have secured huge enthusiasm for different fields, for example, photocatalysis, sensors, microelectronics, biological activities, etc. [1,2]. These particles are found to have points of interest emerging because of their reduced size, huge surface area, electrical conductivity, chemical and optical properties [3]. CuO NPs have sparked researchers' interest in a variety of areas due to their wide applications, for example, solar cells [4], biodiesel [5], photocatalysis [6], expulsion of polluted water [7], super capacitors, electrocatalysis [8] and so on., because of their alluring properties, like minimal effort, nontoxicity and simple structures.

For many years, scientists have been interested in using light energy to remove hazardous contaminants [9]. Toxic waste has been removed by numerous initiatives. Polluted water has a number of long-term repercussions on the environment; the majority of contaminants are non-biodegradable and hazardous to humans and marine ecology [10,11]. Many methods exist for reducing contaminants, including biodegradation, ion exchange, chemical precipitation, enhanced oxidation and photocatalysis [12]. Researchers are particularly interested in preparing transition metal oxide NPs because of their crystal forms, diverse oxidation states, magnetic properties, low cost and ecologically benign nature [13–15]. Transition metal oxides have exhibited excellent catalytic properties in oxidative processes due to the high mobility of oxygen ions at the materials' surface, making them good candidates for sensor development [16–18].

DNA is a biomolecule with unique molecular recognition, mechanical rigidity and physicochemical stability, as well as the

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# Persistent prevalence of non-covalent interaction in pyrimidine containing sulfonamide derivative: A quantum computational analysis

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## ABSTRACT

A novel pyrimidine containing sulfonamide derivative has been synthesized and characterized by spectroscopic techniques like FT-IR, NMR and Mass. Single crystal X-ray diffraction study revealed that the title molecule is crystallized in the triclinic crystal system with the *P*-1 space group. Structural investigation inferred that the crystal packing is mainly stabilized by N–H...O and C–H...O intermolecular interactions, also by weak C–H... $\pi$  and C–X... $\pi$  [X=Br, Cl] interactions. Further, Hirshfeld surface analysis was employed to explore the noncovalent interactions which are responsible for the crystal packing quantitatively. In addition, quantum chemical calculations have been performed to validate the non-covalent interactions present in the title molecule. The molecular geometry of the compound is optimized at the DFT/WB97XD/6-311G(d,p) level of theory. The NBO analysis was carried out to know the intramolecular charge transfer in the molecule. Finally, the thermodynamic properties of the title compound have been calculated at different temperatures.

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## 1. Introduction

In recent years, the non-covalent interactions (NCIs) have been the focus of intense investigation in chemistry due to their key role in several fields of science and technology, such as biology, nanotechnology, or materials chemistry [1]. NCIs are key components in the dynamics of life; examples can be including the functioning of DNA and proteins, the mechanisms of medications structure, and properties of chemical structure [2,3]. Designing new solid-state materials with desirable features, such as effective biological activity, is gaining more interest. The primary factors that determine the bioactivity of active chemical substances are solubility, stability, and bioavailability. Crystal engineering is the study of how non-covalent interactions can be used to create new crystalline networks with desired physicochemical properties of chemical compounds [4–6]. Physicochemical properties such as pharma-

logical activity are induced by the molecular crystal structures of different polymorphs with varying arrangements [7].

The wide variety of applications of pyrimidine derivatives make them one of the important heterocyclic compounds [8]. The pyrimidine derivatives are also have been found to exhibit a wide range of pharmacological activities, such as anti-bacterial [9], anti-inflammatory [10], anti-cancer [11]. The study of their geometry, physical and electronic properties has become an interesting field in the research of drug design. Sulfonamides have great synthetic and medicinal importance because of their ability to act as precursors for the synthesis of a variety of biologically important heterocyclic compounds and also inhibits the growth of bacteria due to presence of NH and SO<sub>2</sub> group of sulfonamides [12]. Substituted pyrimidines are already well established as key cores in medicinal chemistry, along with that the sulfonamides have lot of biological significance [13]. Synthesis of sulfa drugs required harsh reaction conditions, hazardous and polluting chlorinating agents or oxidants [14]. To overcome these problems, a lead-free catalyzed reaction has been evolved to treat many infectious diseases. Many sulfonamides derivatives show an excellent non-linear optical (NLO) property [15]. Multifunctional ligands with O-, N-, and

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# **Application of Artificial Intelligence in the payment system at shopping malls in Mysore city**

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## **Abstract:**

Globally few billions of people visit malls and shopping centers every month. This reflects not just the integral place that malls hold in retail landscape, but also massive potential of data driven insights waiting to be harnessed. Consumers want to purchase in the shopping malls where they can get all the items under one roof. The major time consuming part is waiting for the bill generation and making payment around 30 minutes. In the modern world, waiting in a line identified as biggest emerging issues. This paper is focusing the impact of artificial intelligence and its use in minimizing the queue system for their payment system. Malls can use big data, machine learning and artificial intelligence to derive meaningful insights to minimize operational cost, build better customer engagement, explore new avenues for revenue, enable tenants to boost productivity and more.

**Key words:** Artificial Intelligence, payment, customers, shopping malls

## **Introduction:**


The Artificial Intelligence system is a technology of computer software that allows human being to expand their business with information technology. It is a process that imitates the action of humans interacting within a digital system to perform a business process. The Artificial Intelligence system involves Robotic Process Automation (RPA) to collect, classify, analyze & report to management for better control & operations.

Artificial Intelligence (AI) is intelligence demonstrated by machines, as opposed to natural intelligence displayed by animals including humans. Leading AI textbooks define the field as the study of "intelligent agents": any system that perceives its environment and takes actions that maximize its chance of achieving its goals. Some popular accounts use the term "artificial intelligence" to describe machines that imitate "cognitive" functions that humans associate with the human mind, such as "learning" and "problem solving".

AI applications include advanced web search engines (e.g., Google), recommendation systems (used by YouTube, Amazon and Netflix), understanding human speech (such as Siri and Alexa), self-driving cars (e.g., Tesla), automated decision-making and competing at the highest level in strategic game systems (such as chess and Go). As machines become increasingly capable, tasks considered to require "intelligence" are often removed from the definition of AI, a phenomenon known as the AI effect. For



# Green and facile synthesis of zinc oxide nanoparticles for enhanced photocatalytic organic pollutant degradation

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## ABSTRACT

ZnO nanoparticles show great potential for photodegradation applications due to their excellent physical and chemical properties. Finding a greener approach to producing nanoparticles is of the utmost importance for multidimensional application purposes. In the present study, the ZnO nanoparticles were synthesized by a simple combustion method at 400 °C, using jackfruit extract. X-ray diffraction (XRD) pattern revealed a crystalline structure of the nanoparticles. Scanning electron microscope (SEM), Raman spectroscopy, BET surface area were used to further characterize the synthesized nanoparticles. Further, it has been used as a photocatalyst for the degradation of one of the organic pollutant methylene blue dye. In general, the method employed here is a greener approach to synthesize ZnO nanoparticles with good photocatalytic activity.

## 1 Introduction

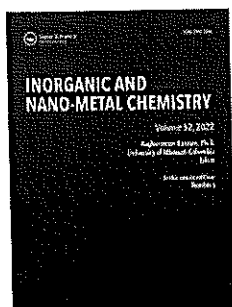
Starting from the development of TiO<sub>2</sub> by Fujishima and Honda in the year 1972 [1] has gradually been increasing in the application of nanomaterials for environmental cleanup. In the present advanced science and engineering fields, nanotechnology is one of the dynamic fields. Nanotechnology mainly deals

with the physical and chemical properties of materials having a size less than 100 nm and it mainly depends on the morphology, size distribution, and atomic and molecular combinations of the materials. Till today researchers have been synthesized modified TiO<sub>2</sub> [2], ZnO [3–5], ZrP<sub>2</sub>O<sub>7</sub> [6], ZrO<sub>2</sub> [7], SnO<sub>2</sub> [8], CuO [9], NiO [10], BiVO<sub>4</sub> [11], Bi<sub>2</sub>WO<sub>6</sub> [12], ZnFe<sub>2</sub>O<sub>4</sub> [13], BiOCl [14], Mn<sub>2</sub>V<sub>2</sub>O<sub>7</sub> [15], ZrO<sub>2</sub> [7, 16],

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## Green synthesis of bismuth tungstate nanoparticles, evaluation of their applications favouring photocatalytic and bio-sensing

S. Pramila, V. Lakshmi Ranganatha, G. Nagaraju & C. Mallikarjunaswamy

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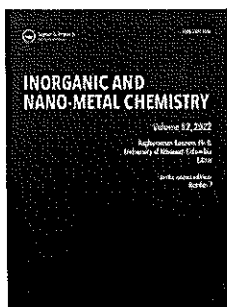
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## A review on synthesis and applications of versatile nanomaterials

G. N. Kokila, C. Mallikarjunaswamy & V. Lakshmi Ranganatha

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# Indian bael mediated eco-friendly synthesis and performance evaluation of zirconium oxide nanoparticles: An efficient anti-microbial agent

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Antimicrobial activity

## ABSTRACT

In this study, we have synthesized zirconium oxide nanoparticles by green, cost-effective solution combustion method using Indian bael extract as a fuel. The zirconium oxide nanoparticles are confirmed by spectroscopic techniques. The phase and crystalline property of the material was confirmed by powder X-ray diffraction analysis, surface morphology was checked by scanning electron microscope, and the energy dispersive X-ray spectrum confirmed the purity and elemental composition of zirconium oxide nanoparticles. Further, the zirconium oxide nanoparticles were subjected for antimicrobial activity against different bacterial strains, the biogenic zirconium oxide nanoparticles showed good activity against all tested bacterial and fungal strains. Overall, this study confirms that the biogenic zirconium oxide nanoparticles could be used as a possible antimicrobial agent.

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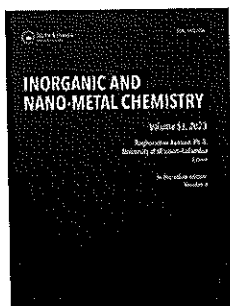
Selection and peer-review under responsibility of the scientific committee of the International Conference on Emerging Trends in Material Science and Technology – 2022.

## 1. Introduction

From the last few decades healthcare requires the largest attention due to high-cost antibiotics, this calls many researchers to find alternatives [1]. The metal oxide nanoparticles are considered to be more potent towards bacterial and fungal strains [2]. In developing countries, the infection of drug-resistant bacteria causes more threats. In India alone, about 60,000 babies died due to drug-resistant bacteria [3]. To find solutions to this problem researchers aim to synthesize metal oxides to give resistance to bacteria [4,5]. The metal oxides exhibit properties due to their unique morphology, small surface area, size, particle distribution, and other physical and chemical properties. Nanomaterials are having varied kinds of applications in the environment [6], medicine [7], energy [8], etc., in the last few years nanomaterials used in the field of disease detection [9], drug discovery [10], tumor imaging [11], cytotoxic activity [12] because conventional methods are not so effective to target diseased cells. The main advantage of nanomaterials

in the medical field is their small size, nanomaterials can easily enter into biological systems without affecting the untargeted area. Many metal oxide nanoparticles like, ZnO [13], CuO [14], NiO [15], BiVO<sub>4</sub> [16], Mn<sub>2</sub>V<sub>2</sub>O<sub>7</sub> [17], Bi<sub>2</sub>WO<sub>6</sub> [18] show significant activity due to their high-density edge surfaces. Zirconium is one of the fascinating having different properties, Zr is used as interference to immobilize radioactive isotopes [19]. ZrO<sub>2</sub> has optoelectronic, dielectric, optical, electrical, and piezoelectric properties. ZrO<sub>2</sub> has three polymorphic structures, namely monoclinic, tetragonal and cubic. ZrO<sub>2</sub> have been synthesized by many techniques like hydrothermal [20], sol-gel [21], microwave [22], and sonochemical [23], etc. all these methods are harmful because of the usage of chemical as surfactants. Here, we have synthesized ZrO<sub>2</sub> nanoparticles using an eco-friendly, simple, and cost-effective combustion method using Indian bael fruit extract as a fuel [24]. Green methods have advantages in synthesizing nanomaterials with low pressure, temperature and pH without leaving toxic materials into the environment. In this study, we have synthesized nanomaterial using fruit extract and subjected it to XRD,

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## Microwave and combustion methods: a comparative study of synthesis, characterization, and applications of NiO nanoparticles

S. Pramila, V. Lakshmi Ranganatha, G. Nagaraju & C. Mallikarjunaswamy

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## Synthesis and characterization of 4-Hydroxy benzophenone (Ph<sub>2</sub>CO)/ Polyvinyl alcohol (PVA) composites for ultraviolet (UV)-Shielding applications

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### ABSTRACT

Exposure of Ultraviolet (UV) light cause negative health effects to human and also reason for the photodegradation of organic compounds. In this framework study and development polymer based of UV shielding materials with visible transparency gains lot of attention. In the present research work, Poly (VinylAlcohol) (PVA) polymer based UV-shielding material fabricated by using 4-Hydroxy Benzophenone (Ph<sub>2</sub>CO) as UV-absorber. 4-Hydroxy Benzophenone (Ph<sub>2</sub>CO) is an organic compound were synthesized by Fries rearrangement. Subsequently, (PVA)/Ph<sub>2</sub>CO composite films were synthesized by an employing simple solvent casting technique. Optical studies revealed that PVA/Ph<sub>2</sub>CO films shows good UV-shielding competency and practically shield the whole UV region (200–400 nm). This outstanding UV shielding properties of the fabricated films arises mainly because of interaction of Ph<sub>2</sub>CO with polymer matrix. Additionally, optical constants are also calculated by using optical absorbance data. Surface properties of the fabricated films is evaluated using Scanning Electron Microscopy (SEM) and structural properties by X-ray Diffractometer (XRD). Elemental analysis is carried out using EDAX. The obtain results shows that the developed composite film have improved optical properties like short band gap with UV shielding possessions. Hence, the prepared composite films can be employed as a novel next generation transparent UV shielding materials.

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### 1. Introduction

The exposure of human body to UltraViolet (UV) radiation for prolong period can severely leads human health issues also damage some materials. UV light also has the capacity degrade organic and also trigger photodegradation of some polymer substance. In this framework, UV shielding material research has gained lot of attentions of the researchers. In particularly optical visible transparent with UV- protective polymer composites materials at low cost is the current importance of research. In UV protecting agents they are two types of UV absorbers namely organic based agents such as benzone derivatives and cinnamates and inorganic based

compounds such as Titania, silica, etc, which are efficient in scattering and reflecting UV radiations. Inorganic nanomaterials like Titaniumdioxide (TiO<sub>2</sub>), Zincoxide (ZnO), Silicondioxide (SiO<sub>2</sub>), etc, proved has good UV radiation absorbing materials [1]. But these materials have intrinsically large band gaps and their UV shielding properties is not complete. Nevertheless, these UV absorbers have many limitations like in their preparation and their discarding methods may have environmental health concerns. Additionally, these materials also suffer from aggregation and constantly evidence for photodegradation and also degrade the polymer matrices also have restrictive to use in food packaging, cosmetics and medical applications. Hernan Miguez et al synthesized ZrO<sub>2</sub>/SiO<sub>2</sub> NP based UV shielding materials. The prepared multilayers presents good shielding properties without photocatalytic activity but less transparent [2,3]. On the other perspective use organic compound as a UV-shielding materials is also gain

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Article

# Synthesis, Characterization, Hirshfeld Surface Analysis, Crystal Structure and Molecular Modeling Studies of 1-(4-(Methoxy(phenyl)methyl)-2-methylphenoxy)butan-2-one Derivative as a Novel $\alpha$ -Glucosidase Inhibitor

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**Abstract:** The crystal compound was synthesized and characterized using conventional analytical techniques. The compound  $C_{19}H_{21}O_3$  crystallizes in a monoclinic crystal system with the space group  $P2_1/c$ . The crystal structure is stabilized by C-H...O interactions. The structure is further reinforced by  $\pi$ - $\pi$  interactions. During in vitro inhibition of  $\alpha$ -glucosidase, the crystal compound exhibited a significant inhibition of the enzyme ( $IC_{50}$ :  $10.30 \pm 0.25 \mu\text{g/mL}$ ) in comparison with the control, acarbose ( $IC_{50}$ :  $12.00 \pm 0.10 \mu\text{g/mL}$ ). Molecular docking studies were carried out for the crystal compound with the  $\alpha$ -glucosidase protein model, which demonstrated that the crystal molecule has a good binding affinity ( $-10.8 \text{ kcal/mol}$ ) compared with that of acarbose ( $-8.2 \text{ kcal/mol}$ ). The molecular dynamics simulations and binding free energy calculations depicted the stability of the crystal molecule throughout the simulation period (100 ns). Further, a Hirshfeld analysis was carried out in order to understand the packing pattern and intermolecular interactions. The energy difference between the frontier molecular orbitals (FMO) was 4.95 eV.

**Keywords:** crystal structure; Hirshfeld surfaces;  $\alpha$ -glucosidase inhibition; molecular docking simulation; molecular dynamics simulations; binding free energy calculations

## 1. Introduction

Diabetes mellitus is a common chronic metabolic condition that causes high blood sugar levels due to damage to the specialized cells (islets of Langerhans) that produce insulin in the human body. Diabetic individuals either do not produce enough insulin



# Facile green synthesis of zirconium phosphate nanoparticles using *Aegle marmelos*: Antimicrobial and photodegradation studies

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## ABSTRACT

Here, we synthesized zirconium phosphate nanoparticles by a simple, cost-effective, green solution combustion method. The zirconium oxychloride and phosphoric acid were used as precursors for the synthesis of nanoparticles and *Aegle marmelos* fruit extract as a fuel. The synthesized nanoparticles are subjected to different spectroscopic techniques to confirm the structure and morphology of the nanoparticles. The crystalline property of the material was confirmed by X-ray diffraction analysis, surface morphology was checked by scanning electron microscope, and the EDS spectrum confirmed the purity and elemental composition of zirconium phosphate nanoparticles. Further, the nanoparticles were subjected for antimicrobial activity against different bacterial strains, the biogenic zirconium phosphate nanoparticles showed good activity against all tested bacterial and fungal strains and also photodegradation studies. Overall, this study confirms that the biogenic zirconium phosphate nanoparticles could be used as a possible antimicrobial agent.

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## 1. Introduction

In recent years nanomaterials research has progressed significantly due to their various surface morphologies, larger surface area, smaller size, and variable band gaps [1–3]. One of the interesting nanomaterials is zirconium phosphate, because of its enormous properties, widely used in drug delivery [4], ion exchangers [5], composites [6], catalysis, photodegradation [7], and battery applications [8], recently many researchers used zirconium phosphate nanomaterials for photodegradation of organic dyes like methylene blue, crystal violet, and indigo carmine [9]. The synthetic approach has a great impact that affects majorly surface morphology, particle size and particle distribution [10]. Zirconium phosphate has been synthesized in both crystalline and amorphous forms by various conventional methods like hydrothermal [11], microwave [12], sol-gel [13], etc., all these methods are not environment friendly, and they release many toxic materials into the atmosphere. Herein, we have synthesized zirconium phosphate

nanomaterial using a simple, cost-effective, eco-friendly solution combustion method using *Aegle marmelos* fruit extract as a fuel [14–17]. Zirconium phosphate can be obtained in four different forms, namely crystalline, amorphous, crystalline based-composites, and amorphous based-composites. The crystalline zirconium phosphate has been used among other forms, the crystalline zirconium phosphate can be synthesized by  $H_3PO_4$  and zirconium oxychloride. In the structure, Zr is in a + 4 oxidation state, and the three oxygen atoms of phosphate bind to the different Zr and one –OH will be free, these free –OH groups are responsible for the acidic property of zirconium phosphate.

## 2. Materials and methods

### 2.1. Chemicals

The chemicals used for the synthesis of zirconium oxide nanoparticles were procured from SD Fine chemical company. All the chemicals are analytical grade and used without any further purification procedure.

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## Eco-Friendly Green Synthesis, Characterizations and Antimicrobial Activities of Nickel Oxide Nanoparticles

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### Abstract

The simple solution combustion method has been used for the synthesis of NiO nanoparticles using nickel nitrate as an oxidizer, Samanea saman pod extract as a fuel at 500 °C. The crystalline nature of the nanoparticles was confirmed by X-ray diffraction studies and SEM images the information about surface morphology of the nickel oxide. The EDS spectrum confirms the composition and purity of the nanoparticles. Further, the nanoparticles are subjected for antimicrobial activity, the results revealed that NiO nanoparticles exhibit good antimicrobial properties.

**Keywords:** combustion synthesis, photodegradation, antimicrobial

### Introduction

In the field of science and technology, Nanoscience is one of the fastest growing and prominent fields. The size of the nanomaterials range from 1nm to 100 nm. Based on the surface area and morphology, nanomaterials exhibit different chemical, magnetic, mechanical, electronic, sensing, optical, properties. The nanomaterials are prepared mainly by two methods, top-down method and bottom up method. In bottom-up method we have several different methods like Microwave irradiation [1], co-precipitation method [2], thermal decomposition [3], pulse laser ablation [4], solvothermal process [5], sol-gel process [6], micro emulsion technique [7], hydrothermal [8], Chemical precipitation [9], electrode position [10], and have all been used to make nanomaterials. All these methods have one drawback that the procedure contains hazardous chemicals.

## Optical, Electrical and Thermal Behaviors of $\text{CaZnO}_2$ Nanofillers Loaded PVP–PVA Nanocomposite Thick Films

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**Abstract**—Herein, we report the successful fabrication of flexible polyvinyl pyrrolidone–polyvinyl alcohol (PVP–PVA) (50 : 50) nanocomposite (NC) thick films containing 0.0, 0.5, 1.0, 2.0 and 4.0 wt % calcium doped zinc oxide ( $\text{CaZnO}_2$ ) nanofillers by solution intercalation technique. Synthesized polymer nanocomposite (PNCs) films were characterized and their optical, electrical and thermal properties were studied. The scanning electron microscopy (SEM) supports dispersion characteristics and polymer–filler compatibilities. Thermo gravimetric analysis (TGA) and differential scanning calorimetric (DSC) studies demonstrate their thermal behaviors. Finally, the imperative optical and electrical properties of developed PNC films such as band gap,  $I$ – $V$  characteristics, DC and AC conductivity and dielectric constant were also explored and reported. Current–voltage characteristics of PVP–PVA/ $\text{CaZnO}_2$  have been performed at room temperature and the blended films show ohmic behavior. Whereas the dielectric properties (dielectric constant, dielectric loss and tangent loss) decrease with increasing frequency and increase with increasing weight percentage of the filler. It was also observed that AC conductivity also increases with the content of embedded fillers. Fabricated PNCs were used in the study of degradation of indigo carmine (IC) dye, where the 4 wt % of PNCs showed the highest degradation rate.

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### INTRODUCTION





Nanocomposites materials have great interest nowadays both in academic and industrial applications, this is due to the fact that introduction of small amount of nanofiller to polymer matrix enhances the performance of polymer [1]. This is due to the small size of nanofiller, its large surface area, quantum confinement effect and strong interfacial interactions of the added nanofiller [2]. A simple and practical method were new material with various properties is done by blending the polymers and by which novel material with superior properties is obtained [3, 4]. Hence there is a great attention nowadays for blended PNCs so that the optical, mechanical and electrical

properties are modified and used for suitable optoelectronic application [5–7]. Blending of the polymer is extensively used as the properties of the final product can be tailored to the requirement of applications, which cannot be achieved by single polymer. However, the properties of the films obtained by blending, depends on the miscibility of blend. This miscibility of the blends depends on one of the properties such as hydrogen bonding, dipole–dipole forces and charge transfer complexes [8–12]. Accordingly, blending of the polymer such as PVA, PMMA, PVC, PVP is used to design modern devices in optical and photonic applications.



Further, PVA, due to the biocompatibility, biodegradability, non-toxic nature of polymer, easy pro-





# N-[2-(5-bromo-2-chloro-pyrimidin-4-yl)thio]-4-methoxy-phenyl]-4-chlorobenzenesulfonamide: The existence of H-bond and halogen bond interactions assisted supramolecular architecture – A quantum chemical investigation

T.N. Lohith<sup>a</sup>, M.K. Hema<sup>a</sup>, C.S. Karthik<sup>b</sup>  , S Sandeep<sup>b</sup>, L Mallesha<sup>c</sup>  , P Mallu<sup>b</sup>, R.Jothi Ramalingam<sup>d</sup>, M.A. Sridhar<sup>a</sup>, Muthusamy Karnan<sup>e</sup>, N.K. Lokanath<sup>a</sup>

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## Abstract

Different types of noncovalent interactions like hydrogen bond and halogen bond are analyzed for the pyrimidine containing sulfonamide derivative. Detailed structural, noncovalent, halogen interactions present in the title compound has been investigated by the single crystal X-ray diffraction study. The compound is crystallized in the triclinic crystal system with the space group  $P\bar{1}$ . The crystal structure analysis revealed that various N-H...N, N-H...S, C-H...N, and C-H...O interactions are responsible for crystal packing. The different components are connected by a network of hydrogen bonds and halogen...halogen interactions. Also, The Hirshfeld surface analysis were done to validate the interactions quantitatively. The results obtained from *ab initio* calculations described herein reveal a major contribution from the electrostatic interaction on the stability of the systems considered. Beside the electrostatic interaction, the charge-transfer force and the second-order orbital interaction also play an important role in the formation of the title molecule, as suggested by the NBO analysis. The presence of halogen bonds in the molecule has been identified in terms of the QTAIM and NCI analyses, and several linear relationships have been established to provide more insight into halogen bonding interactions.

## Introduction





# REVIEW ON BIOLOGICAL ACTIVITY AND CORROSION STUDIES OF 1, 2, 4-TRIAZOLE DERIVATIVES

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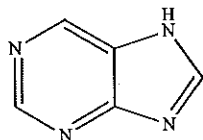
**Abstract:** The present review aims to summarize the synthesis of 1,2,4-triazole and its derivatives along with its complexes and which are characterized by some analytical techniques. These molecules are act as antifungal, antibacterial, anticancer, anticonvulsant, antituberculosis, antiviral agents etc. and also act as corrosion inhibition of metals in some acid media. Along with structure-activity relationship the molecules are compared with the reference drug. Among the molecules some of them shows better inhibition activity compared to the standard one.

**Keywords:** 1,2,4-Triazole, Characterization, Biological activity.

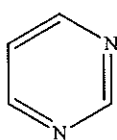
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## I. Introduction

Heterocyclic compounds are the one having cyclic structure and has at least two different elements in a ring. In organic chemistry the heterocyclic chemistry is the separate field in which the life is totally depends on it, such as purine and pyrimidine bases which are the building units of the DNA and RNA.

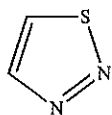


purine

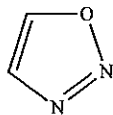


pyrimidine

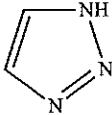
Azoles are the one of the heterocyclic compounds which contain five-membered ring and which is a compound containing sulphur, nitrogen and oxygen in the ring system. The thiadiazole, oxadiazole, triazole, imidazole, isoxazole, pyrazole etc. are the azole compounds.



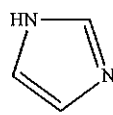
Thiadiazole



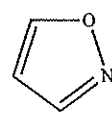
Oxadiazole



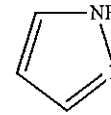
Triazole



Imidazole

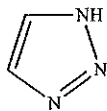


Isoxazole

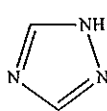


Pyrazole

In 1855 for describing the carbon-nitrogen ring system Blandin first use the name triazole. The triazole molecules are fused/single heterocyclic molecules which show the wide variety of biological spectrum (Kumari *et al.* 2021). The triazole is the nitrogen containing five-membered ring having the molecular formula  $C_2H_3N_3$  in general. It possesses aromaticity and it is an electron rich system. The 1,2,3-triazole and 1,2,4-triazole are the two sets of isomers that differ in the position of nitrogen atoms.



1,2,3-Triazole



1,2,4-Triazole



Review

**Recent Developments of Coumarin Products as Potential Anticancer Agents**

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B. Y. SathishKumar<sup>3</sup> and L. Mallesha<sup>1\*</sup>

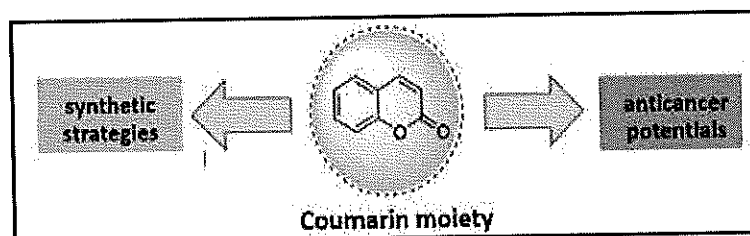
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**ABSTRACT**

*Malignant growth is a recognizable reason for death all over the planet. As of now, the insights of medications that are in clinical practice are having a high recurrence of after effect and multidrug obstruction. Analysts have endeavoured to expand a fitting anticancer medication that has no Multi Drug Resistance and secondary effects. As there is abroad spectrum of pharmacological events, the coumarin platform is a very important, fascinating study. The subordinates of coumarin are found for exercises of anticancer, as it holds the least secondary effect alongside multi-drug inversion action. Coumarin items can act by a few instruments on divergent growth cell lines relying upon replacement type of the central design of coumarin. Replacement on coumarin core prompts the analysis for more powerful mixtures. In this review, we focused on the mode of action of precisely substituted coumarin items as anticancer specialists, as well as the SAR of the most dynamic compound. Coumarin derivatives have been found to have numerous therapeutic applications including photochemotherapy, antitumor and anti-HIV therapy.*

**Graphical Abstract**



**Keywords:** Anticancer, Clinical, Pharmacological, MDR, SAR.

# Effects of gamma radiation on the electrical properties of biopolymer electrolyte

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## Abstract

Potato starch is known for its minimum ghost microstructure and enhanced conductivity. In this study, we report the effects of gamma radiation on the electrical conductivity of potato starch-based electrolytes. The electrolyte prepared was exposed to gamma radiation at different doses and time intervals. The conductivities of the samples were studied at different temperatures ranging from 313 to 383 K by using Keithley electrometer.

**Keywords:** Gamma source, Potato starch, Electrical conductivity, Keithley electrometer.

## Introduction

Irradiation of energetic radiation such as Gamma rays, electrons and ion beams on the materials certainly modify the physical, chemical and biological properties of the materials.<sup>2</sup> Compared to chemical processes, this irradiation technique is very important for the material processing technology due to its cost-effectiveness and environmentally friendly nature.<sup>3</sup>

Gamma irradiation is commonly used for cross-linking polymeric materials. Natural and synthetic polymers have been treated with ionizing radiation to modify their mechanical, structural, optical and electrical properties for various applications such as dosimetry and electrochemical, optical and electronic devices.<sup>6,7,9</sup> When polymers are exposed to high energy radiation such as gamma rays, there may be cross-linking or scission of the long polymer chains. Both processes may occur simultaneously, but usually one dominates.<sup>11</sup>

Generally, polymeric materials are insulators with very low electrical conductivity. But for device applications such as batteries, supercapacitors and solar cells, one can use electrolytes with higher conductivities. Polymeric materials' electrical conductivities can be tuned to a given purpose by adding appropriate doping elements and by irradiation.<sup>8</sup> Potato starch is completely biodegradable and of low cost among all the biopolymers.<sup>12</sup>

The electrical transport mechanism in polymeric materials is very complex and usually assumed by hopping charge carriers such as ions (cations and anions) and polarons or bipolarons.<sup>4</sup> The conductivity depends on several factors such as the concentration and type of blends added. The

effect of radiation on the conductivity of polymer composites is divided into three stages: the generation of more ionic carriers by radiation scission of organic plasticizers; carrier immobilisation by trapping at localised sites or other recombination mechanisms and finally, carrier motion under the influence of density gradients (diffusion) and existing electric fields.<sup>1</sup>

This study aims to investigate the effect of ionizing radiation on potato starch-based electrolytes for potential applications in electrochemical devices. Further its quantitative and qualitative aspects were studied in terms of their electrical properties for future applications.

## Material and Methods

Commercial potato starch was purchased from Sigma Aldrich Limited. Gel electrolytes were prepared by adding 1gm of potato starch in 10 mL of double distilled water at temperature 70° C. The solution was magnetically stirred for 1 hour at 70° C until it forms the gel and later it was allowed to cool at room temperature. For homogeneous solution, suitable amount of sodium iodide (98.5%) (NaI) and iodine (99%) (I<sub>2</sub>) were added and stirred for another 30 minutes at 70 °C. Then the clear solution of potato starch gel electrolyte was poured onto clean and levelled glass plates (20 cm X 30 cm). It was allowed to evaporate at room temperature for 4-5 days and the films were peeled off from the glass plate. The obtained films were vacuum dried thoroughly and stored in desiccators.

**Instrumentation:** The gamma irradiation for starch films was carried out using <sup>60</sup>Co gamma chamber facility available at Sri Jagadguru Chandrashekaranaatha Swamiji Institute of Technology (SJCIT), Chikkaballapura, Karnataka, India. The source strength 50 mCi of Co-60 was used. Starch films were irradiated in air by <sup>60</sup>Co source with doses ranging from 10-100 kGy, applied at a dose rate of 2 kGy/hour.

The temperature dependent dc conductivity of the biopolymer electrolyte samples was measured in the different temperature range from 313 to 383 K using Keithley Electrometer. The disk sample (around 13mm diameter) was sandwiched between the finely polished SS electrodes. Silver paste was deposited on both sides of well-polished sample pallets for good electrical contact. The change in the resistance with different temperature was noted. The dc electrical conductivity ( $\sigma_{dc}$ ) was calculated using the formula:

# $^{60}\text{Co}$ gamma and high energy ion impacts on threshold characteristics and its recovery in N-channel depletion MOSFETs

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**Abstract:** N-channel depletion MOSFETs are irradiated with 140 MeV silicon ions ( $\text{Si}^{10+}$ ) and  $^{60}\text{Co}$  gamma radiation separately from 100 krad to 100 Mrad of total dose. The current–voltage (I–V) variations in MOSFETs are characterized systematically before and after 140 MeV silicon ion and  $^{60}\text{Co}$  gamma irradiation. Threshold voltage ( $V_{\text{TH}}$ ), leakage current ( $I_{\text{L}}$ ), density of oxide trapped charges ( $\Delta N_{\text{ot}}$ ) and density of interface trapped charges ( $\Delta N_{\text{it}}$ ) are measured. The impact of  $^{60}\text{Co}$  gamma radiation on  $V_{\text{TH}}$ ,  $I_{\text{L}}$ ,  $\Delta N_{\text{it}}$  and  $\Delta N_{\text{ot}}$  of MOSFETs is found to be more when compared to 140 MeV silicon ions. Isothermal annealing studies are performed on the irradiated devices, and the recovery in  $V_{\text{TH}}$  is observed to be more in the case of 140 MeV silicon ions-irradiated MOSFETs when compared to  $^{60}\text{Co}$  gamma-irradiated MOSFETs.

**Keywords:** MOSFET; Ion impact; Leakage current; Threshold voltage; Interface trapped charge; Oxide trapped charge

## 1. Introduction

N-channel depletion metal oxide semiconductor field effect transistors (MOSFETs) are one of the building blocks used in many industries, including in IC (integrated circuits) manufacture, military, high energy radiation environment like in large hadron collider (LHC) and low energy radiation region like in space where high and low energy particles present [[1]]. These high or low energy particles strike the MOS devices and cause functional damage [[2], [3]]. The damage created in MOS devices by ionizing radiation is the result of the production of oxide trapped charges in the gate oxide ( $\text{SiO}_2$ ) and interface trapped charges at the silicon–silicon dioxide ( $\text{Si-SiO}_2$ ) interface. These trapped charges malfunction threshold voltage ( $V_{\text{TH}}$ ) and mobility of MOSFETs. Therefore, for the usage of MOS devices in space, the devices need to resist up to a few Mrad of gamma radiation dose and for high energy physics experiments like in LHCs, the MOS devices are expected to be resist up to 1 MeV equivalent  $10^{16} \text{ cm}^{-2}$  fluence of neutron over years of lifetime which is equal to few hundreds of krad of gamma equivalent total dose. Generally,  $^{60}\text{Co}$  gamma radiations are used to evaluate the radiation hardness of the semiconductor devices. The

required time to reach high doses such as 100 Mrad is explicitly high from the conventional gamma source. But using high energy ion facilities, one can reduce irradiation time period to a larger extent to create radiation impact on MOS devices. Thus, in the present work the 140 MeV silicon ions are used to study the high energy ion irradiation effects on MOSFETs and the obtained results are compared with the  $^{60}\text{Co}$  gamma irradiation results. Recently, some attempts have been made to understand the effect of high energy ions on the bipolar junction transistors (BJTs) [[4], [5]], SiGe heterojunction bipolar transistors (HBTs) [[6], [7]] and MOSFETs [[8], [9]]. The degradation in transconductance ( $g_m$ ) of the MOSFETs at room temperature for total dose has been studied extensively and is attributed to mobility degradation from increased interface traps [[10]–[12]]. A few other investigators have observed the degradation in  $V_{\text{TH}}$  at lower temperature for total dose and showed that both  $\Delta N_{\text{it}}$  and  $\Delta N_{\text{ot}}$  can modulate the resistivity and hence alter the value of  $g_m$  [[13], [14]]. The literature on the impact of high energy ions on the electrical characteristics of the MOSFETs and its recovery are very few [[8], [9]]. The systematic analysis in the functioning of the MOS devices when expose to high energy ions and its comparison with  $^{60}\text{Co}$  gamma irradiation studies is not available. Also, there is a lack of understanding on whether the high LET (linear energy transfer) ions can induce similar degradation when compared with  $^{60}\text{Co}$  gamma radiation for identical total

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## RESEARCH ARTICLE



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## On New Subclasses of Analytic Functions Involving (p,q)-Derivatives

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### Abstract

**Objective:** The objectives of the present study are to introduce some new subclasses of analytic functions involving (p,q)-derivatives by using subordination. We derive Fekete-Szegö inequalities for the functions belonging to the new subclasses. **Method:** Using the concept of (p,q)-derivative of a function and the subordination principle between analytic functions we introduce and study new subclasses. **Findings:** The Fekete-Szegö problem may be considered as one of the most important results about univalent functions. It was introduced by Fekete-Szegö in 1933. Coefficient estimates for the second and third coefficients of functions belonging to class of analytic functions with specific geometric properties were obtained. We obtain the Fekete-Szegö inequalities for functions belonging to the new subclasses. Moreover, some special cases of the established results are discussed. **Novelty:** The results of the paper are new and significantly contribute to the existing literature on the topic.

**Keywords:** Analytic functions; Subordination; q-calculus; Fekete-Szegö inequalities; (p; q)-derivative operator

### 1 Introduction

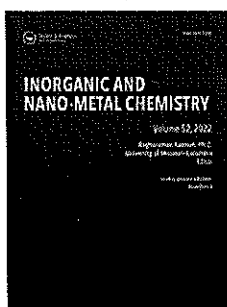
Let  $A$  specify the category of analytic functions  $f(z)$  of the form

$$f(z) = z + \sum_{n=2}^{\infty} a_n z^n \quad (1)$$

in the open unit disc  $U = \{z : z \in C \text{ and } |z| < 1\}$ .

The q-calculus is a generalization of the ordinary calculus without using the limit notation. The theory of q-derivative operators are used in describing and solving various problems in applied science such as ordinary fractional calculus, optimal control, q-difference and q-integral equations, as well as Geometric function theory of complex analysis. The first application and usage of the q-calculus was introduced by Jackson<sup>(1,2)</sup>. After that many researchers have carried out remarkable studies, which play a significant role in the development of Geometric function theory. One may refer the papers<sup>(3-11)</sup> on this subject.

Recently there is an extension of q-calculus, denoted by (p,q)-calculus. The applications of (p,q)-calculus play important role in many diverse areas of the Mathematical, Physical and Engineering sciences. Quite a number of mathematicians



## Green synthesis of Zn/Cu oxide nanoparticles by *Vernicia fordii* seed extract: their photocatalytic activity toward industrial dye degradation and their biological activity

N. A. Chamaraja, B. Mahesh & N. D. Rekha

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## FEKETE-SZEGÖ INEQUALITIES FOR CERTAIN ANALYTIC FUNCTIONS ASSOCIATED WITH $q$ DERIVATIVE OPERATOR

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### Abstract

Using the concept of  $q$  derivative operator and subordination principle we introduce and study new subclasses of analytic functions. We derive Fekete-Szegő inequalities for the functions belonging to the new subclasses. Some special cases of the established results are discussed.

### 1. Introduction

Let  $A$  represent the class of analytic functions  $f(z)$  of the form

$$f(z) = z + \sum_{k=2}^{\infty} \alpha_k z^k \quad (1)$$

in the open unit disc  $U = \{z : z \in \mathbb{C} \text{ and } |z| < 1\}$ .

The  $q$  calculus or quantum calculus is a generalization of the ordinary calculus without using the limit notation. The study of  $q$  calculus was initiated at the beginning of 19th century, it has many applications in the fields of special functions and many other areas. The  $q$  derivative operator is one of the tool used to explore many number of subclasses of analytic

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2020 Mathematics Subject Classification: 30C45.

Keywords: Analytic functions, Subordination,  $q$  derivative operator, Fekete-Szegő inequalities.

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## Partition energy of some lexicographic product of two graphs

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### Abstract

In this paper, we consider some lexicographic product of two graphs  $G$  and  $H$  of the form  $G_m(H_n)$  and determine its  $m$ -partition energy. Also, we determine the partition energy with respect to their  $m$ -complement and  $m(i)$ -complement.

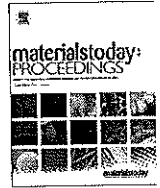
2010 AMS Subject Classification: 05C76, 05C50.

**Keywords:** lexicographic product,  $k$ -partition eigenvalues,  $k$ -partition energy, circulant matrix, block circulant matrix.

## 1 Introduction

The energy of a graph was introduced by I. Gutman [10] as the sum of absolute values of all graph eigenvalues. In connection with graph energy, eigenvalues of several matrices are studied in literature, see [12]. Recently, E. Sampathkumar and M. A. Sriraj in [16] have introduced  $L$ -matrix (also called partition matrix) of  $G = (V, E)$  of order  $n$  with respect to a partition  $P_k = \{V_1, V_2, \dots, V_k\}$  of the vertex





## Larvicidal and antimicrobial activity of zinc oxide nanoparticles synthesized from rain tree pod aqueous extract

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### ABSTRACT

In nanotechnology, green synthesis has gained more attention as an eco-friendly, sustainable protocol for the synthesis of metal oxide nanoparticles. This method reduces the generation of toxic chemicals associated with conventional synthetic methods. In this research work, we have synthesized ZnO nanoparticles by simple solution combustion method using rain tree pod extract as an efficient fuel. The obtained nanoparticles were characterized by various spectroscopic techniques like powder-XRD, SEM, EDS, and FTIR. Further, the ZnO nanoparticles were subjected to larvicidal and antibacterial properties against different fungal and bacterial strains.

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### 1. Introduction

Over the last decades, with rapid urbanization, industrialization, and globalization, the waste released by industries causes water pollution, textile industries are the major contributors, they discharge organic dyes and effluents which are highly toxic to the environment. The degradation of these wastes is a major problem in the world. Even industrial effluents contain heavy metals and suspended particles that cannot be removed easily, they persist more time in the environment. The small amount of these organic dyes causes a major threat to human health and also to the ecosystem. Conventional methods like adsorption, use of permeable membranes, filtration, and coagulation methods are used but they are not much effective.

The nanoscale metal oxide semiconductors, by their physical and chemical properties recognized in various fields from cosmetics to photodegradation to drug delivery applications. Variety of semiconductor metal oxides like Ta<sub>2</sub>O<sub>5</sub> [1], FeVO<sub>4</sub> [2], NiO [3], ZnS [4], ZrO<sub>2</sub> [5], Cu<sub>2</sub>O [6], ZnO, ZnFe<sub>2</sub>O<sub>4</sub> [7,8], BiVO<sub>4</sub> [9], Mn<sub>2</sub>V<sub>2</sub>O<sub>7</sub> [10], Bi<sub>2</sub>WO<sub>6</sub> [11] have been used to degrade wastes and effluents

released from industries. Among this ZnO is good metal oxide has good photostability and biocompatibility. ZnO is non-toxic, but they generate reactive oxygen species (ROS), hence ZnO can be used in many biological applications also. Along with the generation of ROS, sometimes it modifies membranes potential which lowers the generation of ATP thereby decrease in many metabolic activities. In other cases, ZnO nanoparticles inhibit t-RNA binding to Ribosomes. The antimicrobial activity mainly depends on the size of the nanoparticles, smaller particles dysfunctional membranes, and easily enter into the cell. The versatile ZnO nanoparticles have been synthesized by microwave [12], sol-gel [13], hydrothermal [13], combustion [7], sonication methods [14], etc., because of simplicity and cost-effectiveness combustion method widely used. Green synthesis routes are eco-friendly and less toxic synthetic methods, plants, flowers, or fruits extracts are used to prepare nanoparticles because of larger biomass and they contain phytochemicals like terpenoids, amino acids, sugars, ketones [15], etc., for bioreduction of metal salts. Therefore, these extractions are the benign source for the synthesis of metal oxide nanoparticles. Plant sources perform dual role by acting as both stabilizers and reducing agents to facilitate formation of different morphologically, surface modified nanoparticles.

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# Use of smartphone for determination of flutamide in pharmaceuticals: capture on paper approach

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## Abstract

Two simple and inexpensive colorimetric captures on paper methods using PhotoMetrix PRO<sup>®</sup> Application of smartphone for the determination of flutamide (FA), an anti-prostate cancer drug, in pharmaceuticals are presented. The analytical procedure involves the conversion of FA to a free base form of flutamide by reduction, treatment with acetylacetone to obtain a Schiff base, and use of chromatographic paper to spot and capture the colored products of various analyte concentrations. Method-A is based on univariate vector RGB analysis to measure the color intensity of the Schiff base. Method-B on the other hand performed a multivariate partial least square analysis of the same Schiff base. Both methods showed a linear correlation over the range of 3–600 µg/ml reduced FA with respect to the measured intensity. For Method-A, the reported limit of detection and quantification are 0.75 µg/ml and 2.09 µg/ml, respectively. The regression coefficients are 0.986 and 1.000, respectively, for Method-A and B. The validation of the proposed methods was done concerning linearity, accuracy, precision, sensitivity, robustness, and ruggedness according to the current guidelines of ICH. The mean recovery of FA by Method-A (97.9 ± 2.04%) and Method-B (98.9 ± 1.65%) is comparable to the reference method (100.31 ± 0.406%). The accuracy and precision of the developed methods are confirmed by the calculated *t*- and *F*-values, which do not exceed the tabulated values at a confidence level of 95%. Thus, these methods can be successfully used as routine analytical methods for the quantification of FA in quality control laboratories.

**Keywords** Flutamide · Smart phone · Capture on paper · Photometrix PRO<sup>®</sup> · Determination · Pharmaceuticals

## Introduction

Flutamide (FA) is familiar with the IUPAC name 2-Methyl-N-[4-nitro-3-(trifluoromethyl) phenyl] propanamide (Fig. 1). It is a nonsteroidal pure antiandrogen, and it is used in the treatment of prostate cancer (Budavari et al. 1989) and also polycystic ovarian syndrome (PCOS) (Eagleson et al. 2000). The active metabolite of FA, 2-hydroxy-flutamide was found to be mainly responsible for its antiandrogenic activity and acts by blocking and binding to intracellular androgen receptors in target tissues such as testis, prostate, skin, and hair

follicles (Brogden et al. 1989; Adalatkhah et al. 2015; Paradisi et al. 2011).

In addition to the official liquid chromatographic method described in the European pharmacopeia (European Pharmacopeia 2005), there are several analytical techniques such as spectrophotometry (Deepakumari et al. 2012; Basavaiah et al. 2018; Nagaraja et al. 2002a,b; Rangappa et al. 2000; Ryan et al. 2003; Dr. Rao 2015), ESI-MS coupled with Soxhlet apparatus (Khan et al. 2015), HPLC, HPLC-DAD and HPTLC (Salgado et al. 2005; Smith et al. 2009; Abdelwahab et al. 2018; Jalalizadeh et al. 2006; Tevell et al. 2006; Esmacilzadeh et al. 2016; Niopas et al. 2001), flow injection analysis (Tzanavaras et al. 2007), spectrofluorometry (Smith et al. 2008), stripping voltammetry, cyclic voltammetry, linear sweep voltammetry, differential pulse voltammetry and square-wave voltammetry (Hammam et al. 2004; Peckova et al. 2011; Afshan et al. 2020; Karthika et al. 2017; Svorc et al. 2017) and differential pulse polarography (Subba Reddy et al. 2011) have been used by researchers to quantify FA and its metabolites in pure form, in pharmaceuticals, and

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*Full Paper*

## **Fabrication and Validation of Novel Fexofenadine Sensor using Alizarin Red S as Ion Exchanger on PVC Matrix for Assay in Pharmaceuticals and Spiked Human Urine Samples**

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**Abstract-** This study depicts the plan, optimization, validation, and utilization of a novel polyvinylchloride (PVC) lattice-assisted membrane sensor to quantify fexofenadine hydrochloride (FFH) by utilizing Alizarin Red S (ARS),  $\beta$ -cyclodextrin ( $\beta$ -CD) and nitrophenyl octyl ether (NPOE) as an ion-exchanger, ionophore, and plasticizer respectively. The PVC network-assisted FFH-ARS sensor answers in <15s with super Nernstian conduct for FFH over  $2.5 \times 10^{-6}$ - $1.25 \times 10^{-3}$  mol L<sup>-1</sup> in the pH of 2.0 to 5.5 range. The regression coefficient acquired for the alignment plot is 0.9921. The determined Nernstian slope of the line is  $56.18 \pm 1.25$  mV/decade. The detection limit (LOD) is viewed as  $3.5 \times 10^{-7}$  mol L<sup>-1</sup>. Validation results clarified its appropriateness to assay FFH precisely and definitively. The sensor is a decent one for robust and rugged capability with a mean RSD of 4.39%. The outcomes of the interference study confirmed the non-interference of foreign ions while measuring the potentials. Statistical comparison of the outcomes confirms the good agreement of results of the proposed analytical procedure with the reference one. The percentage of mean recovery of FFH utilizing the proposed FFH-ARS sensor was 98.56 and 95.61% for the tablets and spiked human urine respectively, and this affirmed the selectivity of the solid-state electrode for FFH.

**Keywords-** Fexofenadine; Sensor; Alizarin Red S; Nernstian behaviour; Ionophore; Statistically agreed

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## ORIGINAL ARTICLE

# Toxicological effect of *Ricinus communis* aqueous leaf extract on the locomotor activities in *Drosophila melanogaster*

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### ABSTRACT

Plants have been used as a medicinal source since time immemorial, in both traditional and folk medicinal system as a treatment for various diseases due to the presence of various bioactive compounds of therapeutic value. In the present study, an effort has been made to investigate the various phytochemicals present in the aqueous leaf extract of *Ricinus communis* and to determine its effect on the locomotor activities in *Drosophila melanogaster* by using the dipping method. The phytochemical analysis revealed the presence of proteins, carbohydrates, phenols, tannins, saponins, flavonoids, glycosides and steroids. The results of the locomotor assay conducted on the flies that had emerged from the treated 3<sup>rd</sup> instar larvae on day 7 using the negative geotaxis test were expressed in the form of number of flies that were able to climb the 6cm mark in 6 seconds (Mean  $\pm$  SEM) and Performance Index (PI) was calculated for the same. The Mean  $\pm$  SEM obtained for 25%, 50% 75% and control were  $5 \pm 0.179399$ ,  $6.066667 \pm 0.158537$ ,  $5.033333 \pm 0.242038$  and  $5.833333 \pm 0.182621$  respectively and the performance indices obtained were 0.625, 0.758333, 0.629167 and 0.729167 respectively. Statistical analysis was done using ANOVA which revealed that the decreased locomotor activities in *Drosophila melanogaster* induced by both 25% and 75% leaf infusions were significant ( $p < 0.05$ ). This preliminary study paves the way for future studies to explain the exact mechanisms underlying the action of the extract at different concentrations.

**Keywords:** *Drosophila melanogaster*, *Ricinus communis*, locomotory deficits, aqueous leaf extract, dipping method, phytochemical analysis

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## INTRODUCTION

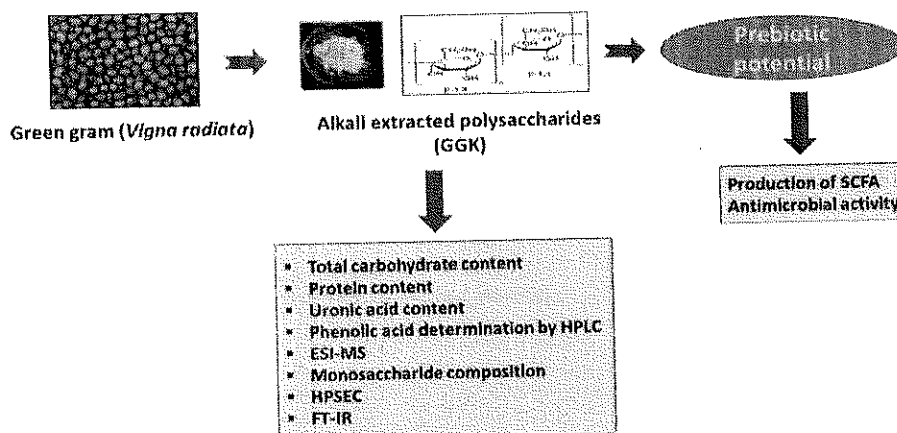
## Structural Features and Prebiotic Properties $\beta$ Glucan from Green Gram (*Vigna radiata*)

M. R. Savitha Prashanth\* and M. K. Monika

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Received: June 15, 2022, Revised and Accepted: July 16, 2022

### Graphical Abstract



### Abstract

Elucidation of structure and knowing the bioactivity of non-starch polysaccharides derived from natural products has become a significant role in the area of health and food science. Due to their wide occurrence in nature and further less toxicity they act as a nutraceutical. Extraction and composition analysis were done for both water and alkali extracted non-starch polysaccharides from Green gram. Yield (12.8%) and total sugar (91%) of GGK was higher compared to GGW. Hence in present study aimed to evaluate the structural features, prebiotic potential and antioxidant ability of only alkali (GKK) extracted non-starch polysaccharides from Green gram. The monosaccharide composition of GGK preponderantly consisted of glucose, in addition to minor amounts of arabinose and mannose indicating that the extracted polysaccharide is rich in  $\beta$ -glucans. Coumaric, caffeic, and cinnamic acids were found to be the major bound phenolic acids along with minor amount of Ferulic acid which was further confirmed by ESI-MS. The purity of GGK was substantiated by HPSEC wherein eluted as single symmetrical peak with retention times of 34.7, with ~ MW of 40kDa with reference to the dextran standards. FTIR spectra further substantiated the structural features of GGK. The radical scavenging activity was around 34 to 42% of inhibition in equivalent to Gallic acid with decrease in concentration from 100 to 1  $\mu$ g. Prebiotic potency of alkali GGK resulted in slow growth at 48 h on both the culture (OD of 0.18 and 0.23 respectively) and pH around 5.9 which slowly increased at 72 h (OD 0.34 to 0.77) and decrease in pH around 4.1. Overall comparison indicated, the utilization of GGK were more by *Lactobacillus fermentum* (156) and *Lactobacillus Mix* which showed high OD 0.558 and 0.77 respectively at 600nm. Acetate was the major SCFA produced in both the culture supernatants along with minor amount of propionate and butyrate. The culture supernatants of both lactic acid bacteria grown on GGK showed bacteriostatic activity towards *S. aureus* FRI 722 and *E. coli* MTCC 118. The result demonstrates that the extracted polysaccharides with potent prebiotic properties could be explored as food grade adjuncts towards symbiotic development.

**Keywords:** Non-starch polysaccharides; FTIR;  $\beta$ -glucan; Prebiotic property; SCFA

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