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Number of research papers per teacher in  
the Journals notified on UGC website

**Academic Year 2017 – 2018**

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## Research papers

### Academic Year 2017 – 2018

S.No.	Title of paper	Name of the author/s	Department of the teacher	Name of journal
1.	Green synthesized silver nanoparticles from <i>Garcinia imberti</i> boud and their impact on root canal pathogens and HepG2 cell lines	Selvankumar, T., Sudhakar, C	Biotechnology	RSC Advances
2.	Process optimization of biogas energy production from cow dung with alkali pre-treated coffee pulp	T. Selvankumar, C. Sudhakar, K. Selvam, M. Govarthan	Biotechnology	3 Biotech
3.	Biosynthesis of silver nanoparticles from <i>Spirulina</i> microalgae and its antibacterial activity	Govarthan M, Selvankumar T, Mythili R, Sudhakar C, Selvam K.	Biotechnology	Environmental Science and Pollution Research
4.	Isolation identification and characterization of arsenic transforming exogenous endophytic <i>Citrobacter</i> sp. RPT from roots of <i>Pteris vittata</i> .	T. Selvankumar, R. Radhika R. Mythili, P. Srinivasan, M. Govarthan,	Biotechnology	3 Biotech
5.	Cellulase enzyme: Homology modeling, binding site identification and molecular docking	K. Selvam, T. Selvankumar, C. Sudhakar, M. Govarthan	Biotechnology	Journal of Molecular Structure
6.	Molecular modeling and docking of protease from <i>Bacillus</i> sp. for the keratin degradation	K Selvam, C Sudhakar, T Selvankumar, A. Sengottaiyan, P. Srinivasan	Biotechnology	Biocatalysis and Agricultural Biotechnology
7.	Biomimetic synthesis of silver nanoparticles using flower extract of <i>Bauhinia purpurea</i> and its antibacterial activity	Sudhakar C, Selvam K Sengottaiyan A, Selvankumar T, Govarthan M	Biotechnology	Environmental Science and Pollution Research
8.	Myco-phytoremediation of arsenic- and lead-contaminated soils by <i>Helianthus annuus</i> and wood	Govarthan, M., Mythili, R., Selvankumar, T.	Biotechnology	Ecotoxicology and Environmental Safety

  
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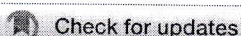
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	rot fungi, Trichoderma sp. isolated from decayed wood			
9.	Biogenic synthesis, characterization and antibacterial activity of gold nanoparticles synthesised from vegetable waste	Mythili, R., Selvankumar, T., Srinivasan, P., Sengottaiyan, A.	Biotechnology	Journal of Molecular Liquids
10.	Utilization of market vegetable waste for silver nanoparticle synthesis and its antibacterial activity	Mythili, R., Selvankumar, T., Sudhakar, C., K.Selvam, M.Govarthanan	Biotechnology	Materials Letters
11.	Ternary Copper (II) complex based chemical probes for DNA targeting: Cytotoxic activity under visible light	S. Mathankumar	Chemistry	Applied Organometallic Chemistry
12.	Role of chromium in tungsten oxide (WO <sub>3</sub> ) by microwave irradiation technique for sensor applications	K. Prabakaran	Physics	Indian Journal of Physics
13.	Generating Sub wavelength pure longitudinal magnetization probe and chain using complex phase plate	K. Prabakaran	Physics	Optics Communication
14.	Generation of Ultra-Long Pure Magnetization Needle and Multiple Spots by Phase Modulated Doughnut Gaussian Beam	K. Prabakaran	Physics	Optics and Laser Technology
15.	Tight focusing properties of spirally polarized LG <sub>(1,1)</sub> * beam with High NA Parabolic mirror	K. Prabakaran	Physics	Optical and Quantum Electronics

  
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## Green synthesized silver nanoparticles from *Garcinia imberti* bourn and their impact on root canal pathogens and HepG2 cell lines

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Nanoparticle biosynthesis using the extract of medicinal plants in a non-hazardous mode has gained wide attention for various applications in nanomedicine. This study aimed to synthesize silver nanoparticles (AgNPs) using the aqueous extract of the *Garcinia imberti* and to evaluate their antibacterial and cytotoxic activities. Structural characterization of synthesized AgNPs was carried out using UV-Vis spectrophotometry, scanning electron microscopy (SEM), X-ray diffraction (XRD) and Fourier transform infrared spectroscopy (FT-IR). SEM showed the formation of particles with average sizes of 25 to 40 nm. Energy dispersive spectroscopy (EDS) was used to analyze the AgNPs within the energy range of 3–3.1 keV to detect the presence of silver. Also, the presence of the face centered solid cubic crystal structure of metallic silver was confirmed with X-ray diffraction (XRD). The functional groups of the biomolecules present in the aqueous extract of *G. imberti* and their interaction with AgNPs were identified through FT-IR analysis. The biosynthesized AgNPs exhibited antibacterial activity against root canal isolates of *Staphylococcus sciuri* S5, *Enterococcus faecalis* S9 and *Enterococcus faecium* S11. The green synthesized AgNPs showed no significant effects on HepG2 cell lines at 75  $\mu\text{g mL}^{-1}$ . Thus, the biosynthesized AgNPs are found to have potential for nano-based drug delivery in future root canal treatment applications.

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### 1. Introduction

The synthesis of nanoparticles and their therapeutic efficacy against infectious and non-infectious disease has, impressively, attracted the attention of scientists and been investigated extensively for the last two decades worldwide.<sup>1–3</sup> Synthesis of noble nanoscale materials is a multidisciplinary approach converging the fields of physics, medicine, biotechnology and chemistry.<sup>4,5</sup> Metal based nanoparticles are very attractive, in particular because of their promising applications in various sectors and cost effectiveness.<sup>6,7</sup> Among them, the biosynthesis of silver nanoparticles (AgNPs) seems to be advantageous for biomedical applications, especially in therapeutic interventions because of their characteristic physiological and biological

properties.<sup>8–10</sup> AgNPs are known to have promising biological potential including antimicrobial,<sup>11</sup> antioxidant,<sup>12</sup> anti-cancer,<sup>13,14</sup> antidiabetic,<sup>15</sup> antifungal,<sup>16,17</sup> anti-inflammatory,<sup>18</sup> antiviral,<sup>19</sup> antiangiogenesis<sup>20</sup> and antiplatelet<sup>21</sup> activities.

Silver nanoparticles emanated as potent antimicrobial compounds with enhanced efficacy against Gram-positive and Gram-negative bacteria, including drug resistant strains, and are the best suited alternatives for antibiotics that pose a menace for bacterial resistance to drugs. Generally, silver in its ionic<sup>22,23</sup> or metallic form has high antimicrobial activity through rapidly binding to a variety of negatively charged molecules (proteins, DNA and RNA) in the pathogens.<sup>24</sup> The search for eco-friendly, more promising and cost effective strategies to synthesize nanoparticles offered a better way of exploring vast biodiversity especially plants sources for greener biosynthesis of nanoparticles. The green synthesis of nanoparticles using herbal extracts has superior biological activities and proven as less toxic to human.<sup>25</sup> Plant extract based synthesis of AgNPs and its bio-potentials are well documented with *Ficussy comorus*,<sup>26</sup> *Myristica fragrans*,<sup>27</sup> *Helianthus tuberosus*,<sup>28</sup> *Tinospora cordifolia*,<sup>29</sup> *Chrysanthemum indicum* L.,<sup>30</sup> *Mimusops elengi* L.,<sup>31</sup> and *Azadirachta indica* L.<sup>32</sup> *Garcinia imberti* bourn is an endangered plant belongs to the family Clusiaceae found evergreen in the South Western Ghats, India, which has better antioxidant<sup>33</sup> as well as antimicrobial activity.<sup>34</sup> However,

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# Process optimization of biogas energy production from cow dung with alkali pre-treated coffee pulp

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K. Selvam<sup>1</sup> · V. Aroulmoji<sup>3</sup> · N. Sivakumar<sup>4</sup> · M. Govarathanan<sup>1,5</sup>

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**Abstract** Biogas production from cow dung with co-substrate agricultural waste is one of the most demanding technologies for generating energy in a sustainable approach considering eco-friendly. In the present study, coffee pulp (CP) was pre-treated with 1% NaOH and combined with various proportions of cow dung (CD) to explore its biogas producing potentiality. The optimization of the process was studied using Response surface methodology. Statistics based on 3-D plots were generated to evaluate the changes in the response surface and to understand the relationship between the biogas yield and other parameters. The highest methane production (144 mL/kg) was achieved after 90 h of incubation with 1:3 of CP and CD at 40 °C. Gas chromatography analyzes

the chemical compositions of the generated biogas and its post combustion emissions. The chemical composition of the substrates before digestion and after fermentation (biogas spent sludge) were measured in terms of fiber content and the values were noted as, total solids (0.53%), ash content (9.2%), volatile fatty acid (100 mg/L), organic carbon (46%) and a total carbohydrate (179 mg/g). The results of the optimization of biogas production presented in this work found to have significance with the process parameters. The outcome of the study has supported the fact of conventional combustion technology that has to be upgraded to prevent these hazardous emissions into the atmosphere.

**Keywords** Biogas · Coffee pulp · Cow dung · Response surface methodology · GC-MS

T. Selvankumar and C. Sudhakar equally contributed this work.

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## Introduction

Biogas production from a variety of agro-industrial wastes through anaerobic digestion is growing worldwide and is considered ideal in many ways due to its economic and environmental benefits (Grisel et al. 2014; Fantozzi and Buratti, 2011; Abbasi and Abbasi 2010; Fantozzi and Buratti 2009; Simpson-Holley et al. 2007; Pandey et al. 2000). Methane fermentation is the most efficient technology for energy generation from biomass in terms of energy output/input ratio (28.8 MJ/MJ) among all the technologies used for energy production through biological and thermo-chemical routes (Deublein and Steinhauser 2008).

Coffee is the second largest traded commodity in the world and generates large amounts of by-products and residues during processing (Grisel et al. 2014). Industrial processing of coffee cherries is performed to separate

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# Biosynthesis of silver nanoparticles from *Spirulina* microalgae and its antibacterial activity

Govarthanan Muthusamy<sup>1,2</sup> · Selvankumar Thangasamy<sup>1</sup> · Mythili Raja<sup>1</sup> ·  
Sudhakar Chinnappan<sup>1</sup> · Selvam Kandasamy<sup>1</sup>

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**Abstract** The present work focuses on a low-cost, simple, and green synthesis of silver nanoparticles (AgNPs) by mixing AgNO<sub>3</sub> solution with the extract of *Spirulina platensis* (SP) without any chemical reducing and/or capping agents. The green synthesis of AgNPs was confirmed by the color change from colorless to yellowish brown. The biosynthesis of AgNPs was further confirmed by UV-visible spectroscopy (UV-vis), Fourier transform infrared spectroscopy (FT-IR), X-ray diffraction (XRD), biological transmission electron microscopy (Bio-TEM), and energy dispersive X-ray analysis (EDX). The UV-vis spectroscopy results showed the surface plasmon resonance (SPR) of AgNPs around 450 nm. Bio-TEM analysis revealed that the Ag nanoparticles were well dispersed with average range of 5–50 nm. XRD results indicated that the green synthetic process produced face-centered cubic structure of AgNPs. FT-IR spectroscopy analysis showed that the bioactive molecules from the SP extract believed to be the responsible for the reduction of Ag ions. Furthermore, the synthesized AgNPs were evaluated against pathogens such as *Staphylococcus* sp. and *Klebsiella* sp. The AgNPs (1–4 mM) extensively reduced the growth rate of the pathogens.

**Keywords** *Spirulina* · Microalgae · Bactericidal · Silver · Green synthesis

## Introduction

Nano-biotechnology is gaining more attention due to its eco-friendly, economical, and green approach to silver nanoparticle synthesis. In recent years, researchers have been attracted by silver nanoparticles due to their unique properties in the field of medicine, science, and technology, such as antibacterial (Govarthanan et al. 2014; Sengottaiyan et al. 2016a), catheters (Roe et al. 2008), food containers (Echegoyen and Nerin 2013), and anticancer (Rajeshkumar et al. 2016). AgNPs can be prepared conventional physico-chemical methods. However, these physico-chemical methods have many disadvantages due to the difficulty of scaling up the process of synthesis, toxic, flammable chemical substances, and required specific equipment and higher costs. Several studies have reported the disadvantages of physical and chemical synthesis of AgNPs (Suman et al. 2013; Yousefzadi et al. 2014). Contemporary to these physico-chemical methods, green synthesis of AgNPs using biological materials has emerged as a simple, environmentally friendly, and cost-effective method.

The natural products involving in the synthesis of AgNPs received tremendous attention in the field of bio-nanomaterial (Gaidhani et al. 2013). Among the biological materials, microorganisms (Reddy et al. 2010; Kumar and Mamidyala 2011; Otari et al. 2012; Gaidhani et al. 2013), plants (Aravinthan et al. 2015; Sengottaiyan et al. 2016b; Senthilkumar et al. 2016), and green algae (Mahdieh et al. 2012; Sinha et al. 2015) have been reported the synthesis of AgNPs. However, the synthesis of microalgae nanoparticles with antibacterial application is less informative.

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## Isolation, identification and characterization of arsenic transforming exogenous endophytic *Citrobacter* sp. RPT from roots of *Pteris vittata*

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**Abstract** The aim of the present study was to assess the arsenic (As) transformation potential of endophytic bacteria isolated from roots of *Pteris vittata* plant. The endophytic bacterium was tested for minimal inhibitory concentration (MIC) against As. The endophytic strain RPT exhibited the highest resistance to As(V) (400 mg/l). Phylogenetic analysis of the 16S rRNA sequence suggested that strain RPT was a member of genus *Citrobacter*. The As transformation assay revealed As(III) oxidation and As(V) reduction potential of *Citrobacter* sp. RPT. The As resistance mechanism was further confirmed by amplification of *arsC* and *aoxB* genes. The growth kinetics of strain RPT was altered slightly in the presence of different concentration (100–400 mg/l) of As stress. Temperature and pH influenced the As removal rate. The maximum As removal was observed at pH 7.0 (74%) and 37 °C (70.9%). The results suggest that strain RPT can survive under the As stress and has been identified as a potential candidate for application in bioremediation of As in contaminated environments.

**Keywords** Arsenic · Transformation · Bioremediation · *Pteris vittata* · *Citrobacter*

### Introduction

Arsenic (As) contamination in environment is a major problem in all over the modern industrialized world. It has received increasing attention due to its carcinogenic impacts on human health. Mining and metallurgical activities lead to As pollution in the environment (Zhu et al. 2014). Due to negative clinical effects of As contamination to humans warrants urgent issue for mitigation and sustainable environmental management. Several physical and chemical techniques have been developed for mitigation of As pollution from soil and water (Yuan and Chiang 2007; Fu and Wang 2011). Although the physico-chemical methods have extensive removal application, the high cost solid and liquid waste generation from the remediation process causes unsustainable environment (Tiwari et al. 2016). Therefore, it is necessary to expand the remediation process to reduce its effects on ecosystem.

Bioremediation is a promising technology to remove As from contaminated soil and water, which is cost-effective and eco-friendly compared to physico-chemical methods (Govarathanan et al. 2013, 2015a). Microorganisms are primarily used in the bioremediation to degrade or detoxify the As into harmless and less toxic forms. Several microbial processes involve the removal of As in soil and water, including oxidation, reduction, adsorption and microbe-mediated electron transfer (Diesel et al. 2009; Guo et al. 2015). Generally As is toxic to microorganisms; however, several microorganisms gain the energy for rapid growth by metabolizing the As (Oremland and Stolz 2003, 2005). The As-resistant microorganisms utilize the As derivatives

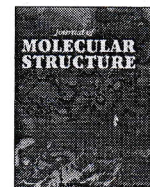
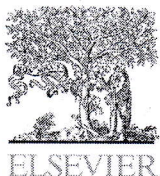
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## Cellulase enzyme: Homology modeling, binding site identification and molecular docking



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### ABSTRACT

Cellulase is an enzyme that degrades the linear polysaccharide like cellulose into glucose by breaking the  $\beta$ -1,4-glycosidic bonds. These enzymes are the third largest enzymes with a great potential towards the ethanol production and play a vital role in degrading the biomass. The production of ethanol depends upon the ability of the cellulose to utilize the wide range of substrates. In this study, the 3D structure of cellulase from *Acinetobacter* sp. was modeled by using Modeler 9v9 and validated by Ramachandran plot. The accuracy of the predicted 3D structure was checked using Ramachandran plot analysis showed that 81.1% in the favored region, compatibility of an atomic model (3D) with amino acid sequence (1D) for the model was observed as 78.21% and 49.395% for Verify 3D and ERRAT at SAVES server. As the binding efficacy with the substrate might suggests the choice of the substrate as carbon and nitrogen sources, the cellobiose, cellotetraose, cellotriose and laminaribiose were employed in the docking studies. The docking of cellobiose, cellotetraose, cellotriose and laminaribiose with cellulase exhibited the binding energy of  $-6.1523$  kJ/mol,  $-7.8759$  kJ/mol,  $-6.1590$  kJ/mol and  $-6.7185$  kJ/mol, respectively. These docking studies revealed that cellulase has the greater potential towards the cellotetraose as a substrate for the high yield of ethanol.

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### 1. Introduction

Cellulases are inducible enzymes, which can be synthesized through microorganisms during their growth on cellulosic substances. They are studied drastically because of their application in the hydrolysis of cellulose, the amplest biopolymer and the potential source of utilizable sugars, which serves as a raw material in the manufacturing of chemicals and fuel [1]. Cellulose is an unbranched glucose polymer composed of D-glucose units connected through a 1,4- $\beta$ -D glucosidic bond. It is degraded by enzymes

produced with the aid of both bacteria and fungi. As cellulose is a completely stable polymer, powerful hydrolysis of it requires the synergistic action of several enzymes, which include endo- $\beta$ -1,4-glucanases, exo- $\beta$ -1,4-glucanases (or cellobiohydrolase) and  $\beta$ -glucosidases [2–6]. The mechanism of cellulose hydrolysis by means of cellulases has been studied enormously [7].

Cellulases are used in lots of biotechnological applications, such as fiber modification in the paper and textile industries, but they also have great ability in the rising industry of ethanol production from lignocellulose. To decrease the water utilization and reduce the expenses of equipment and distillation, the hydrolysis of lignocellulose need to be conducted at an excessive concentration of solids. This approach unavoidably outcomes in excessive concentrations of the hydrolysis end-products cellobiose and glucose, and it has been proposed that the end-product inhibition of cellulases is rate limiting for lignocelluloses hydrolysis in high-solid conditions [8,9]. Thus, relieving the product inhibition becomes a

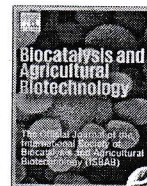
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## Molecular modeling and docking of protease from *Bacillus* sp. for the keratin degradation



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### ARTICLE INFO

#### Keywords:

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### ABSTRACT

In this present study, the 3D structure of protease from *Bacillus* sp. was modeled by using modeler 9v9. The generated structure was accessed for geometrical errors and energy stability using RAMPAGE, VERIFY 3D, ERRAT and PROSA. The proteolytic nature of this modeled protease was determined by docking studies using FlexX. The kartinolytic activity was revealed by using polysacchadire sub units such as arabinose, rhamnase, galactose, and glucose; aminopeptidase activity was revealed by using amino acids like methionine, leucine, rivastigmine and also by protease inhibitor like N-carbobenzyloxy-L-alanine and 4-amidino phenyl methane-sulfonyl fluoride. The docking studies showed that Asp160 and Try246 residues were mainly involved in binding of all the compounds and other important amino acid residues such as His85, Asp97, Glu131, Asp160, Glu131, Glu132, Asp160, Tyr246, and His247 were involved in hydrogen bonding with the substrates. These studies also determined the substrate recognition pattern and the development of suitable protease can potentially enhance its applications in keratin degradation.

### 1. Introduction

Proteases are proteolytic enzymes that catalyze the breakdown of proteins by hydrolysis of peptide bonds. Proteolytic enzymes are ubiquitous in existence, it is being found in all living organisms, and is crucial for cell growth and differentiation. In accordance with global enzyme sales of industrial enzymes, protease accounts for 60–64% and constitutes to be a largest product segment of industrial enzymes (Ch, 2007; Shankar et al., 2011; Annamalai et al., 2014; Satbir and Bijender Kumar, 2014; Selvam et al., 2016). The serine alkaline proteases are one of the most important groups of industrial enzymes. They account for approximately 35% of the total microbial enzyme sales (Bhunia et al., 2012). The proteases are highly valuable commercial enzymes as various applications in food, pharmaceutical, detergent and dairy industries (Gupta et al., 2002; Vellard, 2003; Reddy et al., 2006; Ribitscha et al., 2010; Bhunia and Dey, 2012; Bhunia et al., 2013). Several *Bacillus* sp. like *B. cereus* (Prakash et al., 2014), *Bacillus licheniformis* (Lin

et al., 2015), *Bacillus megaterium* (Asker et al., 2013), *B. stercorophilus* (Sookkheo et al., 2000), *Bacillus mojavensis* (Haddar et al., 2009), *Bacillus pumilus* (Jaouadi et al., 2008) and *B. subtilis* (Maruthiah et al., 2013) were involved in production of a wide variety of extracellular enzymes, including proteases.

The molecular docking approach can be used to model the interaction between the molecule and a protein at the atomic level, which allow us to characterize the behavior of molecules in the binding site of target proteins as well as to elucidate fundamental biochemical processes (Marrone et al., 1997; Huang and Zou, 2010; Ezat et al., 2014). An important type of molecular docking is protein-ligand docking because of its therapeutic applications in modern structure-based drug design. A disadvantage of these methods is their dependence on the molecular data sets used to perform regression analyses and fitting. Protein 3D structure is major pre-requisite for understanding the function and evolutionary relationship. Various studies have reported the potential in silicon application of homology or comparative

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# Biomimetic synthesis of silver nanoparticles using flower extract of *Bauhinia purpurea* and its antibacterial activity against clinical pathogens

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## Abstract

In the present study, we have reported an eco-friendly, rapid, and simple method for the synthesis of silver nanoparticles (AgNPs) using *Bauhinia purpurea* flower extract as non-toxic bioreducing agent. The formation of AgNPs was confirmed by UV-visible spectroscopy, transmission electron microscopy (TEM), scanning electron microscopy and energy-dispersive spectroscopy (SEM-EDS), Fourier transform infrared spectroscopy (FT-IR), and X-ray diffraction (XRD). The synthesized AgNPs were spherical in shape with an average size of 20 nm. Furthermore, the antibacterial activities of the synthesized AgNPs (2–10 mM) against clinical pathogens, *Klebsiella* sp. and *Staphylococcus* sp., were evaluated under *in vitro* conditions.

**Keywords** *Bauhinia purpurea* · Biomimetic synthesis · Silver nanoparticles · Antibacterial activity

## Introduction

In recent years, production and characterization of noble metal nanoparticles gained more attention because of their unique properties compared to other materials. Over the last decades, silver nanoparticles (AgNPs) are gaining important research due to their significant biological properties, such as antibacterial (Govarthan et al. 2014), antifungal (Lee et al. 2013), antidiabetic (Sengottaiyan et al. 2016), anti-inflammatory (Ahmad et al. 2015), and anticancer activities (He et al.

2016). Traditional methods of AgNP production such as sonochemical, electrochemical, and photochemical methods utilized some synthetic chemicals for synthesis, which results in environmental pollution. Thus, researchers have developed several environmentally friendly and cost-effective methods for the synthesis of AgNPs.

Currently, biomimetic synthesis emerged as the most promising method for the synthesis of AgNPs. Several biotic components like plant extracts (Velmurugan et al. 2015), fungi (Abdel Rahim et al. 2017), bacteria (Gopinath and Velusamy, 2013), yeast (Mateus Eugenio et al. 2016), algae (Govarthan et al. 2017), milk (Lee et al. 2013), and oilcakes (Govarthan et al. 2016) have been reported for synthesis of AgNPs. Among the biological components, the use of plant extracts for the production of AgNPs is potentially advantageous due to their low cost, viability, and scale up (Iravani, 2011; Zayed et al. 2012). Several studies prove that extracts from various plants such as *Aloe vera* (Chandran et al. 2006), *Iresine herbstii* (Dipankar and Murugan, 2012), *Pelargonium graveolens* (Shankar et al. 2003), *Prunus yedoensis* (Velmurugan et al. 2015), *Embllica officinalis* (Ramesh et al. 2015), *Abutilon indicum* (Mata et al. 2015), *Lantana camara* (Kumar et al. 2015), *Rosmarinus officinalis* (Ghaedi et al. 2015), *Azadirachta indica* (Ahmed et al. 2016), *Terminalia cuneata* (Edison et al. 2016a), *Tamarindus indica* (Edison

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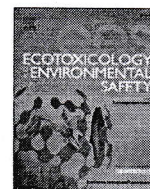
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## Myco-phytoremediation of arsenic- and lead-contaminated soils by *Helianthus annuus* and wood rot fungi, *Trichoderma* sp. isolated from decayed wood

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### ARTICLE INFO

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### ABSTRACT

In the present study, *Helianthus annuus* grown in arsenic- (As) and lead- (Pb) contaminated soil were treated with plant-growth promoting fungi *Trichoderma* sp. MG isolated from decayed wood and assessed for their phytoremediation efficiency. The isolate MG exhibited a high tolerance to As (650 mg/L) and Pb (500 mg/L), and could remove > 70% of metals in aqueous solution with an initial concentration of 100 mg/L each. In addition, the isolate MG was screened for plant-growth-promoting factors such as siderophores, 1-aminocyclopropane-1-carboxylic acid (ACC) deaminase, indole acetic acid (IAA) synthesis, and phosphate solubilisation. Phytoremediation studies indicated that treatment of *H. annuus* with the isolate MG had the maximum metal-accumulation in shoots (As; 67%, Pb; 59%). Furthermore, a significant increase in the soil extracellular enzyme-activities was observed in myco-phytoremediated soils. The activities of phosphatase (35 U/g dry soil), dehydrogenase (41 mg TPF/g soil), cellulase (37.2 mg glucose/g/2 h), urease (55.4 mg N/g soil/2 h), amylase (49.3 mg glucose/g/2 h) and invertase (45.3 mg glucose/g/2 h) significantly increased by 12%, 14%, 12%, 22%, 19% and 14% in As contaminated soil, respectively. Similarly, the activities of phosphatase (31.4 U/g dry soil), dehydrogenase (39.3 mg TPF/g soil), cellulase (37.1 mg glucose/g/2 h), urease (49.8 mg N/g soil/2 h), amylase (46.3 mg glucose/g/2 h), and invertase (42.1 mg glucose/g/2 h) significantly increased by 11%, 15%, 11%, 18%, 20% and 14% in Pb contaminated soil, respectively. Obtained results indicate that the isolate MG could be a potential strain for myco-phytoremediation of As and Pb contaminated soil.

### 1. Introduction

Metals, especially arsenic (As) and lead (Pb), accumulating in soil and/or water via various natural routes as well as anthropogenic activities (e.g., mining and smelting) exerts a significant impact on human health and other living organisms in the ecosystem (Pan et al., 2009). As and Pb are the metal elements without any known biological function and one of the most toxic heavy metals. Soil and/or water contamination with these metals are widespread and pose a substantial threat to the environment. As and Pb contaminated soils are not suitable for feed-crop cultivation and require remediation to reduce risk associated with them (Marques et al., 2013). Most physicochemical methods to remove As and Pb are expensive, inefficient, and labour-intensive (Xiao et al., 2010).

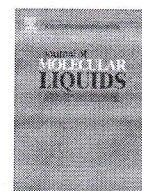
The application of biological remediation techniques, such as phytoremediation appears as an excellent cost-effective alternative, which uses metal tolerant or hyperaccumulating energy-crops. This process may become a promising alternative for renewable energy source (Mlezeck et al., 2010; Antonkiewicz et al., 2016). However, most of the plants produce very less biomass and exhibit stunted growth in metal-contaminated soils. Hence, it is important to propose effective phytoremediation strategy for heavy-metal-contaminated soils (Rajkumar et al., 2009; Weyens et al., 2009). Recently, interaction between plants, microbes, and metals has attracted much attention because of the physiological potential of microorganisms to remove metals directly from contaminated soil and the possible role of microorganisms in promoting plant-growth in metal-contaminated soils (Deng et al., 2011).

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## Short Communication

## Biogenic synthesis, characterization and antibacterial activity of gold nanoparticles synthesised from vegetable waste

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## ABSTRACT

In this study, we report the potential use of market vegetable waste for the synthesis of gold nanoparticles (AuNPs). The AuNPs were synthesised using a green method without using any harmful chemical. The AuNPs obtained from vegetable wastes were characterised by UV–vis spectroscopy, transmission electron microscopy, scanning electron microscopy energy dispersive spectroscopy, X-ray diffraction, and Fourier transform-infrared spectroscopic (FT-IR) analysis. The particles size for the green synthesised AuNPs from vegetable waste were ranged from 10 to 70 nm. The AuNPs showed significant antibacterial activity against clinical pathogens. Hence, this attempt has shown a great potential for utilizing market vegetable waste as a bio-reductant for the synthesis of AuNPs.

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## 1. Introduction

Gold nanoparticles (AuNPs) are some of the most extensively studied nanomaterial in the field of nano biotechnology. AuNPs have attracted wide attention due to their potential applications in catalysis [1], antimicrobial [2], anticancer [3], drug delivery [4], and agriculture [5]. The AuNPs can be easily synthesised and show high chemical as well as thermal stability [6]. The conventional physico-chemical methods attempted over the past several years for AuNPs synthesis are electrochemical [7], photochemical [8], sono-chemical [9] and microwave assisted processes [10]. However, all these physico-chemical methods are complex, cost-intensive, and pressure-required and use toxic chemicals that can harm the human and the eco-system [11]. Currently, the use of biological materials for the synthesis of AuNPs has become a popular alternative. In particular, plants and plant based wastes have been successfully used for the production of AuNPs. Several studies have reported on the synthesis of AuNPs using plants [12–14]. To the

best of our knowledge, the use of market vegetable waste has not been reported so far, for AuNPs synthesis.

In recent years, waste management represents an important challenge in agricultural industries and markets. It demands an integrated approach in the context of reuse for the production of value-added products. India is the largest consumer of vegetable and produces tons of vegetable wastes annually. Such estimates for the worldwide consumption of vegetable are several folds higher. The vegetable wastes were usually discarded in vegetable markets. The vegetables are mainly composed of phytochemicals and many natural polysaccharides. Thus, the use of market vegetable waste attracted for the synthesis of AuNPs.

In the present study, market vegetable wastes were used for the production of AuNPs. The synthesised AuNPs structures have been characterised by using standard spectrochemical methods. In addition, antibacterial activity of the AuNPs has also been investigated.

## 2. Materials and methods

## 2.1. Chemicals

Gold (III) chloride hydrate (HAuCl<sub>4</sub>) was purchased from Sigma-Aldrich (St Louis, MO, USA). All other chemicals were analytical grade and purchased from Hi-Media Laboratories, Mumbai, India.

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## Featured Letter

## Utilization of market vegetable waste for silver nanoparticle synthesis and its antibacterial activity



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## ABSTRACT

In the present study, silver nanoparticles (AgNPs) were synthesized using market vegetable waste extract. The formation of AgNPs was observed by a change in the reaction mixture colour from colourless to brown, after the addition of vegetable waste extract. The bioreduced AgNPs were characterized using transmission electron microscopy, scanning electron microscopy coupled with energy dispersive spectroscopy and other standard techniques. The antibacterial activity of the bioreduced AgNPs was analyzed for both Gram-negative (*Klebsiella* sp.) and Gram-positive bacteria (*Staphylococcus* sp.). The results showed that the bioreduced AgNPs effectively inhibited the growth of the tested bacterial strains. The study revealed the effective method of utilizing market green vegetable waste for the synthesis of AgNPs with high antibacterial efficiency.

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## 1. Introduction

In recent decades, synthesis of silver nanoparticles have blossomed due to their wide range of applicability in the fields of science and technology, and medicine such as catalysis, photocatalysis, chemical and biosensing, antibacterial, catheters, food containers and anticancer [1–7]. In the past decades, several physico-chemical methods have been developed for AgNPs synthesis [8]. Nevertheless, these physico-chemical methods are either costly or involving the use of potential hazardous chemicals that can harm the human and the eco-system [9]. In order to protect the environment from the hazardous chemical pollution, a biosynthesis is proposed as a simple, sustainable alternative, environment friendly and cost-effective method.

Plant extracts derived from various species are regarded as a highly desirable system for nanoparticle synthesis due to their tremendous capability to produce a wide range of phytochemicals with profound reducing potential. Several studies have reported the synthesis of AgNPs using plants [10–12]. However, utilization

of vegetable waste for the production of AgNPs has not been reported. Thus, the present study describes the green synthesis of AgNPs using vegetables waste.

## 2. Materials and methods

## 2.1. Vegetable waste collection

Vegetable waste was collected from a waste disposal yard of a vegetable market (Wednesday Market), Mallasamudram, Namakkal District, Tamil Nadu, India. The trading of vegetable in this city is approximately 2–5 tons/Wednesday. The 200–500 kg quantity of vegetable trading produces a huge amount of wastes in the form of discarded vegetables, fresh skins of vegetables, fresh/damaged leaves etc. The fresh vegetable waste was collected in plastic bags and brought to the laboratory. The vegetable waste was washed thoroughly with tap water and double distilled water until no impurity remained. The mixed vegetable waste (100 g) was separated and added to 500 mL of sterile double distilled water and crushed using mortar and pestle [13]. The extract was filtered through a Whatman No.1 filter paper and stored at 4 °C for further experiments.

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# Ternary Copper (II) complex based chemical probes for DNA targeting: Cytotoxic activity under visible light

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Among the bio-metals, copper derivatives of O, N, S donor salicylaldehyde thiosemicarbazones have been obtained large interest due to their potential biological applications. Multisubstituted thiosemicarbazone ligand HL derived, new ternary Cu (II) complexes of [Cu(L)(bpy)] (1) and [Cu(L)(phen)] (2) (where, bpy is 2,2'-bipyridine and phen is 1,10-phenanthroline) have been synthesized and characterized using different physico-chemical techniques. Complexes 1 and 2 are structurally characterized by single crystal X-ray diffraction analysis, which reveals the trigonal bipyramidal distorted square based pyramid geometry of both the complexes 1 and 2 with ONS-donor thiosemicarbazone bonded at the upper plane. The ground state electronic structures of complexes 1 and 2 have been investigated by using DFT/B3LYP theoretical evaluation with 6-31G (d,p) and LANL2DZ basis set. The affinity towards DNA and human serum albumin has been evaluated using computational docking analysis and complex 2 exposes significant binding ability towards DNA and human serum albumin, because of its immense hydrophobicity. Consequently, complex 2 have higher antimicrobial in addition to the cytotoxic activity than complex 1 and free ligand HL under visible light. Along with, their apoptosis pathway of cytotoxicity has been evaluated by fluorescent microscopic analysis using acridine orange/ethidium bromide (AO/EB) stains. From these preliminary investigations, we believe that complex 2 can play a role as a more robust pharmacological agent.

## KEYWORDS

cu (II) complexes, cytotoxic activity under visible light, docking analysis, structural analyses, thiosemicarbazone ligand



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## Role of chromium in tungsten oxide ( $\text{WO}_3$ ) by microwave irradiation technique for sensor applications

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**Abstract:** Hydrated tungsten oxide ( $\text{WO}_3 \cdot \text{H}_2\text{O}$ )-based nanoparticles were synthesized using a simple and inexpensive facile microwave irradiation process, by doping chromium (2 wt%, 3 wt%, 5 wt% and 7 wt%) at 2.45 GHz with the power of 180 W for 10 min for gas sensor application. The resultant products were annealed at 600 °C at the ambient atmosphere in order to improve the crystallinity and to remove the impurities. The products were characterized by using powder XRD which confirmed the formation of orthorhombic and monoclinic structure of both as-prepared and annealed samples, respectively. Atomic force microscope shows the role of chromium in determining the surface morphology of the resultant products at microscopic level, Fourier transform infrared spectroscopic analysis confirmed the presence of essential functional groups formed through chemical bonds of the end products, room temperature UV-VIS DRS studies showed the optical behavior of the samples through emissions and band gap energy of the respective materials. Cyclic voltammetry study confirmed the suitability of the prepared chromium-doped tungsten oxide ( $\text{WO}_3$ ) materials through electrochemical property for photocatalytic and sensor applications.

**Keywords:** Hydrated tungsten; Tungsten oxide; Nanoparticles; XRD; Electron microscopy; Spectroscopy

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### 1. Introduction

Tungsten oxide ( $\text{WO}_3$ ) is a transition metal oxide semiconductor with a widely tunable band gap, in the range of  $E_g = 2.5\text{--}2.8$  eV at room temperature. Interest was recently put on  $\text{WO}_3$  thin films and nanoparticles [1] for a wide variety of applications in microelectronics and optoelectronics [2], dye-sensitized solar cells [3], colloidal quantum dot LEDs [4], photocatalysis [5], water splitting photocatalyst as main catalyst [6] and methanol oxidation catalyst [7] due to their existence of various structural polymorphs and easily tunable oxygen content of the end product by varying the growth atmosphere. In fact, the optical and electrical properties of this compound strongly depend on

size and morphology of the corresponding end product. Accordingly, the recent scenario for many practical applications is mainly based on morphology and size distribution of the nanoparticles. This can be done by varying the synthesis procedure and growth atmosphere which influence the morphology and size distribution of the nanoparticles.

On the other hand, dopants have offered relatively better morphology and high surface to volume ratio of the nanoscale materials. The fabrication and characterization of tungsten oxide nanofibers using the electrospinning technique and sol-gel chemistry were successfully demonstrated [8]. The potential applications of the electrospun tungsten oxide nanofibers as a sensor materials exclusively for gas detection have been identified. Ultrafine tungsten and tungsten oxide powders with controllable particle size and structure had been synthesized by Xia et al. [9]. The interesting applications in various fields such

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# Generating sub wavelength pure longitudinal magnetization probe and chain using complex phase plate



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## ABSTRACT

Based on inverse Faraday Effect, the three dimensional magnetization field distribution induced by the azimuthally polarized annular multi Gaussian transmitted through a multi belt complex phase filter (MBCPF) is investigated numerically using vector diffraction theory. Numerical results shows that by properly adjusting the radii of different rings of MBCPF, one can achieve sub wavelength ( $0.286\lambda$ ) pure longitudinal magnetic probe with ultra-long focal depth of ( $35\lambda$ ). We also noticed that magnetization chain composed of eight, four and two magnetic spots of subwavelength scale is also achieved by properly modulating the radii of MBCPF. The authors expects such a pure ultra-long subwavelength magnetic probe and magnetic chain can be used to realize all optical magnetic recording (AOMR), multilayer magneto-optical data storage, ultra-compact optomagnetic devices, magnetic particle trapping and transportation, fabricating magnetic lattices for spin wave operation, as well as confocal and magnetic resonance microscopy.

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## 1. Introduction

The increasing interest in developing ultra-compact optomagnetic devices has recently invoked intensive research attention on light-induced schemes, which are capable of steering longitudinal magnetization at the sub-wavelength scale in the magnetic materials. Magneto-optical material has attracted intensive research interest due to its potential and appealing applications in all optical magnetic recording (AOMR) [1–7]. Stanciu et al. first demonstrated the all-optical magnetic recording (AOMR) by a single 40 fs circularly polarized laser pulse by the inverse Faraday Effect (IFE) [8]. To further facilitate those fascinating and practical applications, it is highly desirable to obtain a super-long and sub-wavelength longitudinal magnetization needle, as well as an extra-long and sub-wavelength longitudinal magnetization chain. Based on the vector diffraction theory and the inverse Faraday Effect (IFE) in magneto-optic (MO) film, the circularly polarized beam allows a sub-wavelength magnetic confinement in the tight focusing condition [9–13]. Since then all optical magnetic recording become a topic of much research interest and number of experimental work on

improvement in ultrafast magnetization reversal of optic-magneto materials induced by the inverse Faraday Effect was demonstrated [14–17]. Recently, it has been reported that this doughnut spot produced by the tightly focused azimuthally polarized beam can be changed into a significantly sharper focal spot when a vortical phase encoded on the azimuthally polarized beam [18,19], which shows the intriguing prospect in practical applications due to its sub-wavelength lateral spot size and purely transverse electric field [20–22]. Recently many novel methods such as using hybridly polarized beam and multi belt spiral phase plates are suggested to suppress the side lobe and to improve the focal depth of the transversely polarized focal field [23–27]. Jiang et al., calculated the light-induced magnetization of an azimuthally polarized vortex beam in a high numerical aperture (NA) objective lens [28]. They found that a sub-wavelength ( $0.508\lambda$ ) and pure longitudinal magnetization spot is generated in the focal region. Since then generating a pure magnetization focal field using the azimuthally polarized vortex beam instead of the circularly polarized beam become a topic of great interest. The light-induced magnetization produced by tight focusing of azimuthally polarized beams with helical phase has

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## Generation of ultra-long pure magnetization needle and multiple spots by phase modulated doughnut Gaussian beam



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### ABSTRACT

Based on vector diffraction theory and inverse Faraday effect (IFE), the light induced magnetization distribution of a tightly focused azimuthally polarized doughnut Gaussian beam superimposed with a helical phase and modulated by an optimized multi belt complex phase filter (MBCPF) is analysed numerically. It is noted that by adjusting the radii of different rings of the complex phase filter, one can achieve many novel magnetization focal distribution such as sub wavelength scale (0.29 $\lambda$ ) and super long (52.2 $\lambda$ ) longitudinal magnetic probe suitable for all optical magnetic recording and the formation of multiple magnetization chain with four, six and eight sub-wavelength spherical magnetization spots suitable for multiple trapping of magnetic particles are achieved.

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### 1. Introduction

The possibilities of manipulating magnetization without any applied magnetic field have attracted the growing attention of researchers during the last fifteen years. The emerging Big Data era demanding the ever increasing speed and capacity to store and process information makes magnetization switching on ultra-short time scales a fundamentally challenging topic with implications for magnetic data storage [1]. Gerrits et al. [2] demonstrate that circularly polarized femtosecond laser pulses can be used to non-thermally excite and coherently control the spin dynamics in magnets by way of the IFE. Stanciu et al. [3] first demonstrated the all-optical magnetic recording (AOMR) by a single 40 fs circularly polarized laser pulse by the IFE. Since then all optical magnetic recording become a topic of much research interest and number of experimental works on improvement in ultra-fast magnetization reversal of optic-magneto materials induced by the IFE was demonstrated [4–10]. Recently, Berritta et al. [11] introduced the first materials specific ab initio theory of the magnetization induced by circularly polarized laser light in metals and

compute the effective optomagnetic fields that corresponds to the induced magnetizations. They showed that the IFE is strongly materials and frequency dependent and demonstrated the existence of both spin and orbital induced magnetizations. Freimuth et al. [12] suggested that the ultrafast demagnetization in 3d transition metal ferromagnets is dominated by transverse spin fluctuations rather than by a reduction of the exchange splitting. In All optical Magnetic Recording (AOMR), the magnetization reversal induced by focusing a circularly polarized beam with an objective has been demonstrated to be an essential method for the longitudinal magnetization recording. Since ultra fast high density data storage demands a highly confined pure longitudinal magnetic probe of sub-wavelength scale, several methods utilizing amplitude and phase modulation to the input circularly polarized beam has been suggested for reduction of magnetization spot size and to improve the probe depth [13–16]. However generating pure longitudinal magnetization of ultra-long focal depth within a sub-diffraction limited region by the IFE has remained a challenge toward sub-wavelength AOMR. Recently, Jiang et al. [17] showed that the interaction between the polarization singularity of an azimuthally polarized beam and optical vortices in the tight focus cannot generate longitudinal electric components, which results in the generation of pure longitudinal magnetization. They

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## Tight focusing properties of spirally polarized LG<sub>(1,1)\*</sub> beam with High NA Parabolic mirror

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**Abstract** The tight focusing of double ring shaped spirally polarized beam with high NA Parabolic mirror system is analyzed numerically based on the vector diffraction theory. Calculation results show that intensity distribution in focal region can be altered considerably on changing the spiral parameter (C) and pupil to beam ratio ( $\beta$ ) of the incident double ring shaped beam. Many novel focal patterns such as focal spot, dark hollow focus and flat top profile of sub wavelength scale are achieved by proper tuning  $\beta$  and C.

**Keywords** Spirally polarized beam · High NA parabolic mirror · Vector diffraction theory · Optical trapping

### 1 Introduction

Recently, there is an increasing interest on cylindrical vector beams, mostly driven by the advances made in micro-fabrication techniques and theoretical modelling techniques that were not available with homogeneous polarization (Zhan and Leger 2002; Rao et al. 2009; Wang et al. 2013; Prabakaran et al. 2012). The Radial and azimuthal polarized beams are two special cases of cylindrical vector beam and it is observed that due to the strong longitudinal field component in the radial polarization beam focuses more sharply than the

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