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**Original Research Article** 

# Green Synthesis of Silver (Ag) Nanoparticles with Green Tea Leaf, Its Characterization, and Molecular Docking Analysis against Diabetes

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# Abstract

The Green synthesis method is proved to be one of the simplest and efficient ways for material synthesis. Silver nanoparticles were synthesized using a green synthesis method, with silver nitrate and green tea leaves as precursors. The sample is then characterized using versatile characterization techniques such as Scanning Electron Microscope (SEM), UV Spectroscopy, Raman Spectroscopy and Particle size analyser (PSA). The PSA pattern has shown that the particles are pure. The surface morphology is obtained through SEM image and it has suggested that nano particles were aggregates. The nanoparticles have shown interactions between silver and oxygen atoms supported by Raman. Molecular docking is a pivotal computational technique widely used in drug discovery to predict the preferred orientation of a ligand as it binds to a receptor's active site. This approach is fundamental to understand molecular interactions at the atomic level, thereby facilitating the design of new drugs by high affinity and specificity. The process involves simulating the interaction between molecules to determine the optimal binding configuration, using algorithms that assess the binding energy and stability of the resulting complex.

**Keywords:** Green Synthesis, Silver Nanoparticles, Material Synthesis, Silver Nitrate, Green Tea Leaf, Characterization Techniques, Molecular Docking.

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# 1. INTRODUCTION

Nanotechnology, a multidisciplinary field that operates at the atomic and molecular levels, is revolutionizing various industries and scientific disciplines. It involves designing, producing, and applying materials and devices with dimensions typically ranging from 1 to 100 nanometres. This technology uses the special physical, chemical, and biological properties that appear at the nanoscale to create new advances in medicine, electronics, energy, and environmental example, medicine. science [1-10]. For in nanotechnology has enabled the development of targeted drug delivery systems, which improve treatment efficacy and reduce side effects. In electronics, it has contributed to the creation of smaller, more efficient devices. The potential applications of nanotechnology are vast, offering opportunities to enhance material performance, energy efficiency, and environmental sustainability. As research progresses, the integration of nanotechnology into everyday products and industrial processes is expected to increase, underscoring its transformative impact on society [11-15].

At the nanoscale, typically defined as between 1 and 100 nanometers, materials often exhibit unique properties that differ significantly from their bulk counterparts. These properties can include altered electrical conductivity, chemical reactivity, strength, and optical characteristics. Nanoparticles, which are particles within this size range, possess a high surface area to volume ratio, giving them distinct physical and chemical properties [16-24].

The green synthesis of metallic nanoparticles has emerged as a promising research area in recent years. This approach has gained prominence due to its simplicity, cost-effectiveness, reduced time consumption, non-toxic by-products, environmental friendliness, and scalability for large-scale production. Unlike chemical synthesis methods, which may leave toxic chemical residues on the nanoparticle surfaces, green synthesis is considered a more reliable and economical route. This review aims to highlight the advantages of using various biomolecules as sustainable, eco-friendly components for synthesizing metal and metal oxide nanoparticles [24-35].

Green tea leaves, derived from the Camellia sinensis plant, are renowned for their health benefits, delicate flavour, and cultural importance. Unlike black tea, green tea leaves are not fermented, preserving their natural antioxidants and nutrients. Processing methods such as steaming or pan-firing produce different styles of green tea, including Sencha, Matcha, and Gyokuro, each with distinct flavour profiles. Green tea is rich in catechins, particularly epigallocatechin gallate (EGCG), which is believed to contribute to its antioxidant and potential health-promoting properties. Some reported benefits of green tea include improved brain function, fat loss, and a reduced risk of certain diseases [36-43].

# 1.1 AIM

To evaluate the characterization of silver nanoparticles (Ag NPs) synthesized using green tea leaf extract through a green synthesis method. This approach is chosen for its cost-effectiveness, non-toxicity, biocompatibility, and environmental safety. Additionally, the synthesized Ag NPs have potential applications across various industries and fields.

# 1.2 Objective

The utilize of nanoparticles in pharmaceutical, known as nanomedicine, plays a significant part in diagnosing and treating illnesses. Among different metallic nanoparticles, silver nanoparticles (Ag NPs) are especially prevalent due to their assorted physical, chemical, and organic properties, which incorporate antiviral, antifungal, anti-inflammatory, and anticancer exercises. In this consider, Ag NPs were synthesized employing a nontoxic and eco-friendly strategy. Green tea (GT) leaf extricates served as a decreasing operator, changing over silver particles into free Ag NPs. Based on these discoveries, Ag NPs inferred from GT leaf extricates can be suggested as an antimicrobial operator for treating unremitting diseases. To think about the characterization of silver nanoparticles.

- i. Scanning Electron Microscope (SEM)
- ii. Raman Spectroscopy
- iii. UV Spectroscopy
- iv. Particle Size Analyzer (PSA)

# 2. METHODOLOGY AND MATERIALS USED

**2.1.1** Extraction Procedure for Plant Extracts: Dried, Green Tea (GT) leaves (1 g) obtained in the form of leaves. Purchased from a store.

# 2.2.2 GT Extraction

Add 30 ml of water to 1 g dried ground GT leaves. Heat the mixture for 30 minutes at 50°C under magnetic stirring. Cool the mixture and filter it.

### 2.1 Green Synthesis of Ag NPs 2.2.1 Procedure

**Preparation of AgNO3 Solution**: Dissolve 0.17g AgNO3 in 10ml deionized water to form a 0.1M concentration.

**Add GT Extract**: Mix 0.2g of 20% aqueous GT extract solution into the silver nitrate solution.

# Add NaOH Solution:

Dissolve 0.4g NaOH in 10ml deionized water to form a 0.1M concentration. Add this solution dropwise to the mixture of GT extract and silver nitrate.

**Heating**: Heat the resulting solution for 30 minutes at 50°C to increase the yield of Ag NPs.

**Precipitation Process**: A dark brown or black coloured precipitate is obtained.

**Separation**: Separate the GT Ag NPs by centrifugation (6000 rpm) and wash with 50% acetone/ethanol.

**Drying**: Dry the washed precipitate at 80°C and at pressure 47.4 kPa for 16 hours in a vacuum oven.

Final Product: Ag Nano Particle is obtained [44-58].

The total prepares of green synthesis of Ag NPs by utilizing the dried leaf extricate of green tea leaf was found to be effective. The method is summarized in a stream chart (Figure 1).

# **3. MOLECULAR DOCKING**

Molecular docking is a computational strategy utilized to anticipate the interaction between a small molecule (ligand) and a macromolecule, typically a protein or nucleic acid. This method plays a crucial role in drug discovery and development, as it helps in understanding how a drug binds to its target, the strength and specificity of this interaction, and potential biological effects [100].

The process of molecular docking involves the prediction of the most favorable binding position and orientation of a ligand within the binding site of the target macromolecule. The main goal is to achieve the best fit, considering both the geometric and energetic compatibility between the ligand and the receptor [101].

Insulin is a key hormone involved in the regulation of glucose homeostasis, and its interaction with various ligands can influence its function and stability [102]. The use of silver, a metal with notable antimicrobial properties, in combination with maltose, a disaccharide, as a ligand offers potential therapeutic applications, including enhanced stability or bioavailability of insulin [103].

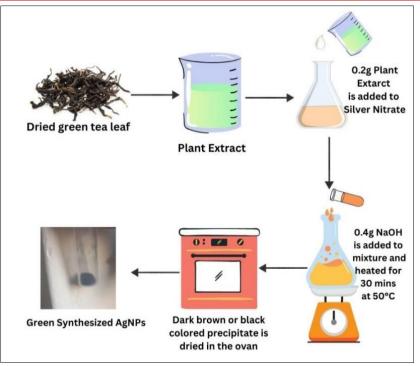


Figure 1: Summary of Green Synthesis of Ag NPs with Green tea leaf

# 3.1 Molecular Docking Process 3.1.1 Protein and Ligand Preparation Protein Preparation:

Obtain the three-dimensional structure of insulin from the Protein Data Bank (PDB I'D: - 2OMI). Prepare the protein by removing water molecules, adding hydrogen atoms, and optimizing the conformation.

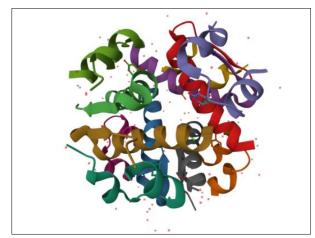


Figure 2: 3D Structure of protein (Insulin)

# **Ligand Preparation:**

Construct the ligand, silver with maltose, ensuring accurate coordination of silver ions. Optimize the ligand's geometry, paying special attention to silver's unique electronic properties.

# Silver-Maltose Ligand:

Silver-maltose complexes are of interest in various fields, including nanotechnology, biomedicine, and material science, due to their potential antimicrobial

and catalytic properties. In silicon studies involve using computational methods to predict and analyse the interactions, structure, and properties of such complexes.

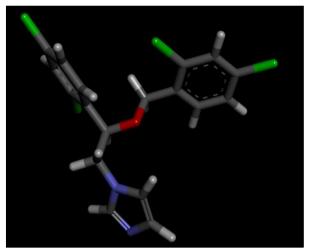


Figure 3: 3D Structure of Ligand

# **3.1.2 Docking Simulation** Software and Algorithms:

Use docking software like Auto Dock. These programs predict binding affinity and ligand orientation using scoring functions.

# **Scoring Functions:**

Evaluate binding affinity based on interactions like hydrogen bonding, hydrophobic interactions, van der Waals forces, and electrostatic interactions. Special focus on the silver ion's role in these interactions.

# **3.1.3 Analysis of Docking Results Binding Affinity and Pose:**

Report binding affinity as a docking score or binding energy. Analyse the ligand's orientation (pose) in the binding pocket to understand potential interactions. The best pose has the lowest binding energy and maximizes favourable interactions.

### **Interaction Mapping:**

Identify key residues in the binding site interacting with the ligand. Include coordination bonds with the silver ion and hydrogen bonds with maltose, among other stabilizing interactions.

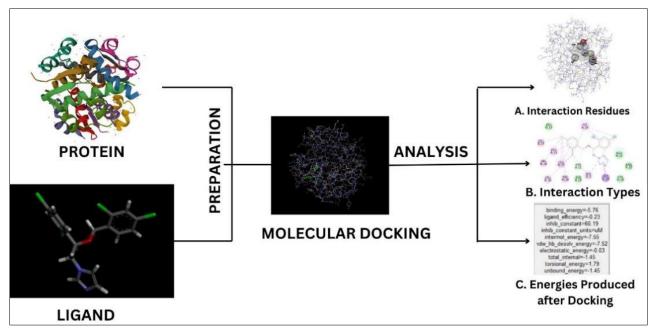


Figure 4: Summary of Molecular Docking

# 3.1.4 Silver-Maltose against Insulin

In silicon studies of silver-maltose complexes against insulin typically involve understanding the interactions between these complexes and the insulin molecule. The goal could be to explore potential applications such as drug delivery, enhancement of insulin stability, or even therapeutic interventions.

### **Molecular Docking:**

This technique helps predict the binding sites and affinity of the silver-maltose complex on the insulin molecule. It can identify potential interaction sites and the nature of these interactions (e.g., hydrogen bonding, Vander Waals forces).

### **Molecular Dynamics Simulations:**

These simulations provide insights into the stability of the silver-maltose complex when bound to insulin and any conformational changes in the insulin molecule. This can reveal how the complex might affect the structure and function of insulin.

# **Quantum Chemical Calculations:**

These calculations can elucidate the electronic properties of the silver-maltose-insulin interaction, such as charge distribution and binding energies, which are crucial for understanding the strength and nature of the interaction. Such insilico studies are crucial for predicting the feasibility and safety of using silver-maltose complexes in clinical settings, particularly in managing insulin-related conditions like diabetes. They provide a foundational understanding that can guide experimental studies and potential drug development [59-75].

# 4. RESULTS AND DISCUSSION

# 4.1 Characterization

The Characterization of Silver Nano particle is carried out Scanning Electron

Microscope (SEM), Raman Spectroscopy, UV Spectroscopy, Particle Size Analyzer (PSA) and Molecular Docking Analysis.

### 4.1.1. Sem Images

Green tea (GT) Ag NPs were observed in SEM images to contain particles of different sizes below 80 nm, with the majority of the particles falling between 58 and 74 nm and mostly distributed as aggregates. Because of the extract's capping agents, which stabilized the aggregates, the nanoparticles inside were probably not in direct contact with one another. It is well known that these phytochemicals actively stabilize and decrease metal nanoparticles [76-80].

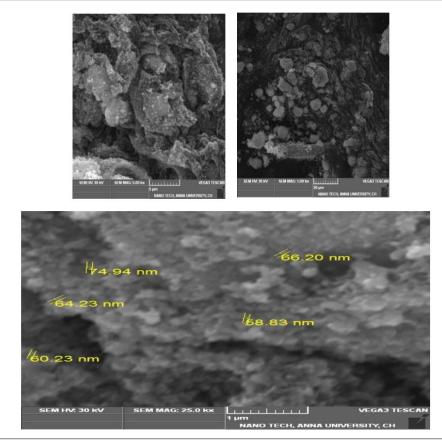


Figure 5: SEM image with nanometer particles

# 4.1.2 Particle Size Analyzer (PSA)

The average particle size of the silver nanoparticles made with green tea leaf extract is 2190

nm, according to the particle size analyzer image [81-83].

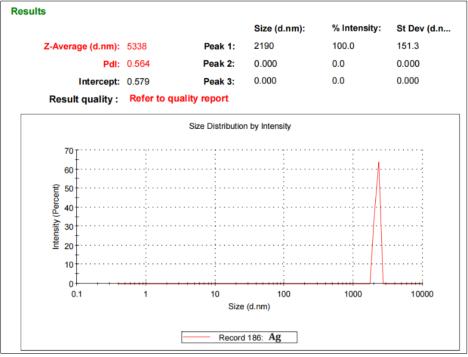


Figure 6: Graph for particale size analyzer

# 4.1.3 Raman Spectroscopy

The Ag NPs exhibit strong Raman enhancement, attributed to their rough surface. The

results indicate that the density of Ag NPs significantly affects the Raman enhancement, with the optimal concentration of sodium citrate being 0.2% [84-90].

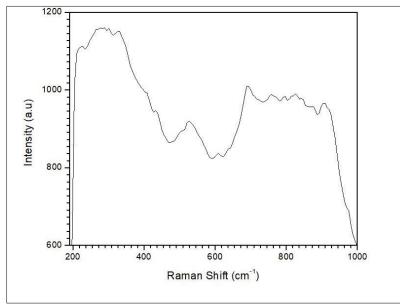


Figure 7: Graph for Raman spectroscopy

# 4.1.4 UV Spectroscopy

A popular instrument for confirming the formation of silver nanoparticles (Ag NPs) in a colloidal solution via the phenomena of surface plasmon resonance in metallic nanoparticles is the UV-vis spectrometer. The size, shape, concentration, and aggregation state of the nanoparticles all affect this optical quality. The GT Ag NP solution's UV-vis scan showed a clear Gaussian-shaped peak at 410 nm. Grand claims that the activation of surface plasmon vibrations is responsible for the characteristic 400–450 nm absorption band that corresponds to Ag NPs [91-99].

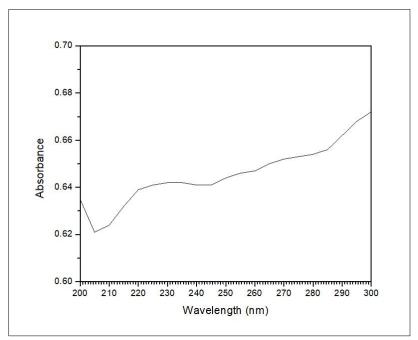


Figure 8: Graph for UV spectroscopy

## 4.2 Antidiabetic Activity by In Silico Analysis 4.2.1 Molecular Docking Analysis

The results from molecular docking can provide valuable information on how the silver-maltose ligand

affects insulin. For instance, if the ligand stabilizes insulin or enhances its bioavailability, it could have significant therapeutic implications. Additionally, understanding the specific interactions can guide the

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design of more effective insulin formulations or delivery systems [104].

The molecular docking study, conducted using Auto Dock 4.2, explored the biological interaction between the silver-maltose ligand and protein insulin. The results, illustrated in Figure 7, indicate that silvermaltose ligand bind to insulin, with the ligand showing a binding energy of less than -5.76 kcal/mol. This negative binding energy suggests a favourable interaction with the protein's binding residues, as detailed in Table 1. The docking process generated 100 poses, all of which localized to a single binding site on the insulin, indicating a high affinity of the silver atoms for these sites. According to Hevener *et al.*, a Root Mean Square Deviation (RMSD) of less than 2.0 Å is required for a docking pose to be considered valid [105]. The redocking results confirmed the reliability of the poses, with RMSD values under 1.0 Å. Interaction analysis revealed that the silver-maltose ligand can effectively interact with the GLY20 and CYS19 residues of insulin [106].

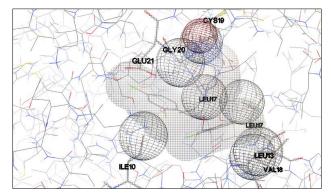


Figure 9: Interactions between silver atoms and the amino acid residues (Insulin)

Table 1. Molecular docking analysis of silver-mattese molecules				
Macromolecule	Binding energy (cal/mol)	Inhibition constant ki (mM)	Metal chelating residues	Distance (Å)
Insulin	-5.76	60.19	Ag—GLY20	2.62
			Ag—CYS19	2.54

 Table 1: Molecular docking analysis of silver-maltose molecules

The results of this study showed that the silvermaltose ligand interact with the glycine and Cysteine residue of insulin. The search algorithm evaluates and generates ligand poses at the target's binding sites by analysing several factors: final intermolecular energy, Van der Waals interaction energy, hydrogen bond energy, solvation energy, electrostatic energy, and the ligand's roto-translational and internal degrees of freedom. Given that the silver-maltose ligand has torsional energy can be disregarded. Although the binding energies for a single silver atom may appear low compared to organic ligands, so, silver-maltose ligand is drawn and interaction has been formed with protein (insulin) [107].

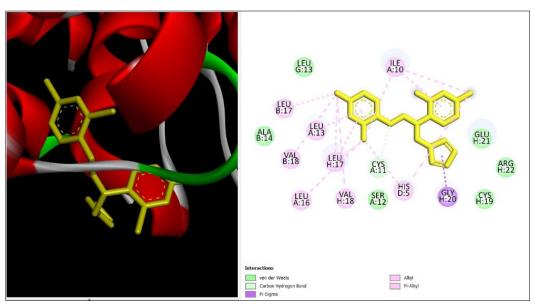


Figure 10: 2D and 3D structure of ligand and protein interaction

# 4 CONCLUSION

The synthesized silver nanoparticles were characterized using UV-vis spectroscopy, particle size analysis (PSA), Raman spectroscopy, and scanning electron microscopy (SEM). The morphology of the green tea (GT) Ag NPs appeared irregular and aggregated. Differences in the UV spectra between the GT extract and the GT Ag NPs indicated the functional groups involved in reducing Ag+ ions into nanoparticles. The silver nanoparticles were synthesized from silver nitrate and green tea leaves using a green synthesis method.

Green synthesis of Ag NPs is a more environmentally friendly, cost-effective, and efficient approach. The characterization of the nanoparticles and composites was performed using PSA, SEM, Raman spectroscopy, and UV-vis spectroscopy.

SEM images revealed that the silver nanoparticles were in the form of aggregates, with sizes in the nanometre range.

PSA confirmed the presence of silver in the particle size distribution.

UV-vis spectroscopy confirmed that the nanoparticles absorb light, indicating the presence of chemical substances.

Raman spectroscopy provided information on the chemical composition.

Molecular docking studies involving insulin and a ligand composed of silver and maltose revealed insights into the binding characteristics of the ligand, suggesting potential therapeutic applications. Future research could include molecular dynamics simulations to validate and refine these docking results, as well as in vitro experiments to confirm the computational predictions.

Based on the results, we conclude that the synthesized Ag NPs have potential applications across multiple disciplines.

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- AZO Nano Classification of Nanomaterials, the Four Main Types of Intentionally Produced Nanomaterials
- Journal of Pharmacy & BioAllied Sciences Iron Oxide Nanoparticles
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