



Role of Phytochemicals in Metal Nanoparticle Synthesis

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DOI - 10.5281/zenodo.18899179

Abstract:

Green synthesis of metal nanoparticles using plant extracts has gained wide attention due to its eco-friendly, safe, and cost-effective nature. The success of this method mainly depends on phytochemicals present in plants. These natural compounds play an important role in the reduction of metal ions, formation of nanoparticles, and their stabilization. Phytochemicals such as phenolics, flavonoids, terpenoids, alkaloids, tannins, sugars, and proteins are actively involved in nanoparticle synthesis through their functional groups. In addition to synthesis, phytochemicals also improve the biological activity and biocompatibility of nanoparticles. This review highlights the role of phytochemicals in metal nanoparticle synthesis and explains how they influence nanoparticle characteristics and biological properties. The advantages, limitations, and future scope of phytochemical-mediated nanoparticle synthesis are also briefly discussed. This review aims to provide a clear understanding of phytochemical involvement in green nanotechnology.

Keywords- Bio-Reduction, Green Synthesis, Metal Nanoparticles, Nanotechnology, Phytochemicals, Plant Extracts

Introduction:

Nanotechnology is an important area of modern science that deals with materials at the nanometer scale. In recent years, **metal and metal oxide nanoparticles** have gained wide attention because of their special physical, chemical, and biological properties. Nanoparticles such as silver, gold, zinc oxide, copper oxide, iron oxide, and cobalt nanoparticles are used in many fields including medicine, agriculture, environmental protection, food packaging, and electronics. Their small size, large surface area, and high reactivity make them very useful in antimicrobial, anticancer, antioxidant, and catalytic applications. (Upadhyay et al., 2023)

Traditionally, metal nanoparticles are produced by **physical and chemical methods** such as chemical reduction, sol-gel method, hydrothermal method, and laser techniques. Although these methods are effective, they often

require high temperature, high pressure, and toxic chemicals. Many chemical reducing agents and stabilizers used in these methods are harmful to humans and the environment. In addition, these processes are costly and generate hazardous waste. Due to these problems, there is a growing need for **safe, eco-friendly, and sustainable methods** for nanoparticle synthesis (Jagdeo, 2023).

In this context, **green synthesis of nanoparticles** has emerged as an attractive alternative. Green synthesis uses biological sources such as plants, bacteria, fungi, and algae to produce nanoparticles. Among these, **plant-based synthesis** is the most preferred because it is simple, fast, cost-effective, and does not require complicated laboratory conditions. Plant extracts contain a wide variety of natural compounds that can convert metal ions into nanoparticles. This method avoids the use of toxic chemicals and

makes the process environmentally friendly (Kanipandian et al., 2014).

The key factor behind plant-mediated nanoparticle synthesis is the presence of **phytochemicals**. Phytochemicals are natural bioactive compounds produced by plants. They include phenolics, flavonoids, terpenoids, alkaloids, tannins, saponins, proteins, amino acids, and sugars. These compounds play a major role in the **reduction, capping, and stabilization** of metal nanoparticles. During synthesis, phytochemicals donate electrons to metal ions such as Ag^+ , Au^{3+} , or Zn^{2+} , leading to their reduction into metallic nanoparticles. At the same time, these molecules bind to the surface of nanoparticles and prevent them from clumping together, thereby improving stability (Khairy et al., 2024).

In addition to their role in synthesis, phytochemicals also improve the **biological activity** of nanoparticles. When nanoparticles are capped with plant compounds, their biocompatibility increases and their interaction with biological systems becomes more effective. Many studies have shown that phytochemical-coated nanoparticles exhibit enhanced antibacterial, antioxidant, anti-inflammatory, antidiabetic, and anticancer activities. This combined effect of metal nanoparticles and plant compounds makes them highly useful in biomedical applications (Marslin et al., 2018).

Although many reports are available on green synthesis of nanoparticles, the **specific role of different phytochemicals** in the synthesis process is not always clearly explained. In many cases, the relationship between phytochemical composition and nanoparticle size, shape, stability, and biological activity is not well discussed. Therefore, there is a need to clearly understand how various classes of phytochemicals contribute to nanoparticle formation and function (Marslin et al., 2018).

The aim of this review is to provide a clear and simple overview of the **role of phytochemicals in metal nanoparticle synthesis**. This review focuses on their involvement in reduction, capping, and stabilization processes and explains how they influence nanoparticle properties and biological activities. The review also discusses advantages, limitations, and future prospects of phytochemical-mediated nanoparticle synthesis. This information will be useful for researchers working on green nanotechnology and plant-based nanoparticle synthesis.

Phytochemicals – An Overview:

Phytochemicals are natural chemical compounds produced by plants as part of their normal metabolic activities. These compounds are mainly involved in plant defense, growth regulation, and protection against environmental stress. Unlike primary metabolites such as carbohydrates, proteins, and lipids, phytochemicals are mostly **secondary metabolites** and are not directly involved in plant growth. However, they play an important role in plant survival and adaptation (Ijaz et al., 2022).

In recent years, phytochemicals have gained great importance in the field of **green nanotechnology**. Plant extracts rich in phytochemicals are widely used for the synthesis of metal nanoparticles because these compounds can act as **reducing, capping, and stabilizing agents**. The chemical structure of phytochemicals contains functional groups such as hydroxyl ($-\text{OH}$), carboxyl ($-\text{COOH}$), carbonyl ($\text{C}=\text{O}$), amine ($-\text{NH}_2$), and thiol ($-\text{SH}$). These functional groups are responsible for the conversion of metal ions into nanoparticles and for stabilizing the formed particles (Ramasubbu et al., 2023).

Phytochemicals can be broadly classified into different groups based on their chemical nature. The major classes involved in nanoparticle

synthesis include **phenolic compounds, flavonoids, terpenoids, alkaloids, tannins, saponins, proteins, amino acids, and sugars**. Each of these groups has unique chemical properties that influence the synthesis and characteristics of nanoparticles (Alhailoul et al., 2023).

Phenolic compounds are one of the most important groups of phytochemicals. They contain one or more hydroxyl groups attached to aromatic rings. These hydroxyl groups easily donate electrons and act as strong reducing agents. Phenolic compounds are commonly found in leaves, fruits, bark, and flowers of many plants and play a significant role in the reduction of metal ions during nanoparticle synthesis (Manik et al., 2022).

Flavonoids are a large subgroup of phenolic compounds and are widely distributed in plants. They possess multiple hydroxyl and carbonyl groups, which help in metal ion reduction and chelation. Flavonoids are known for their antioxidant properties, and this property supports their role in nanoparticle formation. They can also bind to the surface of nanoparticles, providing stability (Thakur & Kaur, 2025).

Terpenoids are another important class of phytochemicals derived from isoprene units. They are responsible for the aroma and flavor of many plants. Terpenoids contain functional groups such as hydroxyl and carboxyl groups, which can participate in the reduction and stabilization of metal nanoparticles. They also influence the shape and size of nanoparticles (Ali et al., 2016).

Alkaloids are nitrogen-containing compounds found in many medicinal plants. They have strong binding ability due to the presence of nitrogen atoms, which can interact with metal ions and nanoparticle surfaces. Alkaloids mainly contribute to the stabilization of nanoparticles and sometimes also take part in the reduction process (Singh et al., 2025).

Tannins are polyphenolic compounds with high molecular weight. They have multiple hydroxyl groups and show strong reducing power. Tannins can form complexes with metal ions and help in the formation and stabilization of nanoparticles. They also improve the biological activity of nanoparticles (Dwivedi et al., 2020).

Saponins are glycosides with soap-like properties. They can act as natural surfactants and help in the dispersion of nanoparticles. Saponins mainly contribute to the stabilization of nanoparticles by preventing aggregation (Dwivedi et al., 2020).

Proteins and amino acids are also present in plant extracts and play a role in nanoparticle synthesis. The amine, carboxyl, and thiol groups present in proteins can bind to metal ions and nanoparticle surfaces. These biomolecules act as capping agents and provide stability to nanoparticles (Sharma et al., 2012).

Sugars and polysaccharides such as glucose, fructose, starch, and cellulose are common in plant extracts. They contain multiple hydroxyl groups that can reduce metal ions and also stabilize nanoparticles. Polysaccharides form a protective layer around nanoparticles, preventing them from clumping together (Barui et al., 2019).

In summary, phytochemicals are the key components responsible for the successful green synthesis of metal nanoparticles. Their chemical nature and functional groups make them suitable for reducing metal ions, stabilizing nanoparticles, and improving their biological performance. Understanding the role of different phytochemical groups is essential for better control and design of plant-mediated nanoparticle synthesis.

Mechanistic Role of Phytochemicals in Metal Nanoparticle Synthesis:

The formation of metal nanoparticles using plant extracts is a complex process, but it

mainly depends on the chemical nature of phytochemicals present in the extract. Phytochemicals play three major roles during nanoparticle synthesis: **reduction of metal ions, capping of nanoparticles, and stabilization of nanoparticles**. These roles are closely connected and often performed by the same compounds.

Role of Phytochemicals as Reducing Agents:

The first and most important step in nanoparticle synthesis is the reduction of metal ions to their metallic form. Metal salts such as silver nitrate, gold chloride, zinc sulfate, or copper chloride contain metal ions in a positive oxidation state. To form nanoparticles, these ions must gain electrons and get converted into neutral metal atoms.

Phytochemicals act as **natural reducing agents** by donating electrons. Compounds such as phenolics, flavonoids, terpenoids, ascorbic acid, and sugars have functional groups like hydroxyl (–OH) and aldehyde groups that can easily lose electrons. When plant extract is mixed with metal salt solution, these functional groups transfer electrons to metal ions. As a result, metal ions such as Ag^+ , Au^{3+} , or Cu^{2+} are reduced to Ag^0 , Au^0 , or Cu^0 atoms. These atoms then start to combine and form small clusters, which grow into nanoparticles (“Reducing Agents in Colloidal Nanoparticle Synthesis,” 2021).

The reducing ability of phytochemicals is strongly related to their antioxidant nature. Compounds with higher antioxidant activity generally show better reducing capacity. This is why plants rich in phenolics and flavonoids are very effective in nanoparticle synthesis.

Nucleation and Growth of Nanoparticles:

After reduction, the newly formed metal atoms undergo a process called **nucleation**, where they come together to form small nuclei. These nuclei act as seeds for further growth. As more

reduced metal atoms deposit on these nuclei, the particles grow in size. This growth continues until stable nanoparticles are formed.

Phytochemicals control this nucleation and growth process. If reduction is fast, many nuclei are formed, leading to smaller nanoparticles. If reduction is slow, fewer nuclei are formed, and particles grow larger. Thus, the concentration and type of phytochemicals present in the extract influence the **size and number of nanoparticles** formed (Basnet et al., 2018).

Role of Phytochemicals as Capping Agents:

Once nanoparticles are formed, they have a strong tendency to stick together due to high surface energy. This leads to aggregation and loss of nanoscale properties. Phytochemicals prevent this problem by acting as **capping agents**.

Capping means that phytochemical molecules attach to the surface of nanoparticles and form a protective layer. Functional groups such as –OH, –COOH, –NH₂, and –SH bind to the metal surface through weak chemical interactions. This layer creates a physical barrier between particles and stops them from coming too close to each other. As a result, nanoparticles remain separated and stable in solution (Lokare et al., 2023).

Different phytochemicals cap nanoparticles in different ways. For example, proteins and amino acids form a strong coating due to multiple binding sites, while flavonoids and phenolics provide both reduction and capping. This dual role is a major advantage of plant-based synthesis (Pirsahab et al., 2024a).

Role of Phytochemicals as Stabilizing Agents:

Stabilization is essential to maintain the nanoparticles in dispersed form for a long time. Phytochemicals help in stabilization by providing **electrostatic and steric repulsion** between particles.

Electrostatic stabilization occurs when charged functional groups on phytochemicals create a surface charge on nanoparticles. This charge causes particles to repel each other, preventing aggregation. Steric stabilization occurs when bulky phytochemical molecules surround the nanoparticles and physically block them from coming close.

Compounds such as saponins, polysaccharides, and proteins are especially effective stabilizers because of their large molecular size. They form a thick layer around nanoparticles and provide long-term stability (Pirsaheb et al., 2024b).

Dual Role of Phytochemicals in Reduction and Stabilization:

One of the unique features of phytochemicals is their ability to perform **multiple functions at the same time**. Many compounds act as both reducing agents and stabilizing agents. For example, flavonoids reduce metal ions and then remain attached to the nanoparticle surface as capping agents. Phenolic compounds also show similar behavior.

This dual role makes plant-mediated synthesis very efficient and simple, as there is no need to add separate reducing and stabilizing chemicals. It also improves the biocompatibility of nanoparticles, which is important for biomedical applications (Pirsaheb et al., 2024a).

Influence of Reaction Conditions on Phytochemical Activity:

The activity of phytochemicals during nanoparticle synthesis is influenced by reaction conditions such as pH, temperature, metal ion concentration, and extract concentration. At higher pH, phenolic groups are more active in electron donation, leading to faster reduction. Temperature affects the speed of reaction and particle growth. Higher extract concentration

provides more phytochemicals, resulting in better reduction and stabilization (Khodade, Shelke, et al., 2025).

Therefore, controlling these parameters is important to obtain nanoparticles with desired size, shape, and stability.

Role of Major Phytochemical Classes in Nanoparticle Formation:

Plant extracts contain a mixture of phytochemicals, and each class contributes differently to nanoparticle formation. Their structural features and functional groups decide how they interact with metal ions and developing nanoparticles.

Phenolic compounds are among the most active components during nanoparticle synthesis. Their aromatic rings with hydroxyl groups make them highly reactive towards metal ions. Because of this, plants rich in phenolics often show faster nanoparticle formation and better control over particle size (Ogidi & Emaikwu, 2024).

Flavonoids play an important role due to their ability to bind metal ions through multiple functional groups. This binding helps in controlled particle growth and uniform distribution. Flavonoids are also known to remain attached to the nanoparticle surface, which improves surface functionality (Casanova et al., 2022).

Terpenoids contribute mainly to shape and structural control. Their diverse structures influence how metal atoms arrange during particle growth, which can lead to variations in morphology (Câmara et al., 2024).

Alkaloids, because of their nitrogen-containing nature, show strong interaction with metal surfaces. They are particularly important in maintaining particle integrity and preventing surface instability (Ijaz et al., 2022).

Tannins have multiple reactive sites and large molecular size. This allows them to form

strong interactions with metal ions and developing particles, helping in compact and well-defined nanoparticle structures (Manik et al., 2022).

Saponins improve dispersion of nanoparticles in solution. Their surfactant nature helps particles remain evenly distributed instead of forming clusters (Wijesekara et al., 2024).

Proteins and amino acids provide structural support to nanoparticles. Their flexible chains and multiple binding sites allow them to wrap around particles, improving stability and surface compatibility (Marslin et al., 2018).

Sugars and polysaccharides form a soft outer layer around nanoparticles. This layer acts as a natural shield and improves particle tolerance in biological systems (Barui et al., 2019).

Overall, nanoparticle formation is not the result of a single compound but the **combined action of multiple phytochemical groups**. The balance between these compounds decides the final properties of the nanoparticles.

Biological Relevance of Phytochemical-Coated Nanoparticles:

Phytochemical-coated nanoparticles show improved **biological performance** compared to chemically synthesized nanoparticles. The presence of plant compounds on the nanoparticle surface enhances their interaction with microbial cells and human cells (Khodade, Sonawane, et al., 2025).

Many studies have reported increased **antibacterial activity** due to combined effects of metal ions and phytochemicals. Similarly, antioxidant and anticancer activities are enhanced because phytochemicals contribute their natural bioactivity along with the metal core. This synergistic effect makes phytochemical-mediated nanoparticles more effective for biomedical applications (Casanova et al., 2022).

Advantages of Phytochemical-Mediated Nanoparticle Synthesis:

Phytochemical-based synthesis is:

- **Eco-friendly** and safe
- **Cost-effective**
- **Simple to perform**
- Does not require toxic chemicals
- Produces **biocompatible nanoparticles**

This approach is suitable for large-scale production and aligns well with sustainable development goals (Li et al., 2020).

Limitations and Challenges:

Despite its advantages, phytochemical-mediated synthesis has some limitations. The **composition of plant extracts varies** depending on plant species, season, and extraction method. This leads to poor reproducibility in some cases. Also, the exact mechanism of action of many phytochemicals is still not fully understood. Standardization of protocols remains a challenge (Gupta et al., 2023).

Future Prospects:

Future research should focus on **phytochemical profiling before synthesis**, standardization of extraction methods, and better control of reaction conditions. Understanding the individual role of phytochemicals will help in designing nanoparticles with specific size and function. This will improve the application of green nanoparticles in medicine, agriculture, and environmental fields.

Conclusion:

Phytochemicals play a central role in the green synthesis of metal nanoparticles. They are responsible for the reduction of metal ions and also help in controlling particle stability and surface properties. The presence of phytochemicals improves the biological activity and safety of nanoparticles. Although challenges

such as variability and lack of standardization exist, phytochemical-mediated synthesis remains a promising and sustainable approach for nanoparticle production. Better understanding of phytochemical mechanisms will further strengthen the development of green nanotechnology.

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