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Green Nanotechnology Using Medicinal Plants: Recent Advances in Sustainable Nanomedicine

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ABSTRACT: Green nanotechnology has become a sustainable method of synthesizing nanoparticles with the help of medicinal plants as natural reducing, capping agents and stabilizing agents. Plant-mediated synthesis does not require harmful chemicals, consumes less energy and facilitates the generation of bio-compatible nanomaterials with higher biological activity. This review highlights recent advancements in green synthesis of metallic and metal oxide nanoparticles, and points out that phytochemicals play vital role in the formation of nanoparticles, characterization techniques, and applications in various biomedical fields such as antimicrobial activity, anticancer activity, antiviral activity, anti-inflammatory activity, antioxidant activity, antidiabetic activity, wound-healing, drug delivery, and diagnostic applications. This review also covers the sustainability issues, environmental impacts, assessment of safety, regulatory issues, and application of artificial intelligence and computational methods to optimize the design of nanoparticles and their clinical translation. In addition, issues of reproducibility, standardization, mass production, and regulatory authorization for current challenges are discussed in detail, as well as future prospects for personalized nanomedicine and industrial commercialization.

In conclusion, green nanotechnology using medicinal plants is a promising platform to create eco-friendly, safe, and multifunctional nanomaterials which can enable environmentally friendly innovation and the next-generation nanomedicine.

1. INTRODUCTION

Green nanotechnology comes as a new multi-disciplinary field, which focuses on implementing environmentally friendly nanomaterials with minimal ecological and human health impacts, through nanoscience and biotechnology, and green chemistry. The potential applications of nanoparticles are very wide ranging, such as in drug delivery, diagnostics, antimicrobial therapy, cancer therapy and tissue engineering/regenerative medicine, due to their unique properties, including high surface area to volume ratio, high catalytic activity, and optical properties and tunable interactions with biological tissues. However, the traditional physical and chemical preparation methods of nanoparticles consume high energy, require expensive preparation equipment, use harmful reducing agents and dangerous organic solvents, and pollute the environment in the preparation process, which causes high production cost, toxic residue of chemicals, and pollution of the environment (1). The drawbacks have led to the development of green synthesis approaches based on the principles of sustainable chemistry and "green" synthesis. The search for biological resources that contain these phytochemicals like flavonoids, phenolic acids, terpenoids, alkaloids, tannins, proteins and polysaccharides, which perform the role of reducing, stabilizing and capping agents in the formation of nanoparticles, has garnered considerable attention for medicinal plants. The synthesis of plant-mediated nanoparticles is easy, fast, simple, scalable, and does not require any hazardous chemicals, produces highly stable and biocompatible nanoparticles, and generates nanoparticles with increased biological activity (2). Besides, the nanoparticles that have phytochemicals often have synergistic therapeutic effects, enhancing antimicrobial, anti-oxidative, anti-inflammatory, antiviral, anti-cancer, wound healing, and targeted drug delivery properties. The use of medicinal plants combined with nanotechnology is also consistent with the principles of green chemistry, which include the use of renewable feedstocks, safer solvents, energy-efficient synthesis, minimization of waste, and environmentally friendly design of products during their life cycle. Nevertheless, there are still several challenges to be addressed: plant extract variability, lack of repeatability, incomplete understanding of the mechanism for the formation of nanoparticles using phytochemicals, and the difficulties of manufacturing phytochemical-based nanoparticles on a large scale, regulatory standardization, and a thorough toxicological evaluation before clinical translation (3). Hence, this review summarizes the recent development of green nanotechnology involving medicinal plants, focusing on biosynthetic mechanisms, phytochemical functions, characterization of nanoparticles, biomedical applications, sustainability issues, toxicity concerns, regulatory issues, and the prospects for the development of safe, effective, and sustainable nanomedicines using plant-derived nanomaterials.

2. MEDICINAL PLANTS AS BIOFACTORIES FOR GREEN NANOPARTICLE SYNTHESIS

Medicinal plants are highly effective biological agents for the sustainable production of metal nanoparticles, as they are rich in various phytochemicals that can reduce, stabilize, and functionalize metal ions to form metal nanoparticles. The secondary metabolites of phenolic acids, flavonoids, terpenoids, alkaloids, tannins, saponins, polysaccharides, proteins, amino acids and reducing sugars are found in the different parts of the plant, such as leaves, stems, root, flower, fruit, seed and bark, and are used in the biosynthesis process (4). The major electron donors present in these are phenolics and flavonoids, which can oxidize the hydroxyl functional groups, converting metal ions to their zero-valence states and metal oxide nanoparticles, such as Ag^{+} to Ag, Au^{3+} to Au, Cu^{2+} to Cu, Zn^{2+} to Zn, and Fe^{3+} to Fe_2O_3. Other components include terpenoids, which are involved in redox reactions and can also be attached to the surface of the nanoparticles, making them even more stable; proteins, enzymes, and polysaccharides are natural capping agents that prevent aggregation, control crystal growth, and ensure colloidal stability. The selection of medicinal plants for the preparation of nanoparticles should take into account several criteria like phytochemical composition, medicinal applications, geographical availability, seasonality, extraction yield, metabolite sustainability and metabolite reproducibility (5). The overall trend is that more polyphenol and antioxidant compounds result in a greater reducing potential and the more uniform the more a smaller size distribution and the higher the biological activity of the nanoparticles.Other experimental parameters like plant extract concentration, metal precursor concentration, reaction time, temperature, pH, mixing condition, incubation period etc., which have a significant influence on the nucleation kinetics, crystal growth, particle morphology and the physicochemical properties of the resulting nanoparticles, also play a role in the efficiency of plant-mediated nanoparticle synthesis (6). The biosynthetic mechanism is the metal ion adsorption with bioactive phytochemicals and subsequent transfer of electrons from the hydroxyl, carbonyl, amine and carboxyl functional groups, leading to the rapid bioreduction of the metal ions to metallic nuclei. These nuclei are then subjected to nucleation, growth and stabilization using an organic phytochemical corona that improves the biocompatibility and stability of nanoparticles in the long term (7). To demonstrate how such reduction, nucleation, growth and surface capping mechanisms occurred in a single mechanism, the following figure (Figure 1) has been provided, which explains the synergistic action of the phytochemicals from the medicinal plants to make the environment-friendly nanoparticles in the absence of any hazardous chemical reducing agents and synthetic stabilizers for various biomedical, pharmaceutical, antimicrobial, catalytic and diagnostic applications.

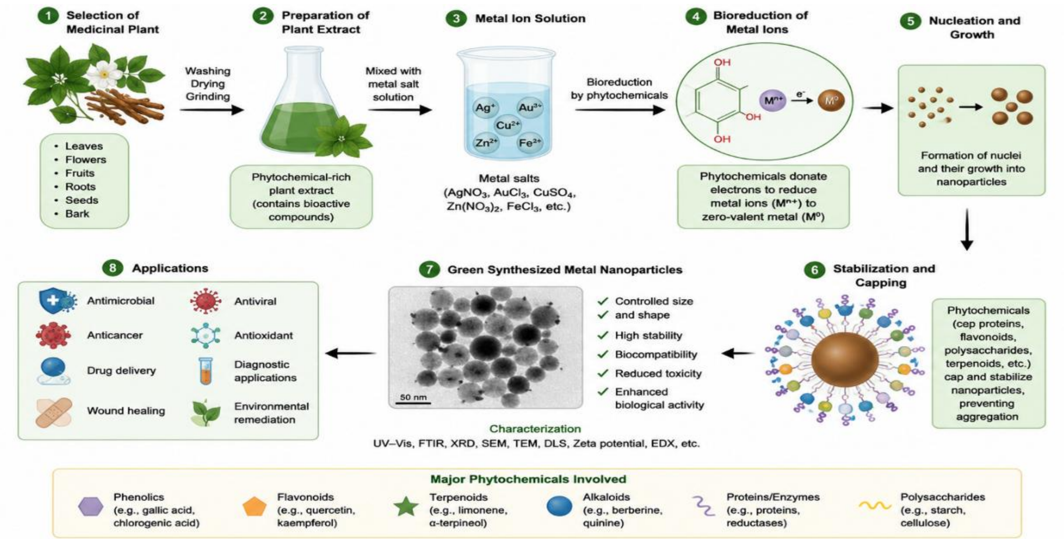

Figure 1. Mechanism of Green Synthesis of Metal Nanoparticles Using Medicinal Plant Phytochemicals

3. GREEN SYNTHESIS STRATEGIES FOR NANOPARTICLES

Green synthesis of nanomaterials using extracts of medicinal plants, ranging from the simplest to the more complex methods, is also growing substantially, and the extracts are utilized as eco-friendly reducing and stabilizing agents for the synthesis of various metallic and metal oxide nanoparticles. Of these, silver nanoparticles (AgNPs) have been studied the most due to their outstanding antimicrobial, antioxidant, anticancer, antiviral, and wound-healing properties (8). The flavonoids, phenolics, and tannins in plants efficiently convert silver ions (Ag^+) into stable AgNPs with controlled morphology and enhanced biological functionality. The gold nanoparticles that are synthesized by the use of medicinal plants are very biocompatible, chemically stable, and possess surface plasmon resonance, which is very useful in targeted drug delivery, biosensing, molecular imaging, photothermal therapy, and cancer diagnosis (9). Likewise, ZnO NPs are also being extensively studied due to their photocatalytic property, UV blocking ability, antimicrobial activity, antioxidant activity, and selective cytotoxicity against cancer cells, and the plant-mediated synthesis process results in reduced toxic by-products as compared to the traditional methods of synthesis. Copper and Copper Oxide nanoparticles (Cu/CuO NPs) have remarkable properties such as Antibacterial, Antifungal, Catalytic, antioxidant, and Environmental Remediation properties; still, the role of phytochemicals extracted from plants is vital to prevent oxidation and to ensure the stability of copper nanoparticles during synthesis while maintaining their cost-effectiveness compared to noble metal nanoparticles. Utilization of the green-synthesized Fe_3O_4 and Fe_2O_3 nanoparticles in magnetic resonance imaging (MRI), drug delivery, magnetic hyperthermia, biosensing, and wastewater treatment can be achieved due to their superparamagnetic properties and functionalization with phytochemicals for biocompatibility (10). Apart from metallic nanoparticles, silica nanoparticles and hybrid nanomaterials based on plant-derived biomolecules have been identified as having high surface area, tunable porosity, mechanical stability, and drug-loading capacity, which are well-suited for advanced applications such as controlled drug delivery, tissue engineering, and multifunctional biomedical devices. In addition, the latest studies are directed towards the synthesis of multifunctional nanocomposites, where nanoparticles of various metals are linked with polymer(s), graphene oxide, carbon nanomaterials, bioceramics or MOFs, which allow the obtainment of synergistic physicochemical and biological properties (11). The hybrid systems have been shown to exhibit improved therapeutic efficacy, controlled drug release, enhanced mechanical properties, and higher catalytic and antimicrobial activity compared with single-component nanoparticles. Type of nanoparticles is dependent on the biomedical application, physicochemical properties of the nanoparticles and the phytochemical composition of the medicinal plant extract utilized for nanoparticles biosynthesis. Finally, medicinal plant-based synthesis is a flexible, scalable, sustainable platform for the production of next-generation nanomaterials with minimal environmental impact, high biocompatibility, and application potential in nanomedicine, diagnostics, therapeutics, environmental remediation, and advanced healthcare nanotechnology, enhancing the role of green nanotechnology for the synthesis of multifunctional sustainable nanomaterials (12).

4. CHARACTERIZATION TECHNIQUES FOR PLANT-DERIVED NANOPARTICLES

The physicochemical characterization of plant-derived nanoparticles is a critical step in green nanotechnology because it provides comprehensive information regarding particle formation, size, morphology, crystallinity, elemental composition, surface chemistry, colloidal stability, and thermal behavior, all of which directly influence their biomedical performance and reproducibility. Following biosynthesis, multiple complementary analytical techniques are employed to confirm successful nanoparticle formation and evaluate their structural and functional properties (13). UV–Visible (UV–Vis) spectroscopy is generally the first analytical tool used to monitor nanoparticle synthesis by detecting characteristic surface plasmon resonance (SPR) bands, which indicate the reduction of metal ions and the formation of stable nanoparticles. Fourier Transform Infrared (FTIR) spectroscopy is subsequently utilized to identify the functional groups of phytochemicals adsorbed on the nanoparticle surface, thereby confirming the involvement of phenolics, flavonoids, proteins, terpenoids, and other biomolecules as reducing, capping, and stabilizing agents during biosynthesis. X-ray Diffraction (XRD) analysis provides information on crystal structure, phase purity, crystallite size, and lattice parameters, enabling the determination of whether the synthesized nanoparticles are amorphous or crystalline (14). Dynamic Light Scattering (DLS) measures the hydrodynamic particle diameter and size distribution in suspension, while zeta potential analysis evaluates the surface charge and colloidal stability; higher absolute zeta potential values generally indicate greater dispersion stability and lower aggregation tendencies. Morphological characterization is achieved using Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM), which reveal particle shape, surface texture, agglomeration patterns, and nanoscale dimensions. SEM provides detailed three-dimensional surface topography, whereas TEM offers high-resolution visualization of internal structures, crystal boundaries, and particle morphology at the nanometer scale. Energy-Dispersive X-ray Spectroscopy (EDX), commonly coupled with SEM or TEM, determines the elemental composition of nanoparticles and confirms the presence of target metals while detecting potential impurities or contaminants originating from synthesis (15). In addition, Thermogravimetric Analysis (TGA) assesses thermal stability, decomposition profiles, moisture content, and the quantity of phytochemical molecules adsorbed onto nanoparticle surfaces, thereby providing valuable insights into the effectiveness of biological capping and long-term storage stability. The combined application of these analytical techniques ensures comprehensive physicochemical characterization and facilitates quality control, reproducibility, and standardization of plant-mediated nanomaterials intended for biomedical applications (16). The principles, analytical functions, and major applications of these characterization methods are summarized in Table 1, highlighting their complementary roles in confirming nanoparticle synthesis and establishing structure–property relationships essential for pharmaceutical development, diagnostics, and sustainable nanomedicine.

Table 1. Common Characterization Techniques Used for Green-Synthesized Nanoparticles and Their Analytical Significance

Characterization Technique	Working Principle	Information Obtained	Analytical Significance in Green Nanotechnology
UV–Visible (UV–Vis) Spectroscopy	Measures the absorption of ultraviolet and visible light by nanoparticles through surface plasmon resonance (SPR).	Surface plasmon resonance peak, nanoparticle formation, reaction kinetics, optical properties.	Confirms successful nanoparticle synthesis and monitors the reduction of metal ions during biosynthesis.
Fourier Transform Infrared (FTIR) Spectroscopy	Detects molecular vibrations and functional groups	Identification of hydroxyl, carbonyl, amine, carboxyl,	Confirms the role of medicinal plant phytochemicals as reducing, capping, and stabilizing agents.

	present on nanoparticle surfaces.	and other phytochemical functional groups.	
X-Ray Diffraction (XRD)	It measures the X-ray diffraction by crystalline materials according to Bragg's law.	Crystal structure, phase purity, crystallinity, crystallite size, lattice parameters.	Determines the crystalline nature and structural integrity of synthesized nanoparticles.
Dynamic Light Scattering (DLS)	Measures fluctuations in scattered light caused by Brownian motion of nanoparticles.	Hydrodynamic diameter, particle-size distribution, and polydispersity index (PDI).	Evaluates nanoparticle dispersion quality, uniformity, and aggregation behavior in suspension.
Zeta Potential Analysis	Determines the electrophoretic mobility of nanoparticles under an applied electric field.	Surface charge (mV), colloidal stability, electrostatic interactions.	Predicts long-term suspension stability; higher absolute zeta potential values indicate better stability and reduced aggregation.
Scanning Electron Microscopy (SEM)	Uses a focused electron beam to scan the nanoparticle surface.	Surface morphology, particle shape, size, texture, aggregation.	Provides high-resolution images for evaluating external morphology and surface architecture.
Transmission Electron Microscopy (TEM)	Transmits high-energy electrons through ultrathin nanoparticle samples.	Internal structure, particle size, morphology, crystal lattice, nanostructure.	Offers direct nanoscale visualization and precise measurement of particle dimensions and morphology.
Energy-Dispersive X-ray Spectroscopy (EDX)	Detects characteristic X-rays emitted by elements after electron-beam excitation.	Elemental composition, elemental distribution, purity, contaminants.	Confirms the presence of target metallic elements and assesses the elemental purity of biosynthesized nanoparticles.
Thermogravimetric Analysis (TGA)	Measures weight changes as a function of increasing temperature.	Thermal stability, decomposition profile, moisture content, organic coating percentage.	Determines thermal behavior and estimates the number of phytochemical capping molecules attached to nanoparticles.

5. BIOMEDICAL APPLICATIONS OF MEDICINAL PLANT-DERIVED NANOPARTICLES

Medicinal plant-derived nanoparticles have attracted great attention due to the unique physical, chemical, and biological properties of nanoparticles and the intrinsic therapeutic effects of medicinal plants, including improved biological efficacy, enhanced biocompatibility, and reduced systemic toxicity, which make them an emerging multifunctional nanomaterial in sustainable nanomedicine (17). They have been utilized in various biomedical applications, including antimicrobial activity, where plant-derived silver, copper, zinc oxide and gold nanoparticles are effective in the destruction of both Gram-positive and Gram-negative bacteria by generating radical oxygen species (ROS), protein denaturation and binding to the DNA of these bacteria with a high activity against multidrug-resistant bacteria (18). In oncology, the use of nanoparticles as carriers of anticancer agents to induce apoptosis, oxidative stress, mitochondrial dysfunction, and cell-cycle arrest in cancer cells has shown great promise for enhancing the efficacy of chemotherapy and PTT. The antiviral and antifungal activity of the plant-derived nanoparticles is also significant, as they inhibit viral attachment, viral propagation within cells, and viral replication, and disrupt fungal cell membranes and fungal biofilm formation, which suggests their possible use for the treatment of emerging viral and fungal infectious diseases. Furthermore, due to the synergistic effect of bioactive phytochemicals and nanoparticles, they have been attributed to potent anti-inflammatory and antioxidant effects, which involve the potent scavenging of ROS, regulation

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of inflammatory cytokines, and reduction of cell damage caused by ROS. Recent studies also indicate their hypoglycemic activity, as nanoparticles ameliorate glucose metabolism, enhance insulin sensitivity, inhibit carbohydrate-hydrolyzing enzymes such as α-amylase and α-glucosidase, and prevent oxidative damage to pancreatic β-cells. Plant-mediated nanoparticles in regenerative medicine stimulate and promote the proliferation of fibroblasts, collagen deposition, angiogenesis, antimicrobial protection, and extracellular matrix remodeling to promote rapid tissue regeneration (19). They are used in drug delivery systems to revolutionize targeted therapeutics by enabling controlled drug release, enhanced bioavailability, prolonged circulation, reduced off-target toxicity, and site-specific delivery of chemotherapeutic agents, proteins, nucleic acids, and natural bioactive compounds. Apart from that, bioimaging and diagnostics applications have been realised based on the optical, magnetic and plasmonic properties of the nanoparticles, like Fluorescence imaging, Magnetic resonance imaging (MRI), computed tomography (CT), biosensing, molecular diagnostics, and real-time monitoring of disease with high sensitivity and specificity (20). Figure 2 provides an overview of the biomedical applications of plant-based nanoparticles and the associated medicinal mechanisms, with a focus on their use in sustainable nanomedicine. While these are remarkable successes, further investigation of pharmacokinetics, long-term biosafety, and standardised manufacturing processes and regulatory approval is required for successful clinical translation and commercialisation of plant-based nanotherapeutics.

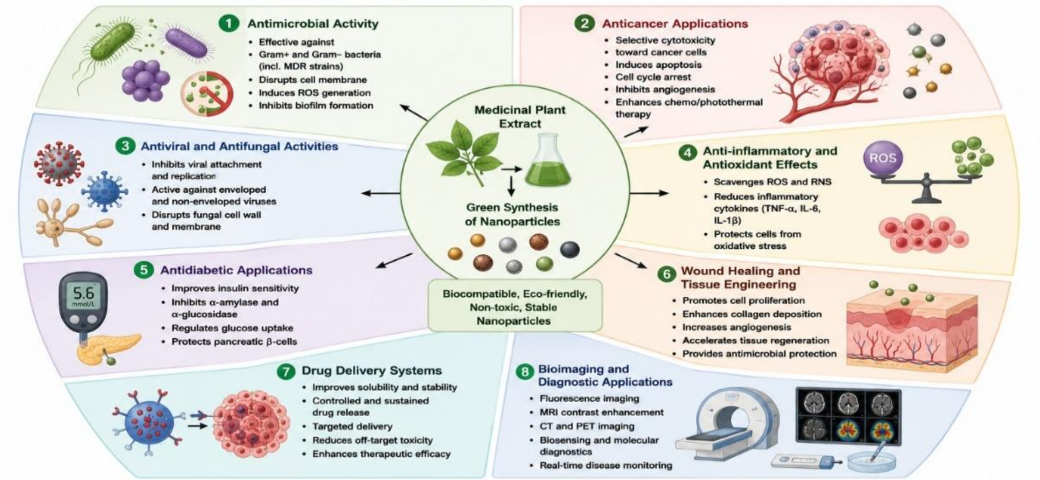

Figure 2. Biomedical Applications of Green-Synthesized Nanoparticles in Sustainable Nanomedicine

6. SUSTAINABLE AND ENVIRONMENTAL PERSPECTIVES

The synthesis of nanoparticles using medicinal plants as bioreactors provides an environmentally friendly alternative to the traditional synthesis of nanomaterials and is one of the main directions of sustainable development of green nanotechnology. The use of renewable resources, safer reaction conditions and solvents, less harmful materials, prevention of pollution, minimization of waste, and design of biodegradable products during the preparation process are all emphasized by the applications of green chemistry in the preparation of nanoparticles (21). Unlike typical chemical synthesis, which uses organic solvents and high-temperature reactions with toxic reducing agents and capping agents to create the product, the synthesis processes do not involve these. Besides adopting eco-friendly approaches to plant-based nanotechnology, the use of nanoparticles from medicinal plants not only helps in reducing chemical wastes but also diminishes the amount of greenhouse gases being released during the energy-intensive production techniques and develops sustainable manufacturing techniques that preserve natural resources (22). Furthermore, the circular bioeconomy concept has inspired the utilization of agricultural residues, pharmaceutical plant waste, fruit peels, leaves, bark, seeds, and other lignocellulosic wastes for synthesizing nanoparticles, thereby converting valuable biological wastes into nanomaterials to boost waste valorization, resource recovery, and sustainable development. This not only reduces landfilling and environmental pollution but also increases the economic viability of green nanotechnology. An increasingly important form of assessment of the environmental sustainability of these biosynthetic processes is the application of a standardized method, called Life Cycle Assessment (LCA), which systematically assesses the environmental impacts associated with the acquisition/extraction of raw materials, the synthesis of NPs, the use of the product, and the disposal of the NP at the end of their use. LCA can be used to quantify the energy, carbon emissions, water use, ecotoxicity, resource depletion, and waste generated in the synthesis process, enabling sustainable synthesis routes to be compared with conventional routes and optimised for sustainable use in industry while maintaining their functionality (23). Even with these benefits, there are still some scaling-up and industrial production issues that are not addressed. There are inter-species, inter-origin, inter-climatic, inter-seasonal, and inter-extraction variations in the phytochemical composition of medicinal plants, which can influence the reproducibility and batch-to-batch consistency of the nanoparticles. Other challenges include a lack of standardisation of processes, quality assurance, purification efficiency, storage stability, regulatory compliance, and economic competitiveness in large-scale production. Continuous-flow bioprocesses, artificial intelligence assistance for process optimization, standardized extraction methods and built-in quality control mechanisms will all be instrumental in tackling these challenges and facilitating commercialization of sustainable plant-based nanomaterials (24). Thus, the path of green nanotechnology using medicinal plants could be a good alternative for environmentally friendly nanomedicine, involving the principles of ecological responsibility, renewability of the biological resources used, innovation in industry, and the concepts of circular bioeconomy, aimed at contributing to global development towards sustainability and responsible manufacturing.

7. SAFETY, TOXICITY, AND REGULATORY CONSIDERATIONS

The great strides achieved in green nanotechnology using medicinal plants; however, a detailed analysis of issues related to safety, toxicology and regulation is still needed to guarantee plant nanoparticles for clinical use and commercialization. Determination of physicochemical properties such as particle size, morphology, surface charge, chemical composition, concentration, aggregation state, and surface functionalization is important for understanding the interaction of nanoparticles with biological systems, although the use of hazardous chemicals is limited (25). To evaluate the toxicity of nanotechnology, a systematic investigation is needed, including in vitro and in vivo studies to measure cytotoxicity, oxidative stress, inflammatory response, genotoxicity, immunotoxicity, and organ-specific toxicity. However, at higher concentrations of nanoparticles, excess production of the reactive oxygen species (ROS), mitochondrial dysfunction, DNA damage, and apoptosis have been reported, calling for the optimization of the dose and the need for long-term safety assessment (21). Recent studies on the biocompatibility and biodistribution are also very important, which are centered on absorption of nanoparticles, circulation, distribution in tissues, uptake by cells, metabolism, clearance and elimination following different administration methods. Medicinal plant-derived surface phytochemicals can enhance biological compatibility, reduce immune recognition, prolong systemic circulation and promote targeted delivery depending on the structure of the nanoparticles and their surface chemistry. Apart from human health, environmental risk assessment is also becoming increasingly relevant because the exposure and/or disposal of nanomaterials on a larger scale may result in effects on aquatic ecosystems, microorganisms, plants and higher organisms through bioaccumulation and ecotoxicological interactions (26). Environmental monitoring and life-cycle assessment therefore need to be standardized to gauge long-term ecological impacts. International regulatory agencies and bodies have made recommendations on the different aspects of the development of nanomedicines, such as characterization, quality assurance and biopharmaceutical testing, manufacturing, and clinical evaluation, for example the United States Food and Drug Administration (FDA), the European Medicines Agency (EMA), the Organisation for Economic Co-operation and Development (OECD), and the International Organization for Standardization (ISO) (27). Regulatory harmonization remains a challenge, however, given that green-synthesized nanomaterials can be produced using many different methods and phytochemical compositions. Also, there are ethical and clinical concerns for translation before larger-scale clinical application, including safety of patients, patient consent, equitable access, environmental responsibility, transparency of data, manufacturing reproducibility, and post-marketing surveillance. While the use of medicinal plants for nanotechnology provides significant benefits in terms of sustainability, biocompatibility, and therapeutic potential, several challenges, such as standardization, toxicity assessment, harmonization of regulations, and industrialization scaling, need to be tackled to ensure safe, effective, and globally accepted applications in sustainable nanomedicine (28).

Table 2. Advantages, Challenges, Safety Concerns, and Future Opportunities of Green Nanotechnology in Sustainable Nanomedicine

Parameter	Key Points
Advantages	Eco-friendly synthesis, renewable plant resources, low toxicity, cost-effective production, enhanced biocompatibility, multifunctional therapeutic applications.
Current Challenges	Lack of process standardization, phytochemical variability, reproducibility issues, scale-up limitations, quality control.

Safety Concerns	Nanotoxicity, oxidative stress, biodistribution, long-term accumulation, environmental exposure, insufficient clinical safety data.
Future Opportunities	AI-assisted synthesis, precision nanomedicine, targeted drug delivery, circular bioeconomy, regulatory harmonization, industrial commercialization.

8. ARTIFICIAL INTELLIGENCE AND COMPUTATIONAL APPROACHES

Artificial intelligence (AI) and computational technologies are transforming green nanotechnology by accelerating the design, optimization, and biomedical translation of medicinal plant-derived nanoparticles through data-driven decision-making and predictive modelling (29). Conventional experimental optimization of nanoparticle synthesis is often labor-intensive and time-consuming and is influenced by numerous variables, including plant species, phytochemical composition, precursor concentration, pH, temperature, and reaction time. AI-assisted nanoparticle design overcomes these limitations by integrating large experimental datasets with computational algorithms capable of predicting nanoparticle size, morphology, crystallinity, stability, and biological performance before laboratory synthesis, thereby reducing experimental cost and improving reproducibility. Among AI techniques, machine learning (ML) has emerged as a powerful tool for optimizing green synthesis processes by identifying complex relationships between synthesis parameters and nanoparticle characteristics. Supervised and unsupervised learning algorithms, including artificial neural networks, random forests, support vector machines, and deep learning models, can accurately predict optimal reaction conditions, enhance process efficiency, and improve product quality while minimizing resource consumption (30). In addition to synthesis optimization, molecular docking has become an indispensable computational approach for investigating nano–bio interactions by predicting the binding affinity of phytochemical-functionalized nanoparticles with disease-associated proteins, enzymes, receptors, nucleic acids, and other biomolecular targets. Docking studies provide mechanistic insights into antimicrobial, anticancer, antiviral, anti-inflammatory, and antidiabetic activities while supporting the rational selection of medicinal plants and bioactive compounds for targeted nanomedicine development (31). Furthermore, the concept of digital twins has recently emerged as an innovative strategy in predictive nanomedicine, where virtual computational models simulate nanoparticle synthesis, physicochemical behavior, biological interactions, pharmacokinetics, biodistribution, and therapeutic responses under different physiological conditions. Such simulations enable rapid optimization of nanoparticle formulations, personalized treatment planning, and reduction of costly experimental iterations. The integration of AI with advanced computational chemistry, molecular dynamics simulations, quantum mechanical calculations, bioinformatics, and high-throughput screening has also facilitated the development of emerging smart nanotechnology platforms capable of self-optimizing synthesis, intelligent drug delivery, real-time biosensing, image-guided therapy, and precision diagnostics (32). These intelligent systems combine nanotechnology with cloud computing, Internet of Medical Things (IoMT), wearable biosensors, and precision medicine to provide adaptive therapeutic strategies and continuous patient monitoring. Although challenges related to data quality, algorithm transparency, computational standardization, cybersecurity, and regulatory acceptance remain, AI-driven computational approaches are expected to significantly accelerate the discovery, optimization, clinical translation, and commercialization of sustainable plant-based nanomedicines, establishing a new paradigm for next-generation green nanotechnology and precision healthcare.

9. CURRENT CHALLENGES AND FUTURE PERSPECTIVES

Despite remarkable progress, medicinal plant-mediated green nanotechnology continues to face several challenges that must be addressed before its widespread clinical and industrial adoption. Variations in phytochemical composition caused by plant species, geographical origin, harvesting conditions, and extraction methods often lead to poor reproducibility and limited standardization of nanoparticle synthesis. Furthermore, the molecular mechanisms underlying phytochemical-mediated reduction, nucleation, growth, and stabilization of nanoparticles remain only partially understood, emphasizing the need for advanced analytical techniques and computational investigations. Clinical translation is another significant challenge because comprehensive studies on pharmacokinetics, biodistribution, long-term toxicity, immunogenicity, and therapeutic efficacy remain limited, and internationally harmonized regulatory guidelines for plant-derived nanomedicines are still under development. Nevertheless, the future of green nanotechnology is highly promising owing to rapid advances in artificial intelligence, machine learning, multi-omics technologies, molecular modeling, and precision medicine, which are expected to improve nanoparticle design, process optimization, and personalized therapeutic strategies. Increasing investment in sustainable

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manufacturing, continuous-flow production systems, automated quality control, and circular bioeconomy approaches will further enhance industrial scalability and commercial feasibility (33). Future research should focus on standardized synthesis protocols, mechanistic studies, comprehensive safety evaluation, regulatory harmonization, and large-scale clinical validation to facilitate successful commercialization. As illustrated in Figure 3, the future roadmap integrates medicinal plant selection, green nanoparticle synthesis, precision nanomedicine, intelligent manufacturing, and sustainable healthcare, providing a comprehensive framework for advancing environmentally responsible nanomedicine and supporting the development of safer, more effective, and globally accessible nanotherapeutic technologies.

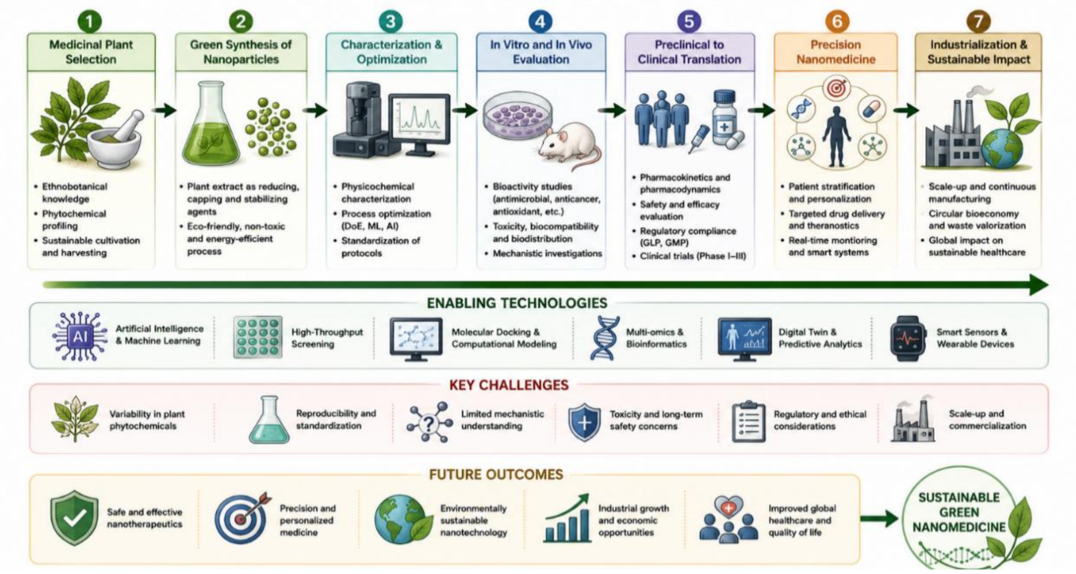

Figure 3. Future Roadmap for Sustainable Green Nanotechnology from Medicinal Plants to Clinical Nanomedicine

10. CONCLUSION

The use of green nanotechnology with medicinal plants has emerged as an eco-friendly approach for synthesizing multifunctional nanoparticles with a wide range of biomedical applications. Plant-derived phytochemicals are used as reducing, capping, and naturally stabilizing agents, and the processing is performed without harmful chemicals, resulting in biocompatible nanomaterials with greater therapeutic potential. They have antimicrobial, anticancer, antiviral, anti-inflammatory, antidiabetic, wound healing, drug delivery and diagnostic properties that have been demonstrated. Moreover, the application of AI, machine learning, molecular docking, and advanced characterization techniques has significantly advanced the clinical applications of green nanomedicine. But there are several hurdles, including reproducibility, standardization, large-scale manufacturing, regulatory approval and long-term safety evaluation, to the commercialization of these devices. The future should be dedicated to standardized synthesis procedures, extensive toxicological testing, harmonizing international regulations, and extensive clinical validation. In conclusion, medicinal plants are considered a promising platform to develop safe, sustainable and innovative nanomedicines that can contribute to precision healthcare and biomedical innovation without affecting the environment.

ABBREVIATIONS

AgNPs, Silver Nanoparticles; AuNPs, Gold Nanoparticles; ZnO NPs, Zinc Oxide Nanoparticles; CuO NPs, Copper Oxide Nanoparticles; FeNPs, Iron Oxide Nanoparticles; AI, Artificial Intelligence; ML, Machine Learning; DLS, Dynamic Light Scattering; FTIR, Fourier Transform Infrared Spectroscopy; XRD, X-Ray Diffraction; SEM, Scanning Electron Microscopy; TEM, Transmission Electron Microscopy; EDX, Energy-Dispersive X-ray Spectroscopy; TGA, Thermogravimetric Analysis; UV–Vis, Ultraviolet–Visible Spectroscopy; MRI, Magnetic Resonance Imaging; CT, Computed Tomography; PET, Positron Emission Tomography; ROS, Reactive Oxygen Species; LCA, Life Cycle Assessment; FDA, Food and Drug Administration; EMA, European Medicines Agency; ISO, International Organization for Standardization; OECD, Organisation for Economic Co-operation and Development; GMP, Good Manufacturing Practice.

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Author Contributions: All authors contributed substantially to the conception, literature review, manuscript preparation, critical revision, and approval of the final version of the manuscript.

Ethical Approval: Ethical approval was not required because this study is a review article based exclusively on published literature.

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