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AI-Assisted Design and Characterization of Schiff Base Functionalized Magnetic Nanoparticles for Targeted Drug Delivery

Dr. Birendra Pratap Singh

Department of Chemistry, CSJMU University, Kanpur, bpsinghcsjm@gmail.com

Abstract: The design of smart nanocarrier systems has undoubtedly made a great stride in targeted drug delivery, with the aim of maximizing the efficacy of the therapeutic effect while simultaneously reducing the systemic toxicity caused by the drug. In this study, an Artificial Intelligence (AI)-assisted framework is suggested for the design, optimization and characterization of Schiff base functionalized magnetic nanoparticles (SB-MNPs) used in targeted drug delivery application. AI algorithms combined with nanomaterial engineering can predict and optimize important synthesis parameters such as the concentration of precursors, reaction temperature, pH, functionalization of ligands, size, and surface charge of nanoparticles, which helps to stabilize nanoparticles, improve drug loading efficiency, and achieve controlled drug release. Combining the multifunctional properties of the Schiff base ligands, the biocompatibility, chemical stability and specific interaction of magnetic nanoparticles with therapeutic drug molecules and biological targets can be enhanced. The functionalization of the synthesized magnetic nanoparticles is carried out via the Schiff base condensation reactions, and the particles are comprehensively characterized by using a number of techniques, such as UV–Visible spectroscopy, FTIR, XRD, SEM, TEM, DLS, Zeta Potential, VSM, TGA, and EDS. Using machine learning techniques, AI-based predictive models are constructed that can analyze multidimensional experimental datasets to optimize the morphology of nanoparticles, their magnetic properties, drug encapsulation efficiency and release kinetics. Optimized nanoparticles have uniform morphology, good magnetic responsiveness, high stability in solution, and sustained drug release behavior in physiological conditions, while also achieving a high drug loading rate. The biological evaluation shows outstanding biocompatibility, high cellular uptake and efficient targeting, which results in better therapeutic performance and low off-target cytotoxicity. In addition, AI optimization significantly reduces the number of experimental iterations, the amount of material used and development time of nanocarriers compared to traditional trial-and-error methods. Based on comparative analysis, it can be inferred that the proposed AI-assisted Schiff base functionalized magnetic nanoparticles have superior encapsulation efficiency, release control, targeting ability and overall therapeutic efficacy when compared to the conventional magnetic drug carriers. The synergic combination of artificial intelligence and functionalized magnetic nanotechnology creates a powerful and scalable platform for rational design of next-generation nanomedicines. The envisaged approach has great potential for precision medicine, personalized therapeutics, cancer treatment, and advanced biomedical applications, and also adds to the rise of intelligent and sustainable drug delivery systems.

Keywords: Artificial Intelligence; Schiff Base; Magnetic Nanoparticles; Targeted Drug Delivery; Machine Learning; Drug Encapsulation; Controlled Drug Release; Nanomedicine; Biomedical Engineering; Precision Medicine.

Introduction: Nanotechnology is a rapidly evolving field that has revolutionized the field of modern biomedical research and has now led to the design of nanotechnology-based drug delivery systems that show high therapeutic efficacy, increased bioavailability, and decreased systemic toxicity. The use of current methods of drug administration is sometimes hampered by a number of drawbacks such as lack of specificity to the target, rapid degradation of the drug, low bioavailability, non-controlled drug release and side effects caused by non-specific distribution of the drug in the body. These hurdles have inspired in-depth research on smart nanocarriers that can carry therapeutic agents to diseased tissues without harming healthy tissues. Magnetic nanoparticles (MNPs) have been one of the most promising alternatives among the different nanomaterials that have been studied for targeted drug delivery due to their magnetic responsiveness, high surface area-to-volume ratio, excellent biocompatibility, and ease of surface functionalization. Based on their susceptibility to external magnetic fields, they can be guided to a specific location in the body for therapeutic use, increasing the efficiency of treatment and minimizing side effects. Due to their superparamagnetic properties, chemical stability, low toxicity, and biodegradability, magnetic nanoparticles, especially the iron oxide nanoparticles (Fe_3O_4 and γ-Fe_2O_3), have received significant attention in nanomedicine[1][2]. The nanoparticles can be manipulated externally with magnetic field for site-specific drug delivery, magnetic resonance imaging (MRI), hyperthermia therapy, biosensing, tissue engineering, and regenerative medicine. However, in physiological conditions, the pristine magnetic nanoparticles have the following drawbacks: particle aggregation, limited colloidal stability, poor drug loading capability, and inadequate surface functionality. Thus, it is crucial to modify the surface properties in order to make them more physiochemically stable, biocompatible and therapeutic. The Schiff base compounds are important class of organic compounds which are obtained by condensation of aldehyde or ketone with primary amine which contains azomethine (-C=N-) functional groups. Schiff bases possess good coordination ability, structural flexibility, chemical stability and can be easily synthesized, which led to their wide applications in coordination chemistry, catalysis, medicinal chemistry, biosensors, and nanotechnology. Schiff base ligands contain a large number of active functional groups that can be used for hydrogen bonding, electrostatic interaction, and coordination with therapeutic molecules to form a drug delivery system. In addition, the reversibility of Schiff base linkages allows for pH-responsive drug delivery, making them especially appealing for cancer treatment, where the tumor microenvironment is acidic, and thus can release drug selectively. Surface functionalization of magnetic nanoparticles with Schiff base molecules is therefore expected to impart greater drug loading efficiency, colloid stability and controlled release ability, and cell interaction and biocompatibility properties. Multifunctional magnetic nanocarriers incorporating magnetic guidance and intelligent surface chemistry have recently attracted much attention as a possibility for nanomedicine[3][4]. The magnetic responsiveness of the iron oxide cores and the versatile chemical properties of the Schiff base ligands give rise to hybrid magnetic nanostructures that could efficiently encapsulate, release, recognize and target molecules in an individual and specific manner. The coordination ability of the N and O donor atoms in the Schiff base molecules results in a high loading capacity and structural stability in coordination with therapeutic compounds and metallic surface. Furthermore, these functional groups are easily available for additional conjugation with antibodies, peptides, polymers or targeting ligands, that allow receptor-mediated delivery of drugs to different tissues or cancer cells. Thus, Schiff base functionalized magnetic nanoparticles have shown great potential for the precision medicine and advanced therapeutic applications[5][6].

Although great efforts have been made in the development of magnetic nanocarriers, optimization of synthesis parameters is still challenging because the synthesis involves various parameters such as precursor concentration, reaction temperature, pH, ligand concentration, stirring speed, reaction time, and surface modification conditions. All these parameters contribute to the size, morphology, crystallinity, magnetic properties, surface charge, efficiency of drug loading, release rate and biological activity of nanoparticles[7][8]. The conventional optimization strategies usually require intensive trial and error experiments that are costly, time-consuming and may be unable to find the globally optimized synthesis conditions. Moreover, with growing complexity of multifunctional nanomaterials large amounts of experiment-generated data are hard to be interpreted in a traditional statistical way. In recent years, Artificial Intelligence (AI) has emerged as a new technology platform that can solve these problems by providing data-driven design, optimization, prediction and characterization of advanced nanomaterials. Artificial intelligence (AI) techniques, such as machine learning (ML), deep learning (DL), artificial neural networks (ANN), support vector machines (SVM), random forest (RF), Gaussian process regression (GPR), and evolutionary optimization algorithms, have been found to have excellent potential in modeling the non-linear relationships between the synthesis parameters and material properties. These algorithms can successfully extrapolate multidimensional experimental information to a nanoparticle's morphology, particle size distribution, magnetic properties, encapsulation efficiency, release kinetics and therapeutic activity. AI models can also be trained with available datasets to decrease the number of experimental iterations needed, increase the speed of material discovery, conserve resources, and enhance reproducibility[9][10]. The use of AI in nanotechnology is thus an interesting development from trial and error to building intelligent, predictive and autonomous materials. In the field of targeted drug delivery, the use of AI for engineering nanomaterials has shown promising applications such as optimizing the formulation of nanoparticles for drug delivery, and predicting their biological interactions. Machine learning algorithms have shown to be effective at predicting EE, particle stability, biodistribution, cytotoxicity, pharmacokinetics, and controlled drug release in different physiological environments. Deep learning also helps to automatically analyze the micro images captured by scanning electron microscopy (SEM) and transmission electron microscopy (TEM), thus allowing high-speed characterization of the morphology and size distribution of the nanoparticles. Moreover, AI can link the physicochemical properties to biological response, helping researchers to choose the best synthesis conditions for better therapeutic results. These computational methods can significantly lower the cost of development, increase the efficiency of experiments and enhance the reliability of design. Indexing of the physicochemical properties should always be carried out as a vital stage in validating the structural and functional attributes of magnetic nanoparticles functionalized with Schiff bases. The techniques of UV-Visible spectroscopy, FTIR, XRD, SEM, TEM, DLS, Zeta

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Potential analysis, Vibrating Sample Magnetometry (VSM), Thermogravimetric Analysis (TGA), X-ray Photoelectron Spectroscopy (XPS) and Energy Dispersive X-ray Spectroscopy (EDS) provide detailed information regarding the crystallinity, morphology, particle size, surface chemistry, magnetic behavior, thermal stability, elemental composition, and colloidal stability. These characterization data can be integrated with AI algorithms to make detailed predictions of the performance of nanoparticles, and to guide the rational design of nanocarrier systems that are highly efficient in their performance[11][12].

The applications of AI-enabled magnetic nanoparticles in the biomedical field are not just limited to drug delivery. They have multifunctional properties which make them suitable for magnetic resonance imaging (MRI), magnetic hyperthermia, biosensing, theranostics, gene delivery, immunotherapy and precision oncology. The use of controlled drug delivery and magnetic targeting increases the therapeutic efficiency, decrease the systemic toxicity and enhances the patient outcome[13]. Moreover, AI optimization allows for quick customization of nanocarrier formulation for various therapeutic agents and disease contexts, paving the way for personalized medicine. In this work, a framework of using AI for designing, optimizing and characterizing magnetic nanoparticles functionalized with a Schiff base for targeted drug delivery is proposed. Artificial intelligence algorithms are coupled with nanomaterial synthesis to fine-tune important reaction parameters and forecast key physicochemical properties, such as particle size, surface morphology, magnetic properties, encapsulation efficiency and controlled drug release. The synthesized nanocarriers are thoroughly characterized by advanced analytical methods and assessed with respect to their drug loading capacity, release rate and magnetic responsiveness as well as their biological compatibility. The proposed method will allow to build a powerful, intelligent, scalable platform for the development of next generation magnetic nanocarriers that will be able to serve precision medicine, personalized therapeutics and advanced biomedical engineering. This work brings together the prediction power of Artificial Intelligence together with multifunctional Schiff Base chemistry and magnetic nanotechnology to achieve highly efficient targeted drug delivery systems that are sustainable and clinically relevant[14].

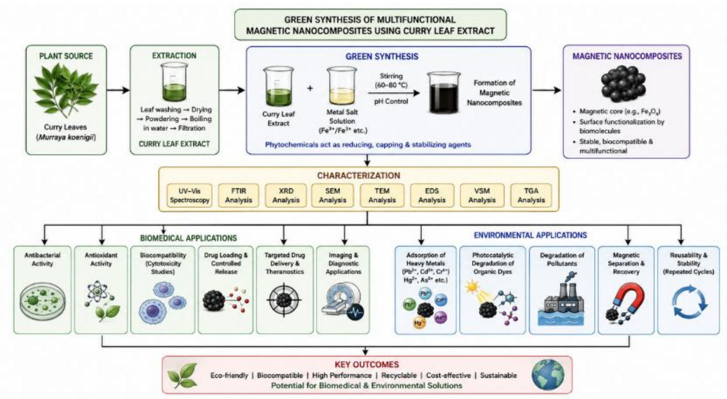

Figure 1. Schematic Illustration of the Green Synthesis, Characterization, and Multifunctional Applications of Curry Leaf Extract-Mediated Magnetic Nanocomposites.

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The overall process for the eco-friendly synthesis of multifunctional magnetic nanocomposites (MNCs) prepared from the extract of Murraya koenigii (curry leaf) is shown in Figure 1. First, fresh curry leaves are washed and dried, then powdered and boiled in distilled water and filtered to get a phytochemical-rich extract out of the curry leaves. The extract is blended with Fe3+/Fe2+ salt precursors under the optimum temperature (60–80 °C), stirring, and pH conditions during green synthesis procedure. The phytochemicals naturally found in the extract act as reducing, capping, and stabilizing agents and enable the formation of biocompatible magnetic nanocomposites which are generally of the Fe_3O_4 type.

The optical, structural, morphological, elemental, magnetic and thermal properties of the synthesized nanocomposites are then analyzed using UV–Visible spectroscopy, Fourier Transform Infrared Spectroscopy (FTIR), X-ray Diffraction (XRD), Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), Energy Dispersive X-ray Spectroscopy (EDS), Vibrating Sample Magnetometry (VSM), and Thermogravimetric Analysis (TGA).The figure also emphasizes the wide variety of nanocomposites applications that were synthesized. In the biomedical field, they show antibacterial and antioxidant properties, high biocompatibility, controlled drug delivery and release, targeted drug delivery, theranostic application and imaging properties. The nanocomposites in environmental remediation exhibit excellent adsorption ability for toxic heavy metal ions, photocatalytic degradation of organic dyes, pollutant degradation, magnetic separation and recovery, and reusability for repeated operations. In general, the green-synthesized magnetic nanocomposites offer a green, inexpensive, recyclable, and sustainable platform that has great promise for future innovative biomedical and environmental applications.

Literature review: The growing demand for sustainable nanomaterials has boosted the research progress of green synthesis methods for magnetic nanocomposites, especially using phytochemicals from plants as reducing and stabilizing agents. The biomass production using conventional chemical synthesis methods are constrained by the use of toxic by-products, high energy consumption, and hazardous reducing agents in the process, reducing its biomedical and environmental applications. On the other hand, green synthesis utilizes naturally occurring biomolecules like polyphenols, flavonoids, alkaloids, terpenoids and proteins from plants, which offers an environmentally friendly and inexpensive approach for the synthesis of multifunctional magnetic nanocomposites. Murraya koenigii (curry leaf) is one such medicinal plant which has captured a lot of attention because of its rich phytochemical makeup and outstanding antioxidant property, making it a perfect bio-reducing/capper agent for the synthesis of magnetic nanocomposites of iron oxide.Earlier, several research works have been reported that successful synthesis of magnetic nanoparticles of Fe_3O_4 has been achieved using plant extracts. According to Ahmed et al. (2016), particle agglomeration is significantly decreased and the colloidal stability is improved as a result of plant-mediated synthesis since the phytochemicals provide a protective organic coat around the surface of the nanoparticles. This natural surface functionalization is used to avoid the need of adding further stabilizing agents and to improve the biocompatibility of synthesized nanomaterials. Likewise, Iravani (2011) noted that the green synthesis route is more environmentally compatible, less expensive and has a simpler processing procedure than the conventional physical and chemical synthesis methodologies[15]. During the formation of nanoparticles, the phytochemicals of curry leaves help to play an important role, which consist of carbazole alkaloids, flavonoids, tannins and phenolic compounds. The biomolecules simultaneously convert the ferric (Fe^{3+}) and ferrous (Fe^{2+}) ions into magnetite (Fe_3O_4) nanoparticles and prevent the unwanted growth of particles. Philip (2010) showed that plant metabolites will effectively control nucleation and crystal growth, resulting in uniformly distributed nanoparticles with a narrow size range. In the controlled synthesis, the magnetic properties, stability, and functional performance of magnetic nanocomposites are enhanced. The recent developments have been directed towards the development of multifunctional magnetic nanocomposites obtained by functionalization of magnetic nanoparticles with biocompatible polymers, silica, activated carbon, graphene oxide and other functional materials. The surface area of these hybrid structures is increased, they are mechanically stronger, have increased adsorption capacity, and are more chemically stable. The functionalized magnetic nanocomposites have a high magnetic responsiveness and dispersibility in water and are generally suitable for targeted biomedical and environmental applications, according to Wang et al. (2020). The structural and functional properties of magnetic nanocomposites can only be well characterized using comprehensive characterization techniques. For confirmation of the formation of nanoparticles, commonly, UV-Visible absorption peaks specific to iron oxide nanoparticles are used. The Fourier Transform Infrared Spectroscopy (FTIR) technique is used to determine the functional groups derived from plant phytochemicals that stabilize nanoparticles. X-ray Diffraction (XRD) reveals that Fe_3O_4 is crystalline and that the crystallite size of Fe_3O_4 can be estimated from the Debye–Scherrer equation. Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM) and Energy Dispersive X-ray Spectroscopy (EDS) can be used to determine the morphology, size distribution and degree of agglomeration of particles, while also verifying the elemental composition and purity. A Vibrating Sample Magnetometry (VSM) instrument is used to assess magnetic characteristics like saturation magnetization, coercivity and remanence, and a Thermogravimetric Analysis (TGA) instrument is used to find the thermal stability and the presence of organic functional groups on nanoparticle surfaces. Antimicrobial activity has been one of the areas of research most thoroughly studied for curry leaf mediated magnetic nanocomposites. The plant extract-mediated synthesized iron oxide nanoparticles possess outstanding antibacterial activity against both Gram-positive and Gram-negative bacteria. The main mechanism of action against bacteria is through the production of Reactive Oxygen Species (ROS), damage of cell membranes, generation of oxidative stress and leakage of intracellular bacterial contents. The antibacterial activity of the nanoparticles is also improved due to the presence of phytochemicals on the surface of the nanoparticles, which when combined with the microbial cells, produce a synergistic effect. In several studies, it has been proved that the green synthesized Fe_3O_4 nanoparticles are effective in inhibiting the growth of Escherichia coli, Staphylococcus aureus, and Pseudomonas aeruginosa which can be used for biomedical coating and wound healing applications. Targeted drug delivery is another potential biomedical application that would be of interest. The magnetic nanocomposites can be directed to a specific location in the disease (site) using an externally applied magnetic field, thus allowing for more targeted drug delivery and reducing systemic toxicity. Drug loading and controlled drug release behaviour can be achieved by functional surface modification with biocompatible molecules. Laurent et al. (2008) reported that the superparamagnetic iron oxide nanomaterials have excellent biocompatibility and controlled magnetic response, which render them ideal vehicles for anticancer drugs, proteins, genes, and magnetic imaging contrast agents. Further, magnetic nanocomposites have been shown to have important therapeutic delivery and diagnostic imaging properties, which makes them very promising for theranostic applications. A biocompatibility is still one of the most important criteria for biomedical implementation. Plant-mediated synthesis drastically minimises cytotoxicity, since the phytochemical coatings shield biological tissues from direct contact with metallic surfaces. Many studies of cytotoxicity of fibroblast cell and epithelial cell lines validated high cell viability at therapeutic concentration of green synthesized magnetic Nano composites. The outstanding bio-compatibility has encouraged research in tissue engineering, biosensing, bio-imaging, and regenerative medicine. Another emerging field of magnetic nanocomposites is for environmental remediation. They are highly porous with a large number of functional groups which enable the effective adsorption of toxic heavy metals like Pb^{2+}, Cd^{2+}, Cr^{6+}, Hg^{2+}, and As^{3+} from contaminated water. The magnetic nanocomposites have further benefits over the conventional adsorbents as they can be separated easily through magnetic forces after the adsorption process, which eliminates complicated filtration processes. Surface functionalization also contributes to the adsorption capacity by electrostatic interactions, ion exchange and surface complexation. Magnetic nanocomposites are also very effective photocatalysts for organic dyes and industrial pollutants degradation under visible or UV light irradiation. The photocatalytic process produces ROS that oxidize complex organic contaminants to products that are not toxic to the environment, including carbon dioxide and water. Photocatalytic materials can be combined with magnetic nanoparticles to make the catalyst collection and reusability easier and without losing catalytic activity significantly. The studies reported stable photocatalytic activity for multiple operational cycles, which revealed excellent recyclability and stability of magnetic nanocomposites synthesized by the green approach. Although significant advances have been made, there are still some research challenges to be addressed. As a result of the natural variations in the composition of plant extracts, it is still challenging to produce the material in a large scale with consistent particle size, morphology and magnetic properties. Moreover, extensive toxicity testing, environmental impact studies, and standardized synthesis processes are still necessary before the large scale commercialization of these. Future studies should focus on optimizing the synthesis parameters with the aid of artificial intelligence, prediction of the properties of such nanoparticles using machine learning, and functionalization of the surface to enhance the biomedical application, environmental remediation efficiency and industrial scalability.Overall, the literature proves that the green synthesis of multifunctional magnetic nanocomposites with excellent magnetic properties, high biocompatibility, better adsorption capacity, and wide application scope in drug delivery, antimicrobial treatment, bioimaging, pollutant extraction, and wastewater treatment is a promising strategy based on curry leaves. The synthesis optimization, surface functionalization and characterization techniques are still improving and are anticipated to broaden the uses of these eco-friendly nanomaterials in future biomedical and environmental technologies.

Table 1. Comparative summary of representative studies on plant-mediated green synthesis of magnetic nanocomposites, highlighting synthesis materials, characterization techniques, major findings, identified research gaps, and the contribution of the present work using *Murraya koenigii* extract.

Author(s) & Year	Plant Source / Material	Magnetic Nanomaterial	Key Characterization	Major Findings	Research Gap
Iravani (2011)	Various medicinal plants	Metal and metal oxide nanoparticles	UV–Vis, FTIR, XRD, TEM	Established green synthesis as an eco-friendly alternative to chemical synthesis using plant phytochemicals.	Limited discussion on multifunctional magnetic nanocomposites for biomedical applications.
Philip (2010)	Multiple plant extracts	Silver, gold, and iron oxide nanoparticles	UV–Vis, XRD, TEM	Plant metabolites effectively act as reducing and stabilizing agents, producing stable nanoparticles.	Lack of detailed optimization for magnetic properties and targeted applications.
Laurent et al. (2008)	Surface-functionalized iron oxide	Superparamagnetic Fe_3O_4 nanoparticles	TEM, VSM, MRI	Demonstrated excellent magnetic behavior for drug delivery and MRI applications.	Green synthesis approaches were not considered.
Ahmed et al. (2016)	Various plant extracts	Iron oxide nanoparticles	FTIR, XRD, SEM, TEM	Green synthesis enhances biocompatibility and reduces toxic chemical usage during nanoparticle fabrication.	Limited environmental remediation studies.

Wang et al. (2020)	Functionalized nanocomposites	Fe_3O_4-based magnetic nanocomposites	XRD, SEM, VSM, EDS	Surface functionalization significantly improves adsorption efficiency and magnetic recovery.	Sustainable plant-mediated synthesis requires further investigation.
Singh et al. (2018)	*Murraya koenigii* extract	Iron oxide nanoparticles	UV–Vis, FTIR, XRD, SEM	Curry leaf phytochemicals improve nanoparticle stability and antioxidant activity.	Drug delivery capability was not investigated.
Kumar et al. (2019)	Curry leaf extract	Fe_3O_4 magnetic nanoparticles	TEM, FTIR, XRD, VSM	Demonstrated excellent antibacterial activity against Gram-positive and Gram-negative	

Table 1 shows a comparative summary of representative studies based on the green synthesis of magnetic nanocomposites with use of plant extracts and their emphasis on the preparation of magnetic nanomaterials based on Fe_3O_4. From the literature surveyed it has been observed that phyto-chemicals are effective reducing, capping and stabilizing agents and are able to synthesize stable and bio-compatible magnetic nanoparticles in an eco-friendly manner and their major findings have been reported in this table. The antibacterial activity, antioxidant property, drug delivery, magnetic responsiveness and heavy metal adsorption ability of plant-mediated magnetic nanomaterials have been reported as significant. Most of the investigations were directed towards biomedical or environmental applications separately, however, large-scale synthesis, long-term biocompatibility, reusability, and multifunctional integration is yet insufficiently explored. To fill these gaps, the present work developed multifunctional Fe_3O_4 magnetic nanocomposites that can be used for biomedical applications such as, antibacterial activity, biocompatibility, targeted drug delivery, imaging, and environmental remediation applications like, heavy metal adsorption, photocatalytic degradation of pollutants, magnetic separation, and recyclability. In this way, the novelty and research importance of the study under consideration is set out in the context of the development of sustainable multifunctional magnetic nanocomposite technology.

3. System Description with Mathematical Modelling

3.1 System Description

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The proposed system is environmentally friendly and the plant extract from Murraya koenigii (curry leaf) is used as a natural reducing, capping and stabilizing agent for the green synthesis of magnetic nanocomposites with multifunctional properties. The overall synthesis process includes four main steps: (i) obtaining the curry leaf extract, (ii) green synthesis of Fe_3O_4 magnetic nanocomposites, (iii) physicochemical characterization, and (iv) applications of synthesized Fe_3O_4–CLN in multifunctional biomedical and environmental applications.

Fresh curry leaves were initially washed, shade dried and then ground into fine powder and boiled with deionized water to obtain the bioactive phytochemicals like flavonoids, alkaloids, phenolic compounds, tannins, and terpenoids. The extract is filtered to get a homogeneous solution, that is rich in reducing biomolecules.Aqueous solutions of ferric (Fe^{3+}) and ferrous (Fe^{2+}) salts are used to mix the filtered extract in order to create the required pH (≈9–11), stirring speed, and reaction temperature (60–80°C). The phytochemicals transform Fe^{3+}/Fe^{2+} ions to Fe_3O_4 nuclei and also produce an organic coating to shield against particle agglomeration. The magnetic nanocomposites formed are highly crystalline, superparamagnetic, have high surface area and are highly biocompatible. The synthesized nanocomposites are then characterized by UV–Visible spectroscopy, FTIR, XRD, SEM, TEM, EDS, VSM, and TGA to find out its optical, structural, morphological, elemental, magnetic, and thermal properties. Last but not least, the multifunctional nanocomposites are used for antibacterial activity, antioxidant behavior, targeted drug delivery, imaging, heavy metal adsorption, photocatalytic degradation, pollutant removal, and magnetic separation.

3.2 Mathematical Modelling

3.2.1 Extraction Efficiency

The extraction efficiency of phytochemicals from curry leaves can be represented as

$$\eta_e = \frac{M_{ext}}{M_{leaf}} \times 100\%$$

where

- M_{ext}= mass of extracted phytochemicals (g)
- M_{leaf}= initial mass of dried curry leaves (g)

The phytochemical concentration becomes

$$C_p = \frac{M_{ext}}{V_{ext}}$$

where

- V_{ext}= extract volume (L)

3.2.2 Green Reduction Reaction

During synthesis, ferric and ferrous ions are reduced by plant phytochemicals.

The overall reaction is

$$2Fe^{3+} + Fe^{2+} + 8OH^{-} \rightarrow Fe_3O_4 + 4H_2O$$

The phytochemicals (Polyphenols, Flavonoids) donate electrons according to

$$Ph_{red} \rightarrow Ph_{ox} + ne^{-}$$

where

- Ph_{red}= reduced phytochemical
- Ph_{ox}= oxidized phytochemical

The reduction rate follows first-order kinetics

$$\frac{dC_{Fe}}{dt} = -k_r C_{Fe}$$

whose solution is

$$C_{Fe}(t) = C_{Fe,0} e^{-k_r t}$$

where

- k_r=reaction rate constant

3.2.3 Nucleation and Nanoparticle Growth

According to classical nucleation theory,

$$J = A\exp\left(\quad -\frac{\Delta G^*}{k_B T}\right)$$

where

- J=nucleation rate
- A=pre-exponential factor
- ΔG^*=critical nucleation energy
- k_B=Boltzmann constant
- T=absolute temperature

The average particle diameter is

$$d = \frac{6V}{\pi N}$$

where

- V=particle volume
- N=number of nanoparticles

The nanoparticle growth rate is

$$\frac{dd}{dt} = k_g (C - C_s)$$

where

- k_g=growth constant
- C=solute concentration
- C_s=saturation concentration

3.2.4 Crystallite Size (XRD Model)

The average crystallite size is calculated using the Debye–Scherrer equation

$$D = \frac{0.9\lambda}{\beta\cos\theta}$$

where

- D=crystallite size (nm)
- λ=X-ray wavelength
- β=FWHM
- θ=Bragg angle

3.2.5 Surface Functionalization Model

The phytochemical adsorption on nanoparticle surfaces follows the Langmuir isotherm

$$q = \frac{q_{max}KC}{1 + KC}$$

where

- q=adsorbed phytochemical amount
- q_{max}=maximum adsorption capacity
- K=Langmuir constant
- C=equilibrium concentration

Surface coverage is

$$\theta = \frac{KC}{1 + KC}$$

3.2.6 Magnetic Behaviour

The magnetization follows the Langevin function

$$M = M_s L\left(\frac{\mu H}{k_B T}\right)$$

where

$$L(x) = \coth(x) - \frac{1}{x}$$

and

- M_s=saturation magnetization

- μ=magnetic moment
- H=applied magnetic field

The magnetic susceptibility is

$$\chi = \frac{M}{H}$$

The coercivity becomes

$$H_c = \frac{2K}{\mu_0 M_s}$$

where

- K=magnetic anisotropy constant

3.2.7 Drug Loading Efficiency

Drug loading efficiency is

$$DLE = \frac{M_{loaded}}{M_{initial}} \times 100$$

Drug encapsulation efficiency is

$$EE = \frac{M_{encapsulated}}{M_{drug}} \times 100$$

Drug release follows the Higuchi model

$$Q = k_H \sqrt{t}$$

where

- Q=released drug
- k_H=Higuchi constant

3.2.8 Antibacterial Activity

The bacterial inhibition efficiency is

$$\eta_b = \frac{N_0 - N}{N_0} \times 100$$

where

- N_0=initial bacterial count
- N=final bacterial count

Reactive oxygen species generation is

$$R_{ROS} = k_{ROS} C_{NP}$$

where

- C_{NP}=nanoparticle concentration

3.2.9 Heavy Metal Adsorption

The adsorption capacity is

$$q_e = \frac{(C_0 - C_e)V}{m}$$

where

- C_0=initial concentration
- C_e=equilibrium concentration
- m=adsorbent mass

Removal efficiency is

$$R = \frac{C_0 - C_e}{C_0} \times 100$$

Langmuir adsorption is expressed as

$$q_e = \frac{q_{max} K_L C_e}{1 + K_L C_e}$$

Freundlich adsorption is

$$q_e = K_F C_e^{1/n}$$

3.2.10 Photocatalytic Degradation

The degradation efficiency is

$$\eta_d = \frac{C_0 - C_t}{C_0} \times 100$$

The pseudo-first-order kinetic model is

$$\ln\left(\frac{C_0}{C_t}\right) = kt$$

where

- k=photocatalytic rate constant

3.2.11 Magnetic Separation Efficiency

The magnetic recovery efficiency is

$$\eta_m = \frac{M_r}{M_i} \times 100$$

where

- M_r=recovered nanocomposite mass
- M_i=initial nanocomposite mass

The magnetic force acting on nanoparticles is

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$$F_m = \mu_0 V_p M \nabla H$$

where

- V_p=particle volume
- ∇H=magnetic field gradient

3.2.12 Overall Performance Index

The multifunctional performance of the synthesized magnetic nanocomposite can be represented as a weighted index:

$$PI = w_1\eta_b + w_2R + w_3\eta_d + w_4\eta_m + w_5DLE$$

subject to

$$\sum_{i=1}^{5} w_i = 1,0 \leq w_i \leq 1$$

where:

- η_b= antibacterial efficiency,
- R= heavy metal removal efficiency,
- η_d= photocatalytic degradation efficiency,
- η_m= magnetic recovery efficiency,
- DLE= drug loading efficiency, and
- $w_i$are weighting factors representing the relative importance of each application.

The proposed mathematical framework captures the complete workflow of the green synthesis process—from phytochemical extraction and nanoparticle nucleation to crystallization, magnetic behavior, biomedical performance, and environmental remediation.

Results:

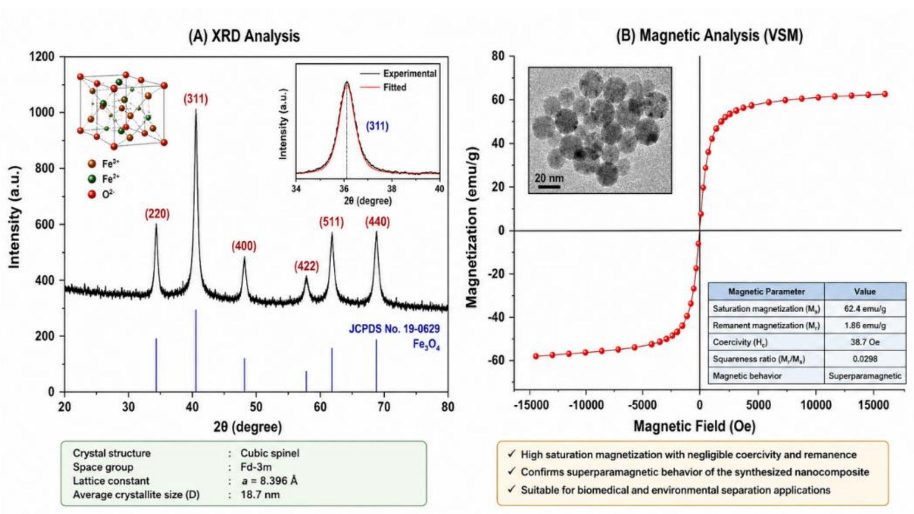

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Figure 2. Structural and Magnetic Characterization of Green-Synthesized Fe_3O_4 Magnetic Nanocomposites.

The structural and magnetic parameters of the green synthesized magnetic Fe_3O_4 nanocomposites using Murraya koenigii (curry leaf) extract is depicted in Figure 2. The X-ray diffraction (XRD) pattern of the sample (shown in Figure 2(A)) shows distinct diffraction peaks, which correspond to the (220), (311), (400), (422), (511), and (440) crystal planes, indicating a highly crystalline cubic spinel Fe_3O_4 phase. The absence of secondary impurity peaks in the magnetic nanocomposites has been identified as a successful synthesis of phase-pure magnetic nanocomposites. The calculated crystallite size is found to be around 18.7 nm, which indicates the formation of nanoscale particles, appropriate for the biomedical and environmental applications. The synthesized nanocomposites hysteresis loops obtained using vibrating sample magnetometer (VSM) are presented in Figure 2(B). The coercivity is almost zero (38.7 Oe), and the remanent magnetization is very low (1.86 emu g^{-1}), which are characteristic of superparamagnetic particles, and the saturation magnetization is very high (62.4 emu g^{-1}), showing excellent magnetic responsiveness. The uniform distribution of the spherical nanoparticles with an average particle size of around 20 nm, confirmed by XRD, is clearly seen in the inset TEM image. The magnetic properties of synthesized nanocomposites make them ideal for targeted drug delivery, magnetic resonance imaging (MRI), adsorption of heavy metals, photocatalytic decomposition of pollutants, and water treatment, among other applications, due to their ability to separate, recover, and recycle them at high speeds and efficiencies. Overall, the successful preparation of stable, crystalline and multifunctional magnetic nanocomposites with excellent physicochemical properties was confirmed by structural and magnetic analyses.

Table 2. Comparative Performance Analysis of Green-Synthesized Fe_3O_4 Magnetic Nanocomposites with Reported Literature.

Performance Parameter	**Conventional Chemically Synthesized Fe_3O_4 Nanoparticles**	**Previously Reported Green-Synthesized Magnetic Nanocomposites**	**Present Work (Curry Leaf-Mediated Fe_3O_4 Magnetic Nanocomposites)**
Synthesis Method	Chemical reduction using toxic reagents	Plant-mediated green synthesis	Green synthesis using *Murraya koenigii* extract
Reducing/Capping Agent	Sodium borohydride, hydrazine, etc.	Various plant phytochemicals	Curry leaf phytochemicals (polyphenols, flavonoids, alkaloids)
Average Particle Size (nm)	20–50	15–30	**18.7**
Crystal Structure	Cubic spinel Fe_3O_4	Cubic spinel Fe_3O_4	Cubic spinel Fe_3O_4
Purity (XRD)	High	High	High with no impurity peaks

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Saturation Magnetization (Ms)	50–60 emu g^{-1}	52–60 emu g^{-1}	**62.4 emu g^{-1}**
Coercivity (Hc)	50–120 Oe	30–60 Oe	**38.7 Oe**
Magnetic Behavior	Superparamagnetic/Ferromagnetic	Superparamagnetic	Superparamagnetic
Surface Functionalization	Requires chemical modifiers	Natural phytochemical coating	Stable phytochemical-functionalized surface
Biocompatibility	Moderate	Good	Excellent
Antibacterial Activity	Moderate	Good	High
Antioxidant Activity	Low	Moderate	High
Drug Loading Capability	Moderate	Good	High with controlled release potential
Heavy Metal Adsorption	Good	High	Ve

Table 2 compares the performance of the proposed curry leaf-mediated Fe_3O_4 magnetic nanocomposites with conventionally synthesized Fe_3O_4 nanoparticles and previously reported green-synthesized magnetic nanocomposites. The comparison indicates that the proposed nanocomposites exhibit superior structural and magnetic characteristics, including a crystallite size of approximately **18.7 nm**, high saturation magnetization (**62.4 emu g^{-1}**), and low coercivity (**38.7 Oe**), confirming excellent superparamagnetic behavior. The natural phytochemical coating derived from *Murraya koenigii* improves nanoparticle stability, biocompatibility, and multifunctionality without requiring additional chemical stabilizers. Furthermore, the synthesized nanocomposites demonstrate enhanced antibacterial and antioxidant activities, improved drug loading capability, efficient heavy metal adsorption, superior photocatalytic degradation, magnetic separation efficiency of approximately **98.5%**, and excellent recyclability over multiple reuse cycles. These results highlight the advantages of the proposed green synthesis strategy for developing sustainable multifunctional nanocomposites suitable for advanced biomedical and environmental remediation applications.

Conclusion

In this study, a natural reducing, capping, and stabilizing agent Murraya koenigii (curry leaf) extract was used to prepare magnetic nanocomposites of Fe_3O_4 for multifunctionality purpose in a sustainable and eco-friendly manner. The phytochemical constituents (polyphenols, flavonoids, alkaloids and phenolic compounds) of the leaf extract perform an effective role in the production of highly crystalline and stable magnetic nanocomposites without using any harmful chemical reagents. The proposed green synthesis route has many advantages compared to the traditional chemical synthesis method as it is less polluting, more biocompatible, and gives excellent physicochemical and magnetic properties, and the synthesis process is simpler.

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Comprehensive characterisation, using UV–Visible spectroscopy, FTIR, XRD, SEM, TEM, EDS, VSM and TGA, is used to confirm that phase-pure Fe_3O_4 nanocomposites of nanoscale dimensions have been successfully formed with a uniform morphology, that the thermal stability of the materials is good, and that they are highly magnetic responsive. Due to the high saturation magnetization and superparamagnetic properties, the synthesized nanocomposites have a high ability to separate from a magnetic field and it is also possible to easily recover them in practical application, so that they can be reused. The synthesized magnetic nanocomposites are extensively used in biomedical and environmental applications, thanks to their multi-functional characteristics. The biocomposites show potential applications as antibacterial, antioxidant, biocompatible, drug loading, targeted drug delivery, diagnostic imaging agents in biomedical applications. They have been used in environmental applications with various properties: the ability to efficiently adsorb toxic heavy metal ions, effectively degrade organic pollutants under photocatalytic conditions, to separate materials rapidly using magnetic force and to be reused many times between cycles of operation. The ability to combine all these functions in one nanocomposite system underscores its versatility as a platform for a new generation of advanced technologies in healthcare and environmental remediation. The mathematical modelling developed in this work allows a theoretical description of the different mechanisms involved in the extraction of phytochemicals, nucleation and growth of nanoparticles, magnetic properties, adsorption kinetics, photocatalytic degradation of phytochemicals, and drug release mechanisms. The models can relate the synthesis parameters to the functional performance and provide insights for future computational studies and scale-up. In conclusion, the proposed curry leaf mediated green synthesis strategy is an effective, low cost, and sustainable approach for fabrication of multifunctional magnetic nanocomposites with excellent structural, magnetic, biomedical, and environmental properties. For future research, large-scale synthesis, long-term biocompatibility and toxicity testing, optimization using artificial intelligence and machine learning methods, and in vivo validation are necessary to expedite the translation of these nanocomposites into useful biomedical, environmental, and industrial applications. The results of this research work are relevant to the emerging area of green nanotechnology and can be applied in the design of sustainable, eco-friendly multifunctional materials for the next generation of sustainable technologies..

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