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EVALUATION OF SOLVENT POLARITY ON THE NANOPARTICLE-FORMING POTENTIAL OF SOLANUM VIRGINIANUM LEAF EXTRACTS

A Comparative Phytochemical, FTIR, and Mechanistic Feasibility Study

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Abstract: The green synthesis of silver nanoparticles via plant-mediated reduction depends fundamentally on the presence of functional biomolecules capable of electron donation and surface stabilization. In the present study, dried Solanum virginianum leaves were extracted separately by 72 h maceration in n-hexane and methanol, yielding 1.60% and 13.60% crude extract, respectively representing an approximately 8.5-fold higher extractive yield for methanol. Qualitative phytochemical screening and FTIR spectroscopy were employed to map functional group profiles and evaluate their capacity to drive Ag^+ bio reduction under solar irradiation. Following aqueous reconstitution, the methanolic extract (CMM) demonstrated distinct bio reduction potential upon reaction with 1 mM $AgNO_3$, yielding a prominent chromatic transition to dark reddish-brown consistent with characteristic of colloidal metallic silver (Ag^0). In contrast, the hexane extract (CMH) exhibited no discernible color change, remaining inactive. Spectral profiling revealed that CMM was enriched with broad hydrogen-bonded O–H stretching (3326.21 cm^{-1}) and intense C–O/C–N stretching vibrations (1016.95 cm^{-1}), representing active electron-donating moieties. Conversely, CMH was dominated by lipophilic aliphatic chains (2856.84–2934.03 cm^{-1}) and an ester carbonyl band (1734.55 cm^{-1}) lacking accessible reduction centers. These findings establish a direct mechanistic link between solvent polarity, secondary metabolite extraction, and the feasibility of plant-assisted silver reduction, identifying methanol as an appropriate solvent system for future nano formulation studies involving S. virginianum leaves.

Index Terms: Solanum virginianum; phytochemical; FTIR; solvent polarity; green synthesis; silver nanoparticles; bio reduction feasibility.

I. INTRODUCTION

Plants represent an indispensable natural reservoir of structurally diverse bioactive secondary metabolites, including phenolics, flavonoids, alkaloids, terpenoids, saponins, and glycosides. These phytochemicals have garnered extensive research interest across pharmaceutical sciences, agricultural biotechnology, and green nanomaterials synthesis. The extraction efficiency and qualitative composition of these phytoconstituents are heavily dictated by extraction parameters, most notably solvent polarity, extraction duration, solid-to-liquid ratio, and temperature. Selecting a solvent system with suitable dielectric and thermodynamic properties is therefore a decisive prerequisite for isolating targeted biomolecules with defined functional capabilities.

Solanum virginianum Burm, widely known as yellow-berried nightshade, is a prickly perennial herb belonging to the family Solanaceae. Distributed extensively across the tropical and subtropical regions of the Indian subcontinent, Southeast Asia, and Australia, S. virginianum holds a distinguished position in classical Ayurvedic medicine as an integral component of the polyherbal formulation Dashamoola (Devi et al., 2015). Various morphological parts of S. virginianum have been reported to exhibit pronounced antimicrobial, anti-inflammatory, antipyretic, anthelmintic, and antioxidant properties. Previous investigations have established that extraction in solvents of differing polarities such as petroleum ether, chloroform, methanol, ethanol, and water yields markedly divergent secondary metabolite profiles and bioactivity spectra (Anburaj, 2019).

In recent years, the biogenic synthesis of noble metallic nanoparticles via plant extracts has emerged as a rapid, cost-effective, and environmentally sustainable alternative to traditional chemical and physical methods. In this green synthesis paradigm, plant secondary metabolites serve dual roles as thermodynamic electron-donating reducing agents and steric capping ligands that stabilize colloidal nanoparticles against agglomeration. Among metallic nanomaterials, silver nanoparticles (AgNPs) have attracted preeminent focus owing to their unique localized surface plasmon resonance (SPR) optical characteristics and potent broad-spectrum antibacterial efficacy (Marukurti et al., 2025). Previous studies utilizing S. virginianum fruit and berry extracts have demonstrated successful AgNP formation, implicating phenolic hydroxyl (O–H, ~3436–3660 cm^{-1}), primary amine/amide (C–N/N–H, ~1021–3375 cm^{-1}), and carboxylic functionalities in the bio reduction and colloidal stabilization of Ag^+ (Anburaj, 2019; Basha, Soundhararajan & Srinivasan, 2025).

Mechanistically, the bio reduction of monovalent silver ions (Ag^+) to zero-valent metallic silver nuclei (Ag^0) is driven by electron- and hydrogen-donating functional groups—primarily phenolic hydroxyls (–OH), free amines ($–NH_2$), and conjugated carbonyls (C=O)—predominantly present in polyphenols, flavonoids, and reducing sugars (Zuhrotun, Oktaviani & Hasanah, 2023; Miyanda & Parveen, 2026). Because these reactive functional groups are concentrated within polar and semi-polar phytoconstituents, the polarity of the extraction solvent directly dictates whether an extract possesses the chemical reducing power

necessary for nanoparticle synthesis. The present investigation provides this empirical baseline, offering a clear mechanistic foundation for solvent selection in plant-mediated nano-biotechnology.

II. MATERIALS AND METHODS

2.1 Plant material and reagents

Fresh, healthy leaves of Solanum virginianum were collected, washed thoroughly with running tap water followed by double-distilled water to eliminate surface detritus, and shade-dried at ambient room temperature (25°C –28 °C) until reaching a constant weight. Analytical-grade n-hexane, methanol, silver nitrate and standard phytochemical reagents were procured from commercial suppliers. Double-distilled water was utilized throughout all aqueous preparations.

2.2 Solvent extraction and yield determination

The shade-dried S. virginianum leaves were pulverized into a fine, uniform powder using an electric blender. For extraction, 10.0 g of dry leaf powder was accurately weighed and placed into separate conical flasks containing 100 mL of either n-hexane (non-polar, relative polarity = 0.009) or methanol (polar, relative polarity = 0.762), maintaining a solid-to-liquid ratio of 1:10 (w/v). Maceration was carried out for 72 h at ambient room temperature (25–28 °C) with regular intermittent agitation. After 72 h, the mixtures were filtered through Whatman No. 1 filter paper. The filtrates were concentrated to complete dryness using a thermostatically controlled water bath (40–45 °C) to yield the crude dry extracts, designated CMH (crude hexane extract) and CMM (crude methanol extract). Extractive percentage yields were computed using the following standard equation:

$$\text{Percentage Extractive Yield (\%)} = \frac{\text{Weight of dried crude extract (g)}}{\text{Weight of initial plant material (10.0 g)}} \times 100$$

2.3 Qualitative phytochemical screening

Crude extracts (CMH and CMM) were systematically screened for major secondary metabolite classes using standard pharmacognostic chemical assays. Mayer's and Wagner's tests were employed for alkaloids; Fehling's and Molisch's tests for carbohydrates and reducing sugars; Salkowski's reaction for phytosterols; the ferric chloride ($FeCl_3$) and gelatin tests for tannins or phenolics; the ninhydrin and xanthoproteic tests for proteins and amino acids; the persistent froth test for saponins; the filter paper spot test for fixed oils or lipids; and the alkaline reagent and Shinoda reduction tests for flavonoids. Assays were conducted in triplicate to verify reproducibility.

2.4 Colorimetric feasibility assessment of Ag^+ bio reduction

To evaluate nanoparticle-forming feasibility, the dried extracts were reconstituted. For CMM, 100 mg of dry extract was dissolved in 20 mL of double-distilled water. For CMH, 100 mg was dissolved in 2 mL of dimethyl sulfoxide (DMSO) and diluted to 20 mL with double-distilled water to ensure homogeneous aqueous miscibility. Each reconstituted extract solution (20 mL) was subsequently combined with 80 mL of freshly prepared 1 mM aqueous $AgNO_3$ solution in 100 mL volumetric flasks. The reaction mixtures were thoroughly homogenized and exposed to direct natural sunlight (solar irradiance ~800–950 W/m²) for 48 h at ambient temperature (28–32 °C) to facilitate solar-assisted photocatalytic bio reduction. Visual observation of chromatic shifts was recorded at regular intervals. The emergence of a dark reddish-brown colloidal coloration served as the primary qualitative benchmark for localized surface plasmon resonance (SPR) excitation and successful reduction of Ag^+ to Ag^0.

2.5 FTIR spectral characterization

Fourier Transform Infrared (FTIR) spectral analyses of the dry CMH and CMM extracts were recorded over the wavenumber range of 4000–400 cm^{-1} in transmittance mode using a spectrophotometer equipped with a deuterated triglycine sulfate (DTGS) detector. Characteristic vibrational absorption peaks were identified and assigned to corresponding chemical functional groups by referencing standard infrared correlation tables and published literature for Solanaceae species.

III. RESULTS AND DISCUSSION

3.1 Comparative extraction yield

Maceration of S. virginianum leaf powder in solvents of contrasting dielectric constants resulted in substantial variations in extractive recovery (Table 1). Extraction with non-polar n-hexane (CMH) produced 0.16 g of crude extract from 10.0 g of dry leaf powder (1.60% w/w), whereas polar methanol (CMM) yielded 1.36 g (13.60% w/w), representing an ~8.5-fold higher extractive recovery for the polar solvent system.

This marked disparity reflects the principle of 'like dissolves like'. Methanol possesses a high dielectric constant ($\varepsilon = 32.7$) and strong hydrogen-bonding capacity, enabling extensive dissolution of polar and semi-polar secondary metabolites including polyphenols, flavonoids, glycosides, and oligosaccharides. Conversely, n-hexane ($\varepsilon = 1.88$) acts as a strictly lipophilic solvent, solubilizing only non-polar epicuticular waxes, phytosterols, and fatty acyl derivatives, which comprise a minor mass fraction of the leaf tissue.

Table 1. Comparative extractive yield of Solanum virginianum leaves in solvents of contrasting polarity.

Sr. No.	Extract Code	Extraction Solvent	Dry Plant Material (g)	Crude Extract Obtained (g)	Percentage Yield (% w/w)
1	CMH	n-Hexane	10.0	0.16	1.60%
2	CMM	Methanol	10.0	1.36	13.60%

3.2 Phytochemical profiling of extracts

Qualitative phytochemical screening highlighted distinct compositional profiles between CMH and CMM (Table 2). Polar methanol successfully extracted major classes of reducing agents, demonstrating positive reactions for alkaloids, carbohydrates/reducing sugars, flavonoids, phytosterols, and polar amino acid/protein fragments. In contrast, n-hexane selectively extracted non-polar lipids, fixed oils, and phytosterols, alongside minor lipophilic alkaloid and flavonoid aglycones.

Tannins and saponins were not detected in either extract under the evaluated maceration conditions. The absence of fixed oils in CMM and the absence of hydrophilic proteinaceous residues in CMH are consistent with the chemical partitioning behaviors expected across non-polar hydrocarbon versus polar alcoholic solvent matrices.

Table 2. Qualitative phytochemical screening of Solanum virginianum leaf extracts.

Phytoconstituent Class	**Hexane Extract (CMH)**	**Methanol Extract (CMM)**
Alkaloids	+ve	+ve
Carbohydrates	+ve	+ve
Phytosterols and Steroids	+ve	+ve
Tannins	-ve	-ve
Proteins and Amino Acids	-ve	+ve
Saponins	-ve	-ve
Fixed Oils and Lipids	+ve	-ve
Flavonoids	+ve	+ve

3.3 Visual monitoring and nanoparticle-forming feasibility

Upon mixing the reconstituted leaf extracts with 1 mM aqueous $AgNO_3$ and exposing the solutions to sunlight, a clear, solvent-dependent visual divergence emerged (Table 3). The methanolic reaction mixture (CMM + Ag NO_3) underwent a distinct, progressive color transformation from an initial pale yellow to a deep reddish-brown within solar exposure. This chromatic transition is the diagnostic visual hallmark of $Ag^+ \rightarrow Ag^0$ reduction, originating from the excitation of localized Surface Plasmon Resonance (SPR) in newly nucleated nanoscale metallic silver colloids (Anburaj, 2019; Basha et al., 2025; Marukurti et al., 2025).

In contrast, the hexane extract mixture (CMH + Ag NO_3) displayed no discernible color shift across the entire 48 h period, remaining pale and translucent. This lack of visual reaction confirms that n-hexane failed to extract the functional biomolecules required to drive the reduction of monovalent silver ions under identical photochemical conditions.

Methodological Note on Physical Characterization: Visual color transition serves as an effective preliminary screening tool to establish chemical feasibility. Definitive physical verification—including average hydrodynamic diameter, polydispersity index, crystalline face-centered cubic (fcc) lattice planes, and surface charge stability—requires subsequent instrumental validation via UV-Visible spectrophotometry (monitoring the characteristic SPR absorption maximum at ~400–450 nm), Dynamic Light Scattering (DLS), Zeta potential, X-ray Diffraction (XRD), and High-Resolution Transmission/Scanning Electron Microscopy (HR-TEM/SEM). Nevertheless, within this comparative screening framework, the colorimetric divergence establishes a definitive baseline regarding the reducing capability of the two extracts.

Table 3. Visual colorimetric observations and silver bio reduction` feasibility of Solanum virginianum extracts.

Extract Code	**Visual Observation (1 mM $AgNO_3$ + 48 h Solar Irradiation)**	**Bio reduction Feasibility Inference**
CMH (n-Hexane)	No color change observed; solution remained pale translucent	Inactive: Ag^+ bio reduction did not occur
CMM (Methanol)	Distinct chromatic transition to dark reddish-brown (SPR excitation)	Feasible: Rapid $Ag^+ \rightarrow Ag^0$ reduction and nucleation

3.4 FTIR spectral mapping and functional group correlation

FTIR spectroscopy provided clear structural insight into the chemical functional groups isolated by each solvent system (Tables 4a and 4b). The methanolic extract (CMM) showed a broad, intense absorption band centered at 3326.21 cm^{-1}, corresponding to the stretching vibrations of hydrogen-bonded hydroxyl (–OH) groups from polyphenols, flavonoids, and reducing sugars. This broad phenolic band was absent in the hexane spectrum, which displayed only weak, sharp high-frequency vibrations (~3755–3758 cm^{-1}).

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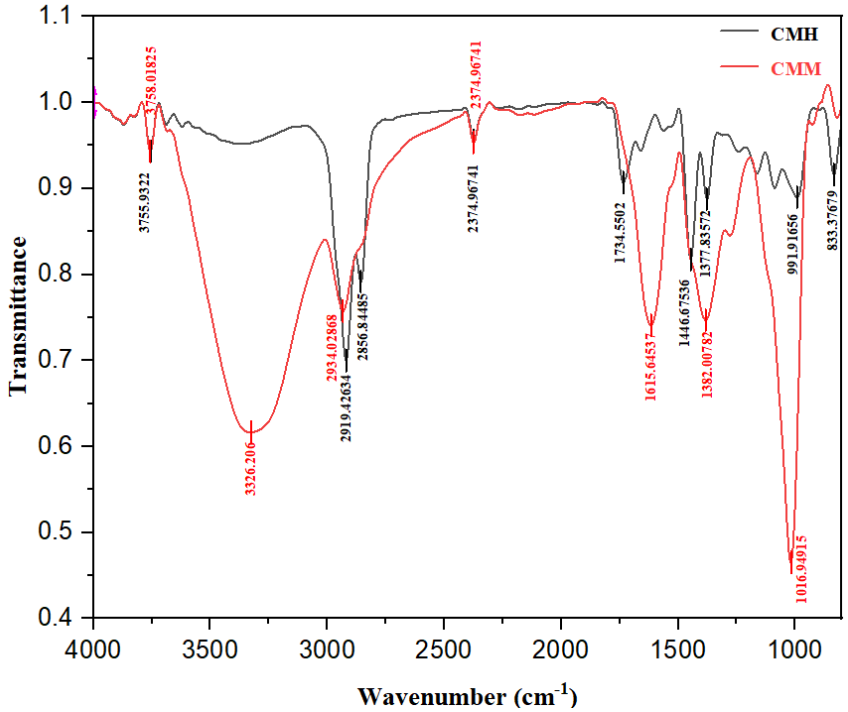


Figure 1. FTIR spectra of the hexane extract (CMH, black) and methanol extract (CMM, red) of Solanum virginianum leaves, recorded over 4000–400 cm^{-1}.

Furthermore, CMM displayed a distinctive absorption at 1615.65 cm^{-1}, assigned to aromatic ring C=C skeletal vibrations and amide N–H bending, and a very strong absorption band at 1016.95 cm^{-1}, attributed to overlapping C–O stretching (in polyols and glycosides) and aliphatic C–N stretching (in primary amines and alkaloids). In sharp contrast, the CMH spectrum was dominated by intense aliphatic C–H stretching modes (2934.03, 2919.43, and 2856.84 cm^{-1}) and a sharp ester carbonyl band at 1734.55 cm^{-1}, confirming the predominance of fatty acid esters, waxes, and lipophilic hydrocarbons.

Table 4a. FTIR peak positions and functional group assignments for Hexane Extract (CMH).

Wavenumber (cm^{-1})	**Vibrational Mode Assignment**	**Probable Functional Group / Phytoconstituent**
3755.93	Weak, sharp O–H vibration	Trace non-bonded hydroxyls / trace moisture
2934.03 / 2919.43	Asymmetric / symmetric C–H stretch	Aliphatic methylene (-CH_2-) and methyl (-CH_3) chains
2856.84	Symmetric C–H stretching	Lipophilic aliphatic hydrocarbon backbone
1734.55	Intense C=O stretching	Ester carbonyl (fixed oils, triglycerides, wax esters)
1446.68	C–H bending (scissoring)	Aliphatic alkyl chains / sterols
1377.84	C–H in-plane bending / O–H deformation	Alkane gem-dimethyl groups / trace sterols
991.92 / 833.38	C–O stretch / Aromatic C–H out-of-plane	Ether linkages / substituted ring structures

Table 4b. FTIR peak positions and functional group assignments for Methanol Extract (CMM).

Wavenumber (cm^{-1})	**Vibrational Mode Assignment**	**Probable Functional Group / Phytoconstituent**
3758.02	Sharp, weak O–H vibration	Trace non-associated hydroxyls / free moisture
3326.21	Broad, intense H-bonded O–H stretch	Polyphenols, flavonoids, alcohols, reducing sugars
2934.03	C–H stretching vibration	Aliphatic -CH_2- / -CH_3 backbone of bioactive compounds

1615.65	Aromatic C=C stretch / N–H bending	Flavonoid/alkaloid aromatic skeleton, amides
1382.01	In-plane O–H bend / C–H deformation	Phenolic hydroxyls, flavonoid pyrone ring structures
1016.95	Intense C–O / C–N stretching	Polyols, glycosides, reducing carbohydrates, primary amines

3.5 Mechanistic rationale: electron donation and reduction feasibility

The distinct visual and chemical differences between CMH and CMM clarify the mechanistic basis of plant-mediated nanoparticle synthesis. The reduction of Ag^+ to elemental Ag^0 is fundamentally an electron-transfer reaction driven by the coupled oxidation of reducing functional groups. In the presence of sunlight, solar photons excite electronic transitions within conjugated polyphenol and flavonoid ring systems, lowering the activation energy for single-electron transfer to silver ions (Zuhrotun et al., 2023; Miyanda & Parveen, 2026)

$$Ag^+ + e^- \text{ (donate by -OH/ -NH}_2\text{/C=O groups)} \xrightarrow{[h\nu \text{ (solar)}]} Ag^0$$

During this reduction process, phenolic hydroxyls (–OH) undergo oxidative dehydrogenation to form quinonoid derivatives (C=O), simultaneously releasing electrons and protons that reduce Ag^+ into metallic silver nuclei (Ag^0). Additionally, free amino groups (–NH_2) and carbonyl moieties interact with newly formed Ag^0 clusters via coordinate covalent bonding and steric shielding, preventing aggregation.

Because methanol solubilizes high concentrations of these polar, electron-rich phytochemicals (confirmed by the intense 3326.21 cm^{-1} and 1016.95 cm^{-1} FTIR bands), CMM provides the chemical driving force necessary for rapid bio reduction under sunlight. In contrast, the hexane extract contains predominantly long-chain aliphatic waxes, neutral lipids, and esterified fatty acids (evidenced by the 1734.55 cm^{-1} ester carbonyl band and C–H stretching modes). These non-polar structures lack readily oxidizable electron-donating centers, leaving CMH unreactive toward silver reduction

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IV. CONCLUSION

This comparative investigation demonstrates that solvent polarity is a primary determinant governing the silver nanoparticle-forming potential of Solanum virginianum leaf extracts. Maceration in polar methanol achieved an ~8.5-fold higher extractive recovery (13.60% vs. 1.60%) and selectively concentrated functional secondary metabolites bearing oxidizable hydroxyl (3326.21 cm^{-1}) and amine/polyol (1016.95 cm^{-1}) functional groups. This phytochemical profile facilitated successful Ag^+ bio reduction under solar irradiation, as evidenced by the development of characteristic reddish-brown surface plasmon resonance. Conversely, non-polar n-hexane extracted predominantly unreactive aliphatic waxes and fatty acid esters (1734.55 cm^{-1}), resulting in no observable reduction.

While visual colorimetric monitoring establishes the chemical reducing capacity of the extracts, comprehensive physical and structural characterization—including UV-Visible spectrophotometry (SPR peak at 400–450 nm), Dynamic Light Scattering (DLS), Zeta potential analysis, X-ray Diffraction (XRD), and HR-TEM/SEM imaging—alongside quantitative antimicrobial and antioxidant evaluations, represents the essential next phase of research to fully determine nanoparticle morphology, size distribution, and biomedical efficacy.

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