WORLD JOURNAL OF PHARMACEUTICAL RESEARCH
Coden USA: WJPRAP Impact Factor 8.63
Volume 15, Issue 16, 1180-1191. Research Article ISSN 2277–7105

PHYTOCHEMICAL PROFILING AND ANTIOXIDANT EVALUATION OF *SOLANUM NIGRUM* LEAF EXTRACTS USING GC-MS AND LC-MS ANALYSES

Avni Nayyar[1], Manaal Zahera[2], Mohammad Fahim Khan[3], Mohammad Ahsan[3], Sonika Bhatia[1], Archna Talwar[1]*

[1]Department of Chemistry, Isabella Thoburn College, University of Lucknow, Lucknow, Uttar Pradesh, India, 226007.

[2]Department of Biotechnology, Era University, Lucknow, Uttar Pradesh, India, 226003.

[3]Chemistry Division, Department of Biotechnology, Era University, Lucknow, Uttar Pradesh, India, 226003.

Article Received on 15 July 2026,
Article Revised on 05 August 2026,
Article Published on 16 August 2026,

https://doi.org/10.5281/zenodo.21917842

***Corresponding Author**

Prof. Archna Talwar

Department of Chemistry, Isabella Thoburn College, University of Lucknow, Lucknow, Uttar Pradesh, India, 226007.

How to cite this Article: Avni Nayyar[1], Manaal Zahera[2], Mohammad Fahim Khan[3], Mohammad Ahsan[3], Sonika Bhatia[1], Archna Talwar[1]*. (2026). Phytochemical Profiling and Antioxidant Evaluation of Solanum Nigrum Leaf Extracts Using Gc-Ms And Lc-Ms Analyses. World Journal of Pharmaceutical Research, 15(16), 1180–1191.

ABSTRACT

Solanum nigrum is a medicinal plant containing a wide variety of bioactive substances that can be used for various biomedical applications. The purpose of this article is to analyze the phytochemicals present in the hexane and methanol leaf extracts of *S. nigrum* using GC-MS and LC-MS to separate non-polar and polar metabolites, respectively. The evaluation of the antioxidant capacity of the extracts will be considered as a measure of their biological activity. The combination of phytochemical and antioxidant analyses gives a comprehensive view of the biologically active substances in *S. nigrum*.

KEYWORDS: Antioxidant activity, GC-MS, LC-MS, phytochemicals, *Solanum nigrum*.

1. INTRODUCTION

The bioactive components present in plants have been used to control agricultural pests and treat several diseases since ancient times.[1] These plants have multifaceted value due to their non-toxic and environmentally friendly nature, making them reliable for sustainable strategies. Only 2% of the approximately 300,000 known medicinal

plants have been scientifically studied for their phytochemical composition and biological activities, highlighting a gap between traditional knowledge and scientific validation.[2] The growing problem of resistance to various disease-causing pathogens has reduced the effectiveness of conventional strategies and increased interest in plant-based therapeutic alternatives.[2,3] Hence, the discovery and scientific validation of lead bioactive compounds become a crucial step in bridging traditional knowledge and modern biomedical and agricultural applications. The bioactive compounds present in plants have been extensively used not only to cure diseases but also to control agricultural pests with considerable effectiveness.[4,5] *Solanum nigrum*, commonly known as black nightshade, has been utilized in conventional Oriental medicine due to its significant therapeutic potential.[6] Various studies report the antimicrobial potential of the *S. nigrum* plant against various microorganisms due to the presence of numerous bioactive compounds, such as saponins, alkaloids (solasodine, solanine), polyphenolic compounds (rutin, caffeic acid), and others.[6,7] Hence, the utilization of plant-based antibiotics or synthetic pesticides may reduce the risk of multi-drug resistance, while allowing lower dosages of drugs, enhancing their efficacy, and minimizing their toxicity and environmental damage.[6]

The present work focuses on analyzing the non-polar and polar bioactive compounds present in the hexane and methanol leaf extracts of *Solanum nigrum* by GC-MS and LC-MS analyses. Furthermore, the current study on *S. nigrum* examines the complex phytochemical matrix by assessing the antioxidant properties of these leaf extracts, which may modulate their biological activity, thus increasing their scientific significance in the context of integrated phytochemical research.

2. METHODOLOGY

2.1 Chemicals

The extraction process was carried out using n-hexane (99% purity) and methanol (99% purity), which were bought from Thermo Fisher Scientific India Pvt. Ltd., Mumbai, India. The antioxidant activity was performed using 2,2-Diphenyl-1-picrylhydrazyl (DPPH), which was procured from SRL Chemicals.

2.2 Sample Collection

Solanum nigrum leaves were collected from Isabella Thoburn PG College, Lucknow, Uttar Pradesh, India, located at 26°52′18″N 80°56′32″E, and authenticated at the CSIR-National Botanical Research Institute, Lucknow, by Dr. K.M. Prabhukumar, Senior Scientist and

Herbarium Curator, under the accession number 117235. The plant material was subsequently deposited in the herbarium for future reference.

2.3 Preparation of plant extracts

To ensure a comprehensive phytochemical analysis, solvents of varying polarities were used in the present study. Hexane, a nonpolar solvent, was used for the extraction of lipophilic compounds, such as fatty acids, sterols, terpenoids, and hydrocarbons, which can be analyzed using GC-MS. On the other hand, methanol, a polar solvent, was used for the extraction of hydrophilic secondary metabolites such as phenolics, flavonoids, glycosides, and organic acids, which are primarily responsible for their antioxidant properties and were analyzed using LC-MS.

2.3.1 Preparation of hexane extract

The fresh *S. nigrum* leaves were washed with water, dried in the sunlight, and then ground into powder. 5 g of powdered leaves were soaked in 75 mL of hexane over a period of 1-2 days. The extract was filtered using a cotton plug to remove particulate matter. The extract was dried in a hot air oven at 55°C. The dried extract was stored at 4°C for subsequent analysis.[8] The extract yield was approximately 5%, obtained from 5 g of dried leaf powder.

2.3.2 Preparation of methanol extract

The maceration method was employed to extract phytochemicals using methanol over a period of 2-3 days. 5 g of powdered leaves were soaked in 75 mL of methanol, and the solvent was subsequently evaporated to yield a viscous methanol extract under controlled conditions at 45-50°C. The methanol extract yield was approximately 8%, and the dried methanol extract was further analysed using LC-MS.[9]

2.4 DPPH Assay

The antioxidant activity of the leaf extract was determined by the DPPH (2,2-diphenyl-1-picrylhydrazyl) assay.[10] The hexane and methanol extracts of *Solanum nigrum* leaves at 50, 100, and 150 µg/mL were prepared. 1 mL of a freshly prepared 0.1 mM DPPH solution in methanol was added to 1 mL of each extract, and the mixture was incubated in the dark for 30 min. Ascorbic acid was used as a standard. The absorbance was measured at 517 nm using a UV-Vis spectrophotometer, and the percentage of inhibition was calculated using the formula

$$\%\ Inhibition = \frac{Absorbance\ of\ control - Absorbance\ of\ sample}{Absorbance\ of\ control} \times 100$$

2.5 GC-MS Analysis

The analysis of the hexane extract was performed on a GC–MS/MS (GC-8890 gas chromatograph equipped with a 7010C GC/TQ mass spectrometer) using the capillary column HP-5MS (5% phenyl)-methylpolysiloxane phase, 30 m length, 0.25 mm diameter, 0.25 µm film thickness) obtained from Agilent Technologies (USA). The GC starting oven temperature of 60˚C (hold time 1 min) and a single ramp 1 of rate 10˚C/min to 120˚C (hold time 2 min), ramp 2 of rate 10 ˚C/min to 250˚C (hold time 2 min), and ramp 3 of rate 5˚C to 290˚C (hold time 1 min). The injector and MS transfer lines were at 250 and 290 °C, respectively. The total GC run time was 33 min. The column flow rate was maintained at 1.0 mL/min, with helium serving as the carrier gas at a split ratio of 20:1. The solvent delay was set to 2.5 min, and 1 µL of the diluted samples was automatically injected using an Autosampler 7693A coupled with the GC in split mode. The EI mass spectra were collected at an ionization voltage of 70 eV over the m/z range of 50–600 in full scan mode, with the ion source temperature set to 230°C.

2.6 LC-MS Analysis

The chemical constituents of the leaf extract were identified using LC-MS. LC-MS analysis was performed using a Waters Alliance e2695 system equipped with a quaternary, low-pressure mixing pump. The HPLC was interfaced with an HPLC-TQD Mass spectrometer with LC-ESI/MS(LC-MS)2ChScan. Full-scan mode from m/z 150 to 2000 was performed with a source temperature of 150°C. Separation was achieved using an ACCUCORE C18 column (150 × 2.1 mm, 2.6 µm), with methanol containing 0.1% formic acid as the mobile phase. A gradient elution was applied at a flow rate of 1 mL/min. The MS spectra were recorded in both positive and negative ion modes. The temperature of the drying gas (N_2) was maintained at 350^0C, with a flow rate of 950 L/hour. The nebulizing pressure (N_2) was adjusted to 21.75 psi. 25 mg of the sample was dissolved in 1mL of methanol and filtered through a 0.22 µm nylon filter. 2 µL of the extract was injected onto the analytical column for analysis. and transferred to LC vials for analysis.

3. RESULTS AND DISCUSSIONS

3.1 DPPH Assay

The DPPH scavenging activity of the leaf extracts and ascorbic acid exhibited dose-

dependent activity. The highest percentage inhibition at 150 µg/mL was recorded for ascorbic acid (90%), followed by leaf extracts in methanol (58.87%) and hexane (50.30%) **(Fig. 1, Table 1)**. The IC_{50} value was calculated by linear interpolation and found to be 98.1 µg/mL for the hexane extract, 69.7 µg/mL for the methanol extract, and 35.7 µg/mL for ascorbic acid.

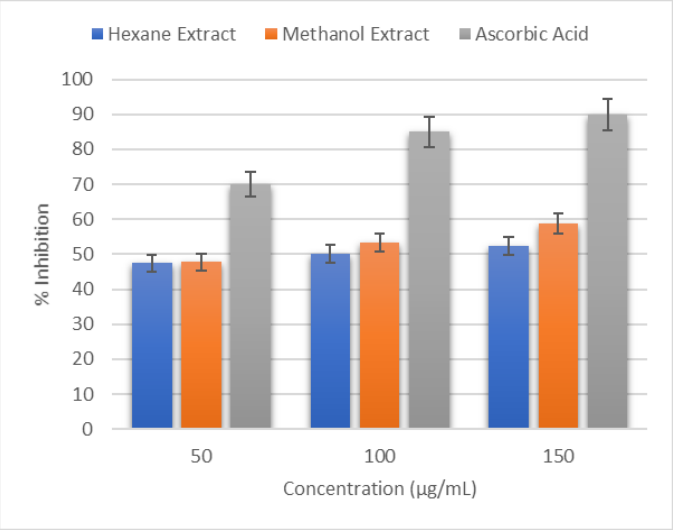

Fig. 1: DPPH assay of *S. nigrum* leaf extracts and ascorbic acid.

Table 1: DPPH radical scavenging activity of *S. nigrum* leaf extract and ascorbic acid at different concentrations (Values are expressed as mean ± standard deviation).

Concentration (µg/mL)	% Inhibition		
	Hexane Extract	Methanol Extract	Ascorbic Acid
50 µg/mL	47.42±0.13	47.83±0.35	70±0.40
100 µg/mL	50.10±0.25	53.32±0.38	85±0.40
150 µg/mL	52.36±0.20	58.87±0.40	90±0.40

The antioxidant activity of *S. nigrum* leaf extracts was evaluated using the DPPH radical scavenging assay with different solvents of varying polarity, such as hexane and methanol. The findings revealed that antioxidant activity is dependent on the type of solvent used for extraction. Between the two extracts, the methanolic extract exhibited the highest radical-scavenging activity, followed by the hexane extract, which showed relatively lower activity. This can be attributed to the extraction efficiency of phytochemicals, which is dependent on the polarity of the solvents. Methanol, a polar solvent, facilitates the extraction of phenolic compounds and flavonoids, which have been reported to exhibit high hydrogen-donating and electron-transfer capacities. These compounds neutralize DPPH radicals by stabilizing them through resonance mechanisms.[11] In contrast, hexane, a nonpolar solvent, extracts lipophilic

compounds such as fatty acids and sterols, which have been shown to have low antioxidant activity.[12]

3.2 GC-MS Analysis

The GC-MS chromatogram of the hexane extract of *S. nigrum* leaves identified a total of seven compounds by comparing the mass spectra with the NIST library **(Table 2)**. The GC-MS analysis of the hexane extract from *S. nigrum* leaves revealed a phytochemical composition rich in non-polar bioactive substances such as hydrocarbons, fatty acids, carotenoids, and high-molecular-weight lipid-like compounds **(Fig. 2)**. The major chromatographic peak observed at RT 17.77 min was identified as 2-methyldecane, emphasizing the predominance of hydrocarbon components within the non-polar fraction. Furthermore, notable peaks associated with palmitic acid (RT 23.78 min) and stearic acid (RT 26.40 min), identified in their trimethylsilyl derivative forms, validated the presence of long-chain saturated fatty acids, which are commonly associated with antioxidant and antimicrobial activities. Several other medium-intensity peaks were identified as fatty acid ester derivatives and carotenoid or lipid-like substances, indicating a complex lipid-rich chemical profile. A minor peak corresponding to low-molecular-weight polar compounds, such as glycerol, was also detected following derivatization. The presence of trimethylsilyl (TMS) derivatives in the GC-MS analysis is due to the derivatization method used to improve the volatility and thermal stability of polar phytochemicals, including fatty acids, alcohols, and amines, facilitating their effective separation and identification. Therefore, the predominance of hydrocarbons and fatty acids in the hexane extract underscores the effectiveness of hexane in selectively extracting nonpolar phytoconstituents from the leaves of *S. nigrum*.

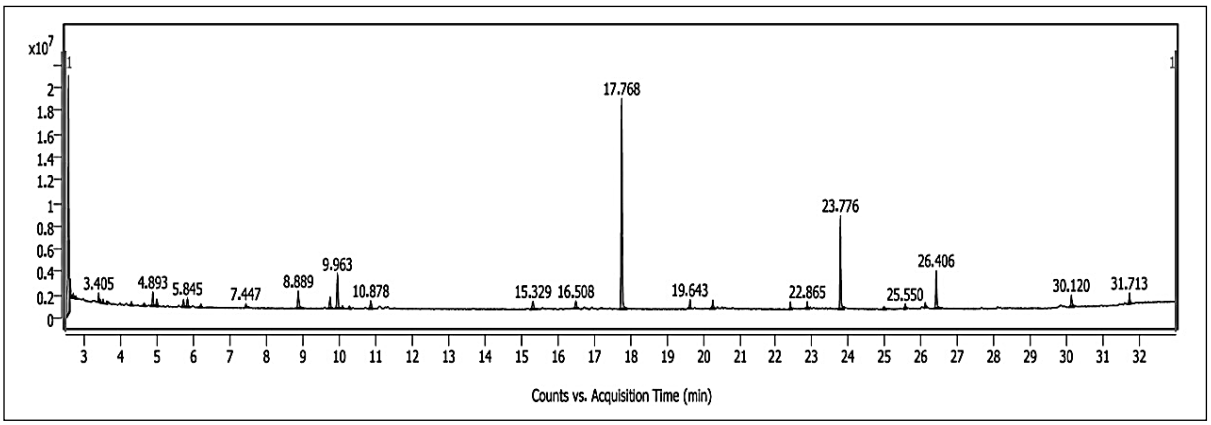

Fig. 2: GC-MS chromatogram of hexane extract of *S. nigrum* leaves.

Table 2: Major phytoconstituents identified from the hexane extract of *S. nigrum* leaves.

S. No.	Retention Time (min)	Compounds	% Peak Area	Phytochemical Class
1.	9.72	2,4,6,8,10-Tetradecapentaenoic acid, 9A-(acetyloxy)-1A,1B,4,4A,5,7A,7B,8,9,9A-decahydro-4A,7B-dihydroxy-3-(hydroxymethyl)-1,1,6,8-tetramethyl-5-oxo-1H-cyclopropa[3,4]benz[1,2-E]azulen-9-yl ester, [1ar-(1A.alpha.,1B.beta.,4A.beta.,7A.alpha.,7B.alpha.,8.alpha.,9.beta.,9A.alpha.)]-	1.62	Fatty acid ester
2.	9.93	Glycerol (3TMS)	4.79	Polyol
3.	15.28	Rhodopin	1.44	Carotenoid
4.	17.73	2-methyldecane	26.91	Hydrocarbon
5.	23.75	Palmitic Acid (TMS)	10.37	Saturated fatty acid
6.	26.38	Stearic Acid (TMS)	4.89	Saturated fatty acid
7.	30.09	6-(9a-Hydroxy-4a-(hydroxymethyl)-2b-methyl-1a,1b,2a,2b,3,4a,5,6,7,7a,9,9a,9b-tetradecahydro-2c,9-epoxycyclopenta[7,8]phenanthro[1,2-b:3,4-b']bis(oxirene)-5-yl)-2,3-dimethylhept-4-enoic acid, (3TMS)	1.60	Terpenoid derivative

3.3 LC-MS Analysis

The phytochemical profiles reported in the LC-MS spectra of the methanol extract consist predominantly of polar compounds, particularly flavonoids and steroidal alkaloids, known for their antioxidant, antidiabetic, and anticancer properties. The LC-MS analysis of the methanol extract showed a dominant ion peak at m/z 327.3 (RT 8.40 min), which is consistent with the known solasodine-type aglycone fragment, representing the steroidal core after loss of a small neutral fragment. The analysis revealed a diverse range of compounds in a 30 min elution using LC-MS spectra. The extract was primarily composed of phenolics, flavonoids, steroidal alkaloids, fatty acids, and lipids **(Table 3)**. Mass spectra were matched with those reported in the literature to identify tentative classes of phytocompounds. In the negative ion mode, the primary putative class of compounds at a retention time of 2.22 min was phenylpropanoid acid. Other prominent classes include flavonoid glycosides (flavonoids) at a retention time of 12.43 min. The less polar and lipid-rich constituents, including fatty acids and lipids, elute between 19.86 and 25.94 min **(Fig. 3)**. In the positive ion mode,

phenylpropanoid acids elute between 1.50 and 2.21 min. However, steroidal glycoalkaloids specific to the Solanaceae family elute at 13.22 min **(Fig. 4)**. Flavonoid glycosides constituted the principal class of phytocomponents in the late-eluting region.

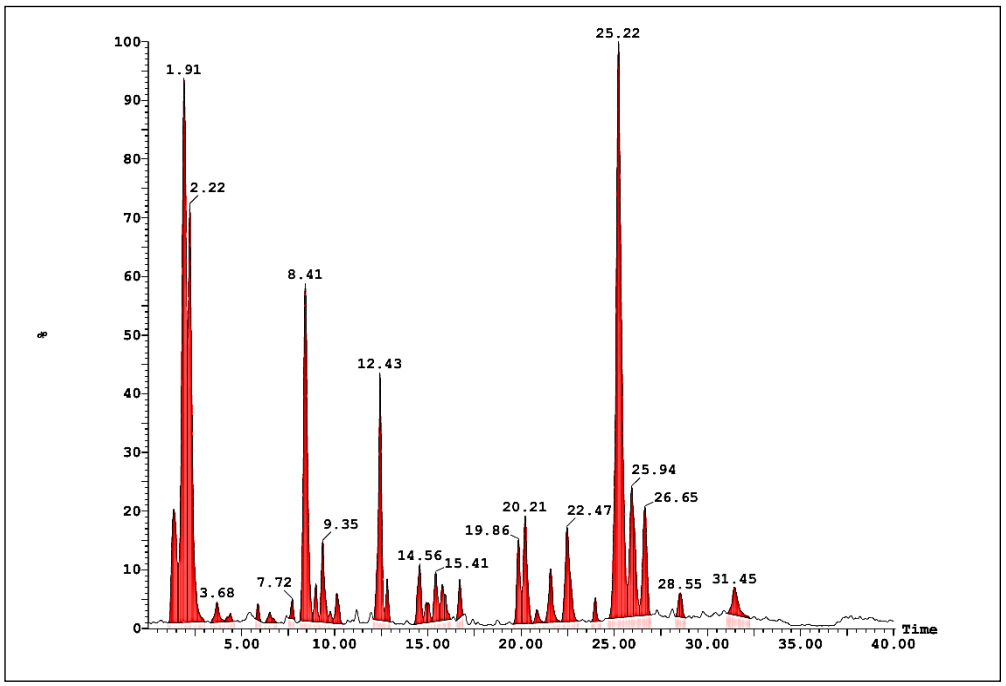

Fig. 3: Total ion chromatogram of the negative ion mode of the methanol extract of *S. nigrum* leaves.

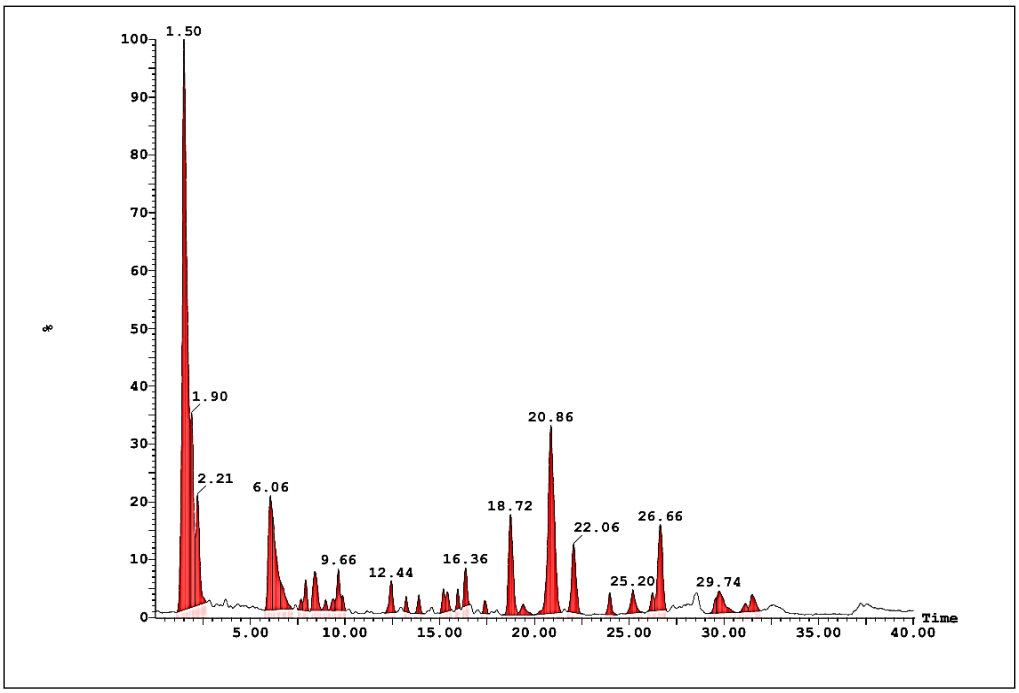

Fig. 4: Total ion chromatogram of the positive ion mode of the methanol extract of *S. nigrum* leaves.

Table 3: List of compounds identified from the LC-MS of the methanol extract of *Solanum nigrum* leaves.

Retention Time	m/z	Ion Type	Compounds	Phytochemical Class	References
2.22	201.1, 183	$[M-H]^-$	Chlorogenic Acid	Phenylpropanoid Acid	[13,14]
12.43	643, 613	$[M-H]^-$	Flavonoid O-diglycoside (Quercetin-O-dihexoside)	Flavonoid	[15,16]
19.86	277, 279	$[M-H]^-$	Linoleic acid	Fatty Acid	[16,17]
25.22	255.3, 256.3	$[M-H]^-$	Palmitic Acid	Fatty Acid	[18]
25.94	281.3, 282.3	$[M-H]^-$	Oleic Acid	Fatty Acid	[19]
26.65	815.7, 816.7	$[M-H]^-$	Triacylglycerol	Lipid	[20]
1.91	167, 203	$[M+H]^+$	Chlorogenic acid	Phenylpropanoid Acid	[21]
2.22	185	$[M+H]^+$	Ferulic Acid	Phenolic Acid	[22]
6.06	303, 447.3	$[M+H]^+$	Quercetin	Flavonoid	[23,24]
13.22	868.7, 869.7	$[M+H]^+$	Solamargine	Steroidal Alkaloids	[25]
18.72	610.4, 611.3	$[M+H]^+$	Rutin	Flavonoid	[26,27]
20.85	593, 594	$[M+H]^+$	N-docosanoyl-sphingosine	Sphingolipid	[28]
26.65	834.7, 835.7	$[M+H]^+$	Solasodine monoglycoside	Steroidal Glycoalkaloids	[29]

4. CONCLUSION

Therefore, the present study revealed that the antioxidant activity of *Solanum nigrum* is strongly influenced by the polarity of the solvent and its phytochemical composition. The enhanced radical scavenging activity in methanolic extracts demonstrated the presence of phenolic and flavonoid compounds, thereby indicating stronger antioxidant potential. Conversely, the relatively lower activity of hexane extracts indicates that non-polar compounds play a limited role in the free radical scavenging activity. Furthermore, GC-MS and LC-MS analyses provided chemical confirmation of these results by identifying structurally diverse phytoconstituents, such as phenolic acids, flavonoids, fatty acids, and sterols. Hence, these findings suggest a relationship between the architecture of phytochemicals and their biological activity. In this regard, the current study provides a comprehensive chemical basis for the application of these plant extracts in green nanobiotechnological and various biomedical applications.

ACKNOWLEDGEMENT

The authors are grateful to Prof. Abbas Ali Mahdi, Vice Chancellor, and Pro-Vice Chancellor Prof. Farzana Mahedi, Era University, Lucknow, India, for providing analytical and laboratory facilities.

REFERENCES

1. El-Saadony MT, Zabermawi NM, Zabermawi NM, Burollus MA, Shafi ME, Alagawany M, et al. Nutritional Aspects and Health Benefits of Bioactive Plant Compounds against Infectious Diseases: A Review. Food Rev Int., May 19, 2023; 39(4): 2138–60. doi:10.1080/87559129.2021.1944183
2. Yang X, Xu Q, Le L, Zhou T, Yu W, Wang G, et al. Comparative histology, transcriptome, and metabolite profiling unravel the browning mechanisms of calli derived from ginkgo (Ginkgo biloba L.). J For Res., Jun. 2023; 34(3): 677–91. doi:10.1007/s11676-022-01519-9
3. Farnsworth NR, Akerele O, Bingel AS, Soejarto DD, Guo Z. Medicinal plants in therapy. Bull World Health Organ, 1985; 63(6): 965–81. PubMed PMID: 3879679; PubMed Central PMCID: PMC2536466.
4. Gębarowska E, Łyczko J, Rdzanek M, Wiatrak B, Pląskowska E, Gołębiowska H, et al. Evaluation of Antimicrobial and Chemopreventive Properties and Phytochemical Analysis of Solanum nigrum L. Aerial Parts and Root Extracts. Appl Sci., Jul. 6, 2022; 12(14): 6845. doi:10.3390/app12146845
5. Fragkouli R, Antonopoulou M, Asimakis E, Spyrou A, Kosma C, Zotos A, et al. Mediterranean Plants as Potential Source of Biopesticides: An Overview of Current Research and Future Trends. Metabolites, Aug. 22, 2023; 13(9): 967. doi:10.3390/metabo13090967
6. Gębarowska E, Łyczko J, Rdzanek M, Wiatrak B, Pląskowska E, Gołębiowska H, et al. Evaluation of Antimicrobial and Chemopreventive Properties and Phytochemical Analysis of Solanum nigrum L. Aerial Parts and Root Extracts. Appl Sci., Jul. 6, 2022; 12(14): 6845. doi:10.3390/app12146845
7. Chen X, Dai X, Liu Y, Yang Y, Yuan L, He X, et al. Solanum nigrum Linn.: An Insight into Current Research on Traditional Uses, Phytochemistry, and Pharmacology. Front Pharmacol, Aug. 16, 2022; 13: 918071. doi:10.3389/fphar.2022.918071
8. Goti D. Screening of Phytochemicals from Leaf Extracts of Argyreia nervosa. Afr J Biomed Res., Oct. 1, 2024; 530–7. doi:10.53555/AJBR.v27i2S.2231
9. Abubakar AR, Haque M. Preparation of Medicinal Plants: Basic Extraction and Fractionation Procedures for Experimental Purposes. J Pharm Bioallied Sci., 2020; 12(1): 1–10. doi:10.4103/jpbs.JPBS_175_19 PubMed PMID: 32801594; PubMed Central PMCID: PMC7398001.
10. Singh RP, Chidambara Murthy KN, Jayaprakasha GK. Studies on the Antioxidant

Activity of Pomegranate (*Punica granatum*) Peel and Seed Extracts Using in Vitro Models. J Agric Food Chem., Jan. 1, 2002; 50(1): 81–6. doi:10.1021/jf010865b

11. Gulcin İ, Alwasel SH. DPPH Radical Scavenging Assay. Processes, Jul. 26, 2023; 11(8): 2248. doi:10.3390/pr11082248
12. Cravotto C, Fabiano-Tixier AS, Claux O, Abert-Vian M, Tabasso S, Cravotto G, et al. Towards Substitution of Hexane as Extraction Solvent of Food Products and Ingredients with No Regrets. Foods, Oct. 28, 2022; 11(21): 3412. doi:10.3390/foods11213412 PubMed PMID: 36360023; PubMed Central PMCID: PMC9655691.
13. Abdallah RH, Hassan WHB, Al-Massarani SM, Abdel-Mageed WM, Eldahmy SI, Basudan OA, et al. UPLC-ESI-MS/MS Profiling of Secondary Metabolites from Methanol Extracts of In Vivo and In Vitro Tissues of Daucus capillifolius Gilli (A Comparative Study). Molecules, Jun. 6, 2024; 29(11): 2694. doi:10.3390/molecules29112694
14. Rohida B, Farman M, George A. Unraveling the bioactive constituents of Typha elephantina: A comprehensive phytochemical analysis by tandem mass spectrometry. Mastinu A, editor. PLOS ONE, Dec. 5, 2024; 19(12): e0311549. doi:10.1371/journal.pone.0311549
15. Shi P, He Q, Song Y, Qu H, Cheng Y. Characterization and identification of isomeric flavonoid O-diglycosides from genus Citrus in negative electrospray ionization by ion trap mass spectrometry and time-of-flight mass spectrometry. Anal Chim Acta., Aug. 2007; 598(1): 110–8. doi:10.1016/j.aca.2007.07.027
16. Pereira P, Cebola MJ, Oliveira MC, Bernardo Gil MG. Antioxidant capacity and identification of bioactive compounds of Myrtus communis L. extract obtained by ultrasound-assisted extraction. J Food Sci Technol, Dec. 2017; 54(13): 4362–9. doi:10.1007/s13197-017-2907-y
17. March RE, Lewars EG, Stadey CJ, Miao XS, Zhao X, Metcalfe CD. A comparison of flavonoid glycosides by electrospray tandem mass spectrometry. Int J Mass Spectrom, Jan. 2006; 248(1–2): 61–85. doi:10.1016/j.ijms.2005.09.011
18. Zhou Y, Wu Z, Li C, Wang N, Zhang X, Chen H, et al. Coupling neutral desorption sampling to dielectric barrier discharge ionization mass spectrometry for direct oil analysis. Anal Methods, 2014; 6(5): 1538–44. doi:10.1039/C3AY41817K
19. National Center for Biotechnology Information, 2025. [Internet]. Available from: https://pubchem.ncbi.nlm.nih.gov/compound/Oleic-Acid
20. Hankin JA, Murphy RC. Relationship between MALDI IMS Intensity and Measured

Quantity of Selected Phospholipids in Rat Brain Sections. Anal Chem., Oct. 15, 2010; 82(20): 8476–84. doi:10.1021/ac101079v

21. Clifford MN, Johnston KL, Knight S, Kuhnert N. Hierarchical Scheme for LC-MS ^{n} Identification of Chlorogenic Acids. J Agric Food Chem., May 1, 2003; 51(10): 2900–11. doi:10.1021/jf026187q
22. Shikweni M, Tavengwa NT, Mokgehle TM. Characterization and chemometric based optimization of bioactive metabolites in Hypoxis hemerocallidea with the aid of UPLC-QqQ-MS/MS. Chem Pap., Feb. 2024; 78(4): 2223–33. doi:10.1007/s11696-023-03232-1
23. Scigelova M, Hornshaw M, Giannakopulos A, Makarov A. Fourier Transform Mass Spectrometry. Mol Cell Proteomics, Jul. 2011; 10(7): M111.009431. doi:10.1074/mcp.M111.009431
24. Stevens JF, Reed RL, Morré JT. Characterization of Phytoecdysteroid Glycosides in Meadowfoam (Limnanthes alba) Seed Meal by Positive and Negative Ion LC-MS/MS. J Agric Food Chem., Jun. 1, 2008; 56(11): 3945–52. doi:10.1021/jf800211k
25. Popova I, Sell B, Pillai SS, Kuhl J, Dandurand LM. High-Performance Liquid Chromatography–Mass Spectrometry Analysis of Glycoalkaloids from Underexploited Solanum Species and Their Acetylcholinesterase Inhibition Activity. Plants, Jan. 20, 2022; 11(3): 269. doi:10.3390/plants11030269
26. Rosenberg E. Characterisation of historical organic dyestuffs by liquid chromatography–mass spectrometry. Anal Bioanal Chem., May 2008; 391(1): 33–57. doi:10.1007/s00216-008-1977-0
27. Wang Y, Fu J, Zhang C, Zhao H. HPLC-DAD-ESI-MS Analysis of Flavonoids from Leaves of Different Cultivars of Sweet Osmanthus. Molecules, Sep. 14, 2016; 21(9): 1224. doi:10.3390/molecules21091224
28. Bartke N, Fischbeck A, Humpf H. Analysis of sphingolipids in potatoes (*Solanum tuberosum* L.) and sweet potatoes (*Ipomoea batatas* (L.) Lam.) by reversed phase high-performance liquid chromatography electrospray ionization tandem mass spectrometry (HPLC-ESI-MS/MS). Mol Nutr Food Res., Dec. 2006; 50(12): 1201–11. doi:10.1002/mnfr.200600140
29. Lelario F, De Maria S, Rivelli AR, Russo D, Milella L, Bufo SA, et al. A Complete Survey of Glycoalkaloids Using LC-FTICR-MS and IRMPD in a Commercial Variety and a Local Landrace of Eggplant (Solanum melongena L.) and their Anticholinesterase and Antioxidant Activities. Toxins, Apr. 19, 2019; 11(4): 230. doi:10.3390/toxins11040230