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Bioactive Potential of Lantana camara Leaf Extracts: Phytochemical Composition, Antioxidant, Anti-Diabetic, Antimicrobial Activities and Molecular Docking Analysis

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Lantana camara, was analysed for its phytochemicals and biological activities. The leaves were dried (250 g) and subjected to maceration and Soxhlet extraction techniques. Chemical profiling was carried out using GC-MS, and the concentration of phenolics, flavonoids, alkaloids, and other bioactive compounds were determined using UV spectrophotometry. Antioxidant activity was determined using DPPH, FRAP, ABTS, phosphomolybdate, H₂O₂, OH, nitric oxide, and Fe²⁺-chelating methods. The extracts had a relatively high antioxidant capacity, which decreased the oxidative damage at 50, 100, 150, 200, and 250 µg/ml. The antidiabetic activity was confirmed by testing for a-amylase inhibition using starch azure as a substrate. The inhibition profile was assessed at 595 nm, indicating that inhibition was dependent on the extract concentrations (100-1000 µg/ml). The antibacterial activity of the extract was assessed using the agar well diffusion method, showing activity against Escherichia coli, Bacillus subtilis, Staphylococcus aureus and Klebsiella pneumonia. The presence of antifungal activity against bacterial types such as Candida albicans, Aspergillus niger, Aspergillus flavus, and Aspergillus fumigatus showed that the plant has antifungal properties supported by its high-spectrum antimicrobial property. The molecular docking analytical results showed high-affinity interactions between the bioactive compound and the target protein, which further validated the plant's antioxidant and antimicrobial potential.

INTRODUCTION

Lantana camara, a plant deeply rooted in Indian traditional medicine, possesses therapeutic potential despite limited scientific validation. While historically utilized for its medicinal properties, comprehensive studies elucidating its phytochemical composition and pharmacological efficacy remain scarce. This study bridges this gap by exploring its bioactive compounds and assessing key biological activities to substantiate its traditional use.

AIM

This study aimed to profile bioactive phytochemicals in L. camara leaf extracts using GC-MS and UV spectrophotometry, and evaluate their antioxidant (via DPPH, FRAP, ABTS assays), antidiabetic (α -amylase inhibition) and antimicrobial (against bacterial and fungal pathogens) potentials. Molecular docking was employed to validate interactions between identified compounds and target proteins.

METHODOLOGY

Fresh L. camara leaves (250 g) were dried, powdered and subjected to maceration and Soxhlet extraction using hexane, ethyl acetate and methanol. Phytochemical screening via qualitative tests detected alkaloids, phenolics and flavonoids. Quantification employed UV spectrophotometry: Folin-Ciocalteu for phenolics, AlCl₃ for flavonoids and Drage Dorff's reagent for alkaloids. GC-MS analysed chemical profiles. Antioxidant activity was evaluated using DPPH, FRAP, ABTS, phosphomolybdate, H_2O_2 , •OH, nitric oxide and Fe²⁺-chelating assays at 50–250 µg/ml [1]. Antidiabetic potential was tested via α -amylase inhibition (starch azure substrate; absorbance at 595 nm, 10-100 μg/ml) [2]. Antimicrobial activity against bacterial and fungal strains was assessed using agar well diffusion [3]. Molecular docking (Auto Dock Vina) evaluated interactions between bioactive compounds and target proteins (NADPH oxidase, α -amylase, microbial enzymes). Data were analyzed statistically to determine significance (p < 0.05)

RESULTS & DISCUSSION Fig 1, DPPH radical scavenging activity of samples L(S)M and standard antioxidants. Fig 2. Antioxidant activity of sample and standard determined by ABTS radical scavenging assay 201 Fig 3. Total antioxidant capacity (phosphomolybdate method) of s le and standard 00 Cama (um Fig 4. H₂O₂ scavenging activity of samples and standard a ntiovidants

Fig 5. Hydroxyl radical (•OH) scavenging activity of sample compared with standards.

INTRODUCTION

MDPI







Fig 7. Fe²⁺ chelation assay (% inhibition), with citric acid as a reference standard. FRAP ASSAY - The sample showed a ferric-reducing antioxidant power (FRAP) of 83.75 µg/mL, indicating moderate antioxidant capacity.





Fig 8. In-Vitro α-Amylase inhibitory activity of the sample (10–100 µg/mL) using starch-azure method. Table 1. Comparative analysis of antioxidant and antidiabetic activities.

Parameter	L(S)M Value (Mean ± SD)	Ascorbic Acid Value (Mean ± SD)	BHT Value (Mean ± SD)
DPPH	31.75 ± 0.89	30.13 ± 0.35	26.68 ± 0.01
ABTS	30.08 ± 0.58	31.89 ± 0.10	27.69 ± 0.004
Phosphomolybdate	29.15 ± 0.42	30.39 ± 0.07	27.36 ± 0.003
Fe ²⁺ -chelating	30.41 ± 0.64	32.37 ± 0.09(Citric acid)	
FRAP	83.75 μg/ml		
In-Vitro α-Amylase Inhibitory A	72.73 ± 1.89	71.00 ± 0.38(Acarbose)	
H ₂ O ₂	28.59 ± 0.24	29.71 ± 0.06	27.21 ± 0.002
OH	30.54 ± 0.67	32.60 ± 1.12	27.83 ± 0.004
Nitric Oxide	30.19 ± 0.6	32.05 ± 0.11	27.72 ± 0.0

14.5 mm 16.2 mm 18.0 mm 24.3 mi 26.0 mi 22.5 mr 13.7 mn 12.9 mm 11.4 mm 20.4 mn 18.7 mm 19.6 mm

13.1 mm 12.2 mm MOLECULAR DOCKING - The study examined Coniferyl Alcohol (PDB ID: 1M8V) binding to Escherichia coli protein with MOLECULAR DOCKING — The study examined contrely Alcohol (PD ID: INVOY binding to escherichia Con protein Will binding affinity of -7.1 kcal/mol, indicating strong non-covalent interactions. GC-MS analysis identified 10 major compounds w affinities ranging from -7.1 to -3.1 kcal/mol, with Coniferyl Alcohol showing the strongest binding. Further analysis of other micro proteins revealed similar affinities, highlighting Coniferyl Alcohol's versatile potential in microbial protein interactions.



CONCLUSION

The study validates the traditional use of Lantana camara by demonstrating its significant antioxidant (DPPH, FRAP, ABTS), antidiabetic (72.73% α-amylase inhibition), and broad-spectrum antimicrobial activities. Molecular docking revealed Coniferyl Alcohol as a key bioactive compound with strong binding affinities to microbial proteins. These findings highlight the plant's pharmacological potential, warranting further in vivo and clinical investigations

REFERENCES

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