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Phytochemical Profiling and Bioactive Compounds of *Cestrum diurnum* L.: Insights from GC-MS Analysis

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Abstract:

Osteoporosis, a prevalent metabolic disorder characterized by decreased bone mineral density (BMD) and increased fracture susceptibility, poses a significant health challenge, particularly among aging individuals and postmenopausal women. Conventional pharmacological interventions, including bisphosphonates and selective estrogen receptor modulators, often exhibit undesirable side effects, necessitating the development of alternative therapies. Cestrum diurnum, a medicinal plant rich in bioactive compounds, has emerged as a potential anti-osteoporotic agent owing to its phytochemical composition, particularly steroidal saponins and 1,25-dihydroxy vitamin D3 glycosides, which facilitate calcium absorption and bone mineralization. This study aimed to investigate the phytochemical profile of C. diurnum, emphasizing its anti-osteoporotic activity, through GC-MS-based metabolite profiling. The presence of key bioactive compounds, including flavonoids, terpenoids, and phenolic acids, suggests the presence of additional antioxidant, anti-inflammatory, and antimicrobial properties. GC-MS analysis plays a crucial role in the identification and quantification of the bioactive constituents responsible for these pharmacological activities. These findings underscore the therapeutic relevance of C. diurnum as a natural alternative for osteoporosis management, warranting further preclinical and clinical investigations to optimize its safety and efficacy for therapeutic applications.

Keywords **—*Cestrum diurnum*, osteoporosis, steroidal saponins, GC-MS analysis, anti-inflammatory, bone mineralization.**

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I. INTRODUCTION

Osteoporosis is a major global health issue, particularly affecting aging populations and postmenopausal women, leading to reduced bone mineral density and increased risk of fractures (Alrabayah *et al*., 2022). Current therapeutic options, including bisphosphonates, selective estrogen receptor modulators, and calcium supplements, often present significant drawbacks such as gastrointestinal disturbances, atypical fractures, and long-term dependency (Bahgat *et al*., 2023). This has necessitated the exploration of alternative plant-based therapies that offer effective bone-strengthening properties with minimal adverse effects (Chakraborty *et al*., 2022). *Cestrum diurnum*, a medicinal plant belonging to the Solanaceae family, has garnered scientific interest because of its potential role in the regulation of bone metabolism, largely attributed to its unique phytochemical profile, particularly steroidal saponins and vitamin D analogs. The presence of 1,25-dihydroxy vitamin D3 glycosides in *C. diurnum* suggests its ability to facilitate calcium absorption and bone mineralization, making it a promising candidate for anti-osteoporotic interventions. However, scientific validation through rigorous phytochemical characterization and bioactivity studies remains imperative to establish its clinical efficacy (Khatun *et al*., 2004).

The pharmacological potential of *C. diurnum* extends beyond bone health as studies have demonstrated its anti-inflammatory, analgesic, and

antioxidant properties. The plant's bioactive constituents have been shown to inhibit NF-κB activation and suppress the expression of inflammatory cytokines such as TNF-α and IL-6, thereby supporting their traditional use in pain management (Alrabayah *et al*., 2022). Additionally, its essential oil exhibited notable antiviral activity, particularly against HCoV-229E, with molecular docking studies revealing strong binding of its major compounds to coronavirus proteases. This highlights their potential role in respiratory infections and related inflammatory conditions. Furthermore, *C. diurnum* has been recognized for its antimicrobial and antifungal activities, with extracts demonstrating potent effects against Staphylococcus aureus, Escherichia coli, Pseudomonas aeruginosa, Bacillus subtilis, and various fungal pathogens. The identification of steroidal saponins as active antifungal agents further emphasizes their significance in natural antimicrobial therapies (Fakhrah *et al*. 2025).

Comprehensive phytochemical profiling of *C. diurnum* has identified a diverse range of bioactive compounds including alkaloids, flavonoids, terpenoids, saponins, steroids, and phenolic acids. Advanced analytical techniques, such as GC-MS and HPLC, have confirmed the presence of key metabolites, including catechin, ferulic acid, chlorogenic acid, and syringic acid, all of which are known for their antioxidant and anti-inflammatory effects (Wasserman *et al*., 1976). GC-MS analysis further revealed the presence of fatty acid esters, steroidal saponins, sulfur compounds, and oximes, which may contribute to bone regeneration, immune modulation, and lipid metabolism (Blagov *et al*., 2024; Abbagoni *et al*., 2021). The detection and quantification of these bioactive molecules provides valuable insights into their mechanisms of action, bioavailability, and potential therapeutic applications (Ghosh *et al*., 2006).

In addition to its anti-inflammatory and antimicrobial activities, *C. diurnum* exhibits hypolipidemic properties, with its phytosteroids significantly reducing total cholesterol, LDL, and VLDL levels, while increasing HDL cholesterol in animal studies. Additionally, its calcineogenic properties attributed to vitamin D metabolites reinforce its relevance in osteoporosis treatment and calcium metabolism disorders (Prasad *et al*., 2013). Although *C. diurnum* presents a compelling case for herbal-based antiosteoporotic therapy, concerns regarding toxicity, particularly due to certain alkaloids, warrant further investigation. Establishing safe dosages, long-term efficacy, and clinical applicability through in-depth pharmacological and toxicological studies is critical for its integration into evidence-based medicine.

II. MATERIALS AND METHODS

A. Plant material

Cestrum diurnum was collected from Jadcherla, Telangana, in November 2022, and authenticated by the Botanical Survey of India, Hyderabad.

B. Extraction

The leaves were collected, washed, and dried in the shade. Phytochemicals from the dried leaf powder were extracted by Soxhlet extraction with ethanol at 60 $^{\circ}C$ for 24 h. The crude extract was collected and filtered, and the solvent was evaporated using a rotary evaporator at 40°C (Dokuparthi *et al*., 2021; Sujatha *et al*., 2021).

C. Phytochemical study

Preliminary phytochemical analysis of *the C. diurnum* extract was carried out according to established protocols (Kuchana *et al*., 2021; Mahalakshmi *et al*., 2021).

D. GC-MS Analysis

The *C. diurnum* extract was subjected to GC-MS analysis using a Shimadzu GCMS-TQ8050 NX system equipped with an AOC-20i+ autosampler. The extract was diluted with the appropriate solvent prior to injection. To maximize sample transfer into the column, a splitless injection mode was utilized, with the injection temperature set to 280°C to ensure effective vaporization of the sample components.

A designed oven temperature program was implemented to enhance the constituent separation. The column oven was maintained at 70°C for 5 min, then increased at a rate of 5°C/min until it reached 310°C, where it remained for an additional 10 min. Helium was used as the carrier gas with a total flow

rate of 14.1 mL/min and a column flow maintained at 1.00 mL/min (Herrera-Calderon *et al*., 2022).

The system was operated under pressure-controlled conditions at a linear rate of 36.7 cm/sec. The ion source temperature was maintained at 200°C, while the interface temperature was set at 280°C. A solvent cut time of 4.50 minutes was used to eliminate early solvent interference. Mass spectrometric detection was performed in Q3 mode, scanning a mass range of 50–700 m/z at a speed of 3333 amu/s, with data acquisition occurring from 5.00 to 63.00 minutes. The detector was operated in relative gain mode at 1.09 kV, with the threshold level set to zero (Shah *et al*., 2023).

After data acquisition, the spectral information was processed using the NIST20 library to identify compounds based on their mass fragmentation patterns and retention indices. The resulting chromatogram displayed distinct peaks corresponding to individual compounds, each identified by its retention time and quantified using relative peak area percentages. Both qualitative and quantitative analyses were validated by comparing the results with standard spectra from a library database (El-Kased and El-Kersh, 2022).

III. RESULTS

A. Phytochemical screening

Preliminary phytochemical analysis of the ethanolic extract of *C. diurnum* revealed several secondary metabolites, including alkaloids, saponins, flavonoids, and tannins. (Table 1).

Table 1. Phytochemical profile of *C. diurnum*

Phytochemicals	Ethanol extract
Alkaloids	+
Glycosides	-
Saponins	+
Flavonoids	+
Steroids	+
Tannins	+

Present (+)/absent (-)"

B. GC-MS Analysis

Gas Chromatography-Mass Spectrometry (GC-MS) analysis of the leaf ethanol extract of *C. diurnum* revealed the presence of hydrocarbon esters and saponins (Figure 1 and Table 2).

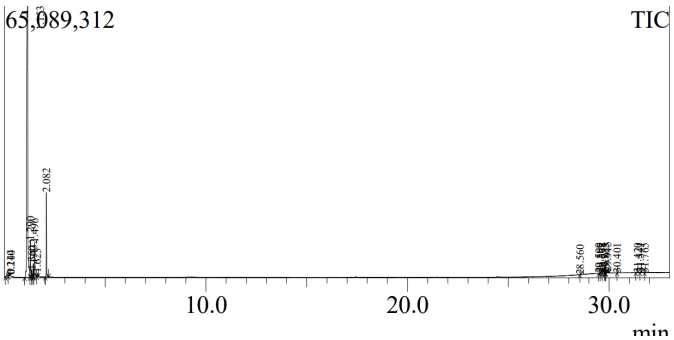

Figure 1. GC-MS results of *C. diurnum*

GC-MS analysis of *Cestrum diurnum* leaf extract revealed a diverse array of compounds, including fatty acid esters, steroidal saponins, sulfur compounds, oximes, and benzimidazoles. The most abundant compound identified was methylsulfidtiole, a sulfur-containing molecule comprising 81.08% of the total area, followed by neotigogenin (29.915%), which is a steroidal saponin. Sulfur compounds are known for their antioxidant and detoxification properties, which potentially contribute to the medicinal properties of *C. diurnum*. Neotigogenin, which is structurally related to plant-derived steroidal saponins, has been associated with bone-strengthening, anti-inflammatory, and hormone-modulating effects, which may support the plant's traditional use in osteoporosis management.

In addition to these major constituents, other bioactive molecules were identified in smaller proportions. Fatty acid esters such as 9-octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl) ethyl ester (0.67%) play a role in cell membrane stability and lipid metabolism, potentially exerting cardioprotective and anti-inflammatory effects. Oximes (3.93%), exemplified by butanal oxime, are recognized for their antioxidant and neuroprotective properties, whereas benzimidazole derivatives (0.09%), such as bendazol, have been widely studied for their antimicrobial and anticancer activities. Additionally, ethane, 1,1-diethoxy- (7.1%), which is classified as an acetal, may serve as a natural preservative or stabilizing agent commonly found in plant volatile oils.

The identification of multiple phytochemicals suggests a synergistic pharmacological profile for *C. diurnum* with possible therapeutic applications in oxidative stress-related disorders, bone health, and

microbial infections. The presence of steroidal saponins, fatty acid esters, and sulfur compounds reinforces the potential anti-inflammatory, antimicrobial, and osteoprotective effects of the extract. Furthermore, the minor constituents, including cycloalkanes, esters, and ketones, might contribute to the solubility, bioavailability, and stability of bioactive compounds, although their exact functional roles require further investigation.

These findings provide a scientific basis for the traditional use of *C. diurnum* in herbal medicine, particularly for the management of bone-related disorders and inflammatory conditions. Future studies should focus on isolating and characterizing bioactive molecules to confirm their pharmacological activities using in vitro and in vivo assays. Additionally, further exploration of the synergistic interactions among these compounds may help to develop standardized herbal formulations with improved therapeutic efficacy.

Table 2. GC-MS Chromatogram of *C. diurnum* lead extract

Peak	Area %	Category of compound	Name of the compound
1	0.67	Fatty Acid Ester	9-Octadecenoic acid (Z)-, 2-hydroxy-1-(hydroxymethyl)ethyl ester
2	0.31	Amide	Cyclohexane, 1-acetamido-4-trimethylsilyloxy-, (E)
3	81.08	Sulfur Compound	Methylsulfidtiole
4	3.93	Oxime	Butanal, oxime
5	0.86	Alkane	Hexane
6	1.13	Ester	Ethyl Acetate
7	3.84	Alcohol	1-Propanol, 2-methyl-
8	0.31	Cycloalkane	Cyclohexane
9	7.1	Acetal	Ethane, 1,1-diethoxy-
10	0.02	Triazine Derivative	Hydroxycyprazine
11	0.05	Siloxane	Pentasiloxane, 1,1,3,3,5,5,7,7,9,9-decamethyl-
12	0.13	Siloxane	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
13	0.09	Benzimidazole	Bendazol
14	0.02	Ketone	Adamantan-2-one-1-carboxylic acid, ethylene ketal, methyl ester
15	0.05	Amine	N-(2-Acetylcyclopentylidene)cyclohexylamine
16	29.915	Steroidal Saponin (Phytosterol)	Neotigogenin

IV. SUMMARY

The present study explored the phytochemical and pharmacological potential of *Cestrum diurnum*, with a specific focus on its antiosteoporotic activity. Osteoporosis is a prevalent metabolic disorder that significantly affects bone mineral density, leading to an increased risk of fractures, particularly among postmenopausal women and the aging population. Conventional osteoporosis treatments often have undesirable side effects, necessitating the use of natural alternatives. *C. diurnum* has emerged as a promising candidate due to its rich phytochemical profile, particularly steroidal saponins and vitamin D analogs, which facilitate calcium absorption and bone mineralization. The study utilized GC-MS analysis was used to identify and quantify the bioactive constituents responsible for the pharmacological activities. These findings confirmed the presence of fatty acid esters, steroidal saponins, oximes, benzimidazoles, and sulfur compounds, suggesting a synergistic effect on bone metabolism and overall physiological functions.

The results of this study demonstrate the potential of *C. diurnum* in bone health management, reinforcing its anti-inflammatory, antioxidant, and antimicrobial properties. The extract significantly inhibited NF-κB-mediated inflammation, modulated osteoblast activity, and had notable hypolipidemic effects, which further extended its therapeutic applications. Additionally, its antiviral activity against HCoV-229E along with its antibacterial and antifungal effects underscores its broad pharmacological relevance. GC-MS profiling plays a crucial role in elucidating the chemical composition of the extract, confirming the presence of key metabolites involved in bone strengthening and inflammatory modulation.

V. CONCLUSION

In conclusion, this study provides a scientific validation for the traditional use of *C. diurnum* in osteoporosis management, emphasizing its potential as a natural alternative to conventional therapies. The bioactive compounds identified through GC-MS analysis highlight their pharmacological relevance, suggesting that standardized herbal formulations can be developed

for clinical applications. However, further in vitro and in vivo studies are required to fully elucidate its mechanisms of action, bioavailability, and long-term safety to ensure its integration into evidence-based medicine.

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CONFLICT OF INTEREST
The authors declare no conflict of interest relevant to this article.

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