



Bioorganic Evaluation Of The Chemical Structure And Biological Activity Of *Phlomoides Labiosa*

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Abstract: *Phlomoides labiosa* is a medicinal plant traditionally used in Central Asian ethnobotany, yet its bioorganic composition and functional properties remain insufficiently studied. This research provides a comprehensive bioorganic evaluation of the plant's chemical constituents and their biological activities. Using chromatographic and spectroscopic methods (GC-MS, HPLC, UV-Vis, FT-IR), the major phytochemical groups—including flavonoids, phenolic acids, terpenoids, sterols, and alkaloids – were isolated and structurally characterized. Quantitative analysis revealed high levels of phenolic and antioxidant compounds, suggesting strong radical-scavenging potential. Biological assays demonstrated antibacterial, antifungal, and moderate anti-inflammatory activities, indicating a synergistic effect among the plant's bioactive components. The results highlight *Phlomoides labiosa* as a promising natural source of biologically active molecules relevant to pharmaceutical, nutraceutical, and bioorganic chemistry applications. Further studies involving purification of individual compounds and mechanism-of-action analysis are recommended to support targeted drug development.

Keywords: *Phlomoides labiosa*, bioorganic chemistry, phytochemical composition, bioactive compounds, antioxidant activity, antimicrobial properties, structure–activity relationships (SAR).

Introduction: Medicinal plants remain an important source of biologically active compounds with significant potential for pharmaceutical and bioorganic chemistry applications. The genus *Phlomoides* (family Lamiaceae) includes numerous species known for their rich phytochemical composition, particularly phenolic compounds, terpenoids, flavonoids, and alkaloids. These constituents are often associated with antioxidant, antimicrobial, and anti-inflammatory effects, making the genus a relevant target for modern natural product research [1,2,3].

Phlomoides labiosa is a less-studied representative of this genus, traditionally used in Central Asian ethnomedicine for its presumed therapeutic properties. Despite its widespread use in folk practice, the plant has not been adequately investigated at the molecular and bioorganic levels. Limited scientific data exist regarding its chemical composition, structural features of its constituents, and the mechanisms underlying its biological activity. A systematic bioorganic evaluation is therefore necessary to validate traditional knowledge, reveal its pharmacologically relevant compounds, and expand the natural product database of regional flora.

Advances in chromatographic and spectroscopic techniques—such as GC–MS, HPLC, FT-IR, and NMR—provide powerful tools to identify, isolate, and structurally characterize bioactive molecules in medicinal plants. Integrating these analytical approaches with biological assays enables a comprehensive understanding of both chemical composition and functional properties. Such studies are crucial for determining structure–activity relationships (SAR), assessing therapeutic potential, and identifying candidate molecules for future drug development.

Given the growing global interest in plant-derived compounds, the present study aims to investigate the phytochemical profile of *Phlomoides labiosa*, elucidate the structural features of its major constituents, and evaluate their biological activity. This research contributes new scientific evidence on a previously underexplored species, supporting its potential role in pharmaceutical, nutraceutical, and bioorganic chemistry fields.

Literature Review

The study of bioactive compounds in medicinal plants has long relied on the integration of phytochemical analysis, biological assays, and advanced extraction methodologies. Foundational chromatographic and spectroscopic techniques remain central to this field, as demonstrated in Harborne's (1998) classic manual on phytochemical methods, which established standardized approaches to isolating and characterizing secondary metabolites. These methodological foundations have been strengthened by modern analytical tools, including ABTS and Folin–Ciocalteu assays described by Re et al. (1999), Singleton et al. (1999), and Slinkard and Singleton (1977), which continue to be extensively used for evaluating antioxidant activity and phenolic contents in natural products research.

The Lamiaceae family, known for its rich phytochemical diversity and pharmacological

activities, has been widely examined through modern extraction and analytical methods. Barros et al. (2013) highlighted significant variations in phenolic profiles of *Melissa officinalis* depending on cultivation and processing conditions, underscoring how environmental and technological factors affect the bioactive potential of Lamiaceae species. In addition, research on essential oils within the family has shown strong antibacterial and anti-inflammatory activities. Burt (2004) and Miguel (2010) provided comprehensive reviews demonstrating how essential oils from aromatic plants exhibit potent antimicrobial and antioxidant properties, largely due to terpenoids and phenolic constituents.

Extraction methodology plays a critical role in obtaining high-quality bioactive fractions. Chemat, Abert Vian, and Cravotto (2012) introduced principles of green extraction that minimize degradation while improving efficiency, which is particularly important when handling heat-sensitive natural compounds. These approaches have become widely adopted in phytochemical research, including studies on Lamiaceae genera.

The genus *Phlomis* and closely related *Phlomoides* have attracted increasing scientific interest due to their diverse bioactive constituents. Taxonomic clarification by Kahraman, Lakušić, and Doğan (2012) helped differentiate Turkish *Phlomis* and *Phlomoides* species, providing a valuable framework for future chemical and pharmacological studies. In a comprehensive review, Nabavi et al. (2015) summarized the ethnobotanical uses, phytochemistry, and pharmacology of *Phlomis* spp., noting the presence of flavonoids, terpenoids, phenolic acids, and sterols with antioxidant, antimicrobial, and anti-inflammatory properties. Kumar and Pandey (2013) further emphasized the importance of flavonoids as major secondary metabolites with broad therapeutic potential, making them critical targets for isolation and characterization.

Several recent studies in Uzbekistan have focused specifically on Lamiaceae plants and related taxa. Mamadjonova, Usmanova, and Abdullayev (2021) compared the ash content and chemical characteristics of *Nepeta* and *Lophanthus* species, demonstrating the biochemical diversity within the family. Yulbarsova et al. (2022) investigated *Phlomoides nuda* as a natural source of β -sitosterol, a sterol known for its anti-inflammatory and cholesterol-lowering effects. The extraction and certification of bioactive compounds from plants in Uzbekistan were also examined by Mamatqulova, Dexqanov, and Abdullayev (2021), who outlined classification strategies for biologically active substances isolated from *Helianthus tuberosus* using national extraction standards. These regional studies complement global findings by highlighting Central

Asian flora as a promising source of pharmacologically significant compounds.

Several works also explore the antimicrobial potential of plant-derived extracts. Parekh and Chanda (2007) demonstrated the antibacterial activity of methanolic extracts from *Woodfordia fruticosa*, indicating the importance of solvent polarity in isolating antimicrobial agents. Their findings correlate with broader evidence from essential oil studies (Burt, 2004; Miguel, 2010) that phenolic- and terpenoid-rich fractions exhibit notable antibacterial effects. These biological properties are mechanistically supported by the antioxidant framework outlined by Halliwell and Gutteridge (2015), who emphasized the role of plant antioxidants in mitigating oxidative stress and enhancing immune responses.

Overall, the accumulated literature demonstrates a strong global and regional interest in Lamiaceae plants, particularly those of the *Phlomis*/*Phlomoides* complex, due to their bioactive metabolites and therapeutic potential. The references collectively highlight advances in extraction technologies, phytochemical profiling, antioxidant assays, and antimicrobial evaluations. However, despite the extensive research on related taxa, species such as *Phlomoides labiosa* remain significantly under-investigated, especially with regard to compound isolation, structural elucidation, and bioorganic characterization. This gap in the scientific record underscores the importance and novelty of research directed at isolating and analyzing active constituents from *P. labiosa*.

Methods

Plant material of *Phlomoides labiosa* was collected during its flowering season from natural habitats in the southern regions of Central Asia. The species was taxonomically identified by specialists at the Department of Botany of a regional university, and a voucher specimen was prepared and deposited in the institutional herbarium. The collected material was washed, shade-dried at room temperature, ground into a fine powder, and stored in airtight containers until further analysis.

Ethanollic and aqueous extracts were prepared from the powdered material. For ethanollic extraction, the plant powder was macerated in 95% ethanol for 72 hours with periodic agitation, followed by filtration and concentration under reduced pressure at 45 °C using a rotary evaporator. For aqueous extraction, the powdered material was boiled in distilled water for 30 minutes, filtered, and lyophilized. All extracts were preserved at 4 °C before chemical and biological evaluation.

Preliminary phytochemical screening was carried out

using standard qualitative tests to detect major groups of secondary metabolites, including alkaloids (Mayer's and Dragendorff's tests), flavonoids (Shinoda reaction), phenolic compounds (ferric chloride test), terpenoids (Salkowski test), sterols (Liebermann–Burchard reaction), and saponins (foam test).

Chromatographic techniques were used to analyze and characterize the chemical constituents. GC–MS was employed for volatile and semi-volatile components using an HP-5MS column with helium as the carrier gas under a programmed temperature gradient. Identification of components was performed by comparing mass spectra with NIST and related libraries. HPLC analysis was conducted on a C18 reverse-phase column with a water–methanol gradient containing 0.1% formic acid, and detection wavelengths of 254 nm and 280 nm. Reference standards such as quercetin, gallic acid, and rosmarinic acid were used to quantify major phenolic and flavonoid compounds.

Spectroscopic methods were applied for structural confirmation of isolated constituents. FT-IR spectra were recorded across 4000–400 cm⁻¹ to determine characteristic functional groups. UV–Vis absorbance between 200 and 800 nm was used to evaluate chromophoric systems. Purified fractions were subjected to ¹H-NMR and ¹³C-NMR spectroscopy to establish molecular structures.

Antioxidant activity of the extracts was assessed using DPPH and ABTS radical-scavenging assays. Extract solutions of varying concentrations were mixed with standard radical solutions, and absorbance was measured at 517 nm for DPPH and 734 nm for ABTS. Ascorbic acid and Trolox served as positive controls. IC₅₀ and TEAC values were calculated to compare the antioxidant potential of the extracts [13].

Antimicrobial activity was evaluated using disk diffusion and minimum inhibitory concentration methods against *Staphylococcus aureus*, *Escherichia coli*, and *Candida albicans*. Mueller–Hinton agar plates were used for bacterial assays and Sabouraud dextrose agar for fungal assays. Extracts at different concentrations were applied to sterile disks, and inhibition zones were measured after incubation.

All experimental procedures were performed in triplicate, and results were expressed as mean ± standard deviation. Statistical evaluation was performed using one-way ANOVA followed by Tukey's post hoc test, with differences considered significant at *p* < 0.05.

Results and Discussion

The phytochemical screening of *Phlomoides labiosa* extracts revealed a diverse range of secondary

metabolites. Both ethanolic and aqueous extracts showed a clear presence of flavonoids, phenolic compounds, terpenoids, sterols, and saponins, while alkaloids were detected primarily in the ethanolic extract. The richness of phenolic and flavonoid constituents indicated that the plant may possess notable antioxidant and antimicrobial activity, consistent with characteristic profiles of Lamiaceae species [4,5,6,7,8].

Chromatographic analysis provided a detailed chemical profile of the plant. GC–MS identified a mixture of volatile and semi-volatile compounds, including terpenoids, fatty acids, sterol derivatives, and phenolic-like molecules. Several compounds known for biological activity, such as phytol, hexadecanoic acid, β -sitosterol, and various sesquiterpenes, were detected. HPLC analysis confirmed the presence of high levels of gallic acid, quercetin, and rosmarinic acid. These compounds are widely recognized for their antioxidant and antimicrobial potential, suggesting that the observed activities result from synergistic interactions among multiple constituents.

Spectroscopic characterization supported the chromatographic findings. FT-IR spectra showed strong absorption bands corresponding to hydroxyl, carbonyl, aromatic, and aliphatic functional groups, indicating the presence of phenolic acids and flavonoids. UV–Vis spectra displayed characteristic peaks associated with conjugated aromatic systems typical of polyphenolic compounds. NMR data provided structural confirmation of selected fractions, further validating the presence of flavonoid cores and terpenoid structures [10,11,12].

Antioxidant activity assays demonstrated that *Phlomoides labiosa* possesses strong radical-

scavenging capacity. In the DPPH assay, the ethanolic extract exhibited higher activity than the aqueous extract, with IC_{50} values approaching those of the standard ascorbic acid. The ABTS assay showed similarly high activity, suggesting broad-spectrum antioxidant potential. The strong performance of the ethanolic extract can be attributed to its higher concentration of phenolic and flavonoid constituents, compounds well-documented for their electron-donating and free radical–neutralizing abilities.

Antimicrobial evaluation showed that the plant extracts exerted inhibitory effects against both Gram-positive and Gram-negative bacteria, as well as against fungal strains. *Staphylococcus aureus* showed the highest sensitivity, followed by *Escherichia coli*, while *Candida albicans* showed moderate susceptibility. Larger inhibition zones were consistently observed with the ethanolic extract, reflecting its higher phytochemical complexity and concentration of bioactive molecules such as terpenoids and flavonoids. These results align with previously reported antimicrobial activities of related species in the Lamiaceae family [9].

Overall, the combined chemical and biological analyses demonstrate that *Phlomoides labiosa* contains a wide spectrum of bioactive compounds with significant antioxidant and antimicrobial properties. The correlation between the phytochemical content and biological activity suggests that phenolic acids, flavonoids, terpenoids, and sterol derivatives contribute collectively to the plant's functional properties. These findings support the potential application of *Phlomoides labiosa* as a natural source of bioactive molecules for pharmaceutical and nutraceutical development. Further purification and in-depth mechanistic studies are recommended to identify individual active compounds and clarify their specific biological pathways.

Parameters

Phytochemical Screening

GC–MS Analysis

HPLC Analysis

FT-IR Spectroscopy

UV–Vis Spectroscopy

NMR Analysis

Antioxidant Activity

Antimicrobial Activity

Results

Presence of flavonoids, phenolic acids, terpenoids, sterols, and saponins; alkaloids mainly in ethanolic extract.

Detected terpenoids, fatty acids, sterol derivatives, and phenolic-like molecules such as phytol, hexadecanoic acid, and β -sitosterol.

Confirmed high levels of gallic acid, quercetin, and rosmarinic acid.

Absorption bands indicating hydroxyl, carbonyl, aromatic, and aliphatic functional groups.

Characteristic peaks of conjugated aromatic systems typical of polyphenolic compounds.

Structural confirmation of flavonoid cores and terpenoid structures.

Strong DPPH and ABTS radical-scavenging capacity; ethanolic extract showed greater activity.

Effective against *Staphylococcus aureus*, *Escherichia coli*, and *Candida albicans*, with highest sensitivity in *S. aureus*.

Conclusion

The study demonstrated that *Phlomoides labiosa* is a

valuable source of diverse bioorganic compounds with significant biological activity. Phytochemical analysis confirmed the presence of flavonoids, phenolic acids, terpenoids, sterols, and other secondary metabolites that collectively contribute to the plant's functional properties. Chromatographic and spectroscopic evaluations verified the structural characteristics of these constituents, supporting their relevance in antioxidant and antimicrobial mechanisms. Biological assays showed strong radical-scavenging potential and notable inhibitory effects against bacterial and fungal microorganisms, particularly in ethanolic extracts. The findings highlight the potential of *Phlomoides labiosa* as a natural source of bioactive molecules suitable for pharmaceutical, nutraceutical, and bioorganic chemistry applications. Further work involving the isolation of individual compounds, mechanistic studies, and in vivo evaluations is recommended to deepen understanding of the plant's therapeutic potential.

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