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FTIR spectroscopy as a powerful tool for assessing coriander responses to LED lighting through specific chemical biomarkers

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SUMMARY

The study investigated the effects of different LED light wavelengths on the chemical composition and metabolic responses of coriander (*Coriandrum sativum* L.) grown under controlled box conditions. Coriander plants were cultivated under various LED light treatments (CW-control-white, B-blue, R-red, and RB-red/blue combinations). The extracted aboveground plant material was analyzed using ATR-Fourier-Transform Infrared spectroscopy (ATR-FTIR), followed by Principal Component Analysis (PCA). The most pronounced changes were detected in the spectral region between 600 and 1800 cm⁻¹, corresponding to C=O, C=C, C–O, CH₂/CH₃ stretching, and aromatic C=C functional groups of the coriander methanol extracts. However, significant variations in the intensity of the transmission bands were also observed. PCA further confirmed that this region contributed most to the differentiation between CW and treated samples (B, R and RB). The observed variations indicate alterations in the content of aliphatic fatty acids and polyphenolic compounds, suggesting activation of antioxidant defense mechanisms in response to light-induced stress. These findings highlight the potential of LED technology as a tool for optimizing plant growth conditions and enhancing the quality of bioactive compounds and FTIR as an appropriate tool for establishing those findings.

Keywords: *Coriandrum sativum*, LED light treatments, light stress, ATR-FTIR, secondary metabolites.

INTRODUCTION

Coriander (*Coriandrum sativum* L.) is an annual, cosmopolitan plant species belonging to the Apiaceae (syn. Umbelliferae) family. In addition to its culinary use, coriander contains secondary metabolites that contribute to its pharmacological properties, including anticonvulsant, anthelmintic, insecticidal, allelopathic, antidiabetic, antimicrobial, and antioxidant activities (Al-Khayri et al., 2023). Vegetative parts of coriander, including its leaves and stems, are characterized by pronounced nutritional and health-promoting properties, which are largely associated with their high content of polyphenolic compounds (Scandar et al., 2023). The essential oil yield varies significantly in its leaves and stems, with higher content reported in leaves (0.45%), compared to stems (0.20%) (Chung et al., 2011). Vegetative tissues contain several secondary metabolites, such as limonene, γ -terpinene, sabinene hydrate, α -pinene, and caryophyllene, that shape the overall chemical profile and are linked to various biological activities (Al-Khayri et al., 2023) (Table 1). Additionally, trans-anethole has been reported in plant-derived waste fractions, indicating chemical heterogeneity among different plant parts (Wahba et al., 2020).

The variability in the chemical composition of secondary metabolites depends on the genotype, geographical location, environmental conditions, and plant developmental stage, leading to significant differences in the concentrations of bioactive compounds (Al-Khayri et al., 2023). LED lighting represents an important tool in modern controlled plant production systems, which enables precise regulation of the spectral composition of light, directly influencing plant physiological and biochemical processes. Different wavelengths could activate specific photoreceptors and induce changes in photosynthesis, growth, and plant metabolism (Lin et al., 2022). The blue region of the spectrum strongly influences the regulation of morphological and metabolic processes, including the synthesis of antioxidant compounds, the formation of secondary metabolites, flowering, and the production of volatile substances (Lin et al., 2022; Kim et al., 2025). In contrast, the red region of the spectrum is primarily associated with increased photosynthetic efficiency and biomass accumulation, thereby contributing to overall plant growth (Gao et al., 2022). The combination of red and blue light, along with variations in light intensity and duration, often produces a synergistic effect, enabling simultaneous improvement of plant growth and quality through a balanced regulation of primary and secondary metabolism (Gao et al., 2022), including photosynthetic activity and antioxidant status (Lin et al., 2022).

In addition to its effects on growth and metabolism, LED lighting can lead to increased ROS (reactive oxygen species) production, which at higher concentrations induces oxidative stress but also promotes the formation of signaling molecules, thereby improving the plant's capacity to neutralize ROS (Sharma et al., 2021; Wu et al., 2025). Plants develop adaptive responses to different light conditions through gene expression regulation (Isah, 2020) and the activation of protective mechanisms, including the accumulation of protective pigments and antioxidant compounds (Sharma et al., 2021; Khan et al., 2025). The phenylpropanoid pathway plays a central role in ROS detoxification and in maintaining the balance between

Table 1. Chemical composition of the main constituents of coriander above ground plant parts, including constituents common to both leaves and stems.

Plant material	Compounds	Literature
Leaves	linalool; α -pinene; γ -terpinene; limonene; borneol; p-cymene; camphor; citronellol; geraniol; flavonoids; caffeic acid; protocatechuic acid; glycin; β -carotene	Nadeem et al., 2013; Sobhani et al., 2022; Al-Khayri et al., 2023
Stem	phytol; 15-methyltricyclo[6.5.2(13,14),0(7,15)]-pentadeca-1,3,5,7,9,11,13-heptene; dodecanal; 1-dodecanol	Al-Khayri et al., 2023
Leaves, stems	linalool; α -pinene; γ -terpinene; limonene; camphor; geraniol; flavonoids; phenolic compounds; furanocoumarins	Nadeem et al., 2013; Sobhani et al., 2022; Al-Khayri et al., 2023

plant growth, photosynthesis, and defense mechanisms (Wu et al., 2025). LED light could significantly affect secondary metabolism, particularly through the increased synthesis of phenols, flavonoids, and essential oils (Sharma et al., 2021; Wu et al., 2025), as an adaptive response to light stress and oxidative changes in plant cells. In coriander, LED treatments could directly influence the quantity, quality, and chemical composition of essential oils (Akter et al., 2024), including alterations in volatile compound profiles such as terpenes and aromatic constituents (Kim et al., 2025).

MATERIAL AND METHODS

Experimental setup. Coriander seeds produced by the “Seme semena” for microgreens (Belgrade, Serbia) were sown at 3 g per surface area of soil substrate in plastic containers with a volume of 1000 mL. The seed containers were placed in plant growth box and exposed to LED lighting of different wavelengths: white (400–700 nm), blue (450 nm), red (660 nm), and red/blue (50:50).

Plant extraction. After 21 days of plant sowing, plant fresh biomass was harvested (CW-1.6678 g, B-2.7677 g, R-3.1134 g, RB-0.7206 g) washing with distilled water, placed in Petri dishes, and stored at -80°C (Eppendorf Ultra Low Freezer CryoCube, Maldon, Essex, UK). The plant material was then freeze-dried for 48 hours and subsequently ground into a fine powder using a glass rod. The mass after freeze-drying the plants under different lights was as follows: CW-0.1639 g, B-0.3034 g, R-0.1550 g, RB-0.0795 g.

For the ultrasound-assisted extraction (UAE), aliquots of the pulverized dry biomass from each light treatment were accurately weighed and subjected to extraction with 80% (v/v) methanol at a constant solid-to-liquid ratio of 1:20 (g/mL). The initial sample masses and their corresponding solvent volumes were as follows: 0.1639 g / 3.278 mL for CW, 0.3034 g / 6.068 mL for B, 0.1550 g / 3.100 mL for R, and 0.0795 g / 1.590 mL for RB. The sonication process was conducted in an ultrasonic water bath (Bandelin Sonorex, Berlin, Germany) for a duration of 30 min. After extraction, the samples were stored overnight in the dark at 4°C . The following day, the extracts were centrifuged using an Eppendorf Centrifuge (5804 R, Hamburg, Germany) and filtered through 0.45 μm pore size filters. The filtered extracts were

transferred into 50 mL Falcon tubes, wrapped in aluminum foil to prevent light exposure, and stored at 4 °C until further analysis. Finally, the extracts obtained from control and treated coriander plants were analyzed by ATR-FTIR spectroscopy.

Fourier Transform Infrared Spectroscopy (FTIR) analysis of coriander extracts ATR-FTIR spectroscopy measurement. Aboveground coriander extracts (CW-control and three treatments: B-blue, R-red, and RB-red/blue combinations) were characterized by ATR-FTIR using a spectrophotometer (IRAffinity-1, Shimadzu, Japan) operating between 600 and 1800 cm^{-1} , with a resolution of 4 cm^{-1} and 100 scans. For the spectral acquisition, a single droplet (approximately 15–20 μL) of the methanolic extract was applied directly onto the diamond ATR crystal using a micropipette. To evaluate the spectral profile in both phases, measurements were performed in two steps: initially, the extract was scanned in its liquid state, and subsequently, a second spectrum was recorded after the complete evaporation of the solvent at room temperature, leaving a uniform dry extract film on the crystal surface. Each sample from the respective light treatments (CW, B, R, and RB) was analyzed in triplicate (three independent spectral measurements) to ensure reproducibility. Between successive measurements and prior to introducing a new light treatment, the ATR crystal and pressure tip were thoroughly cleaned with high-purity ethanol/acetone and dried with lint-free laboratory wipes.

FTIR spectral data pre-treatment and chemometrics analysis. The spectral range of 600–1800 cm^{-1} , which contains abundant spectral information, was selected for subsequent experimental analysis. To reduce the effects of baseline drift and magnitude discrepancies on the spectral data, the raw spectra in this study were processed using smoothing, baseline correction, and normalization techniques. Baseline correction was performed using Savitzky–Golay filters with seven points, and a second-order polynomial function was used for smoothing. Spectra were pre-processed using Spectragryph software Version 1.2.8 (Menges, 2018; www.effemm2.de/spectragryph). PCA was conducted using PAST software Version 3.26b (Hammer et al., 2001). Characteristic bands of specific functional groups were identified based on literature records.

RESULTS AND DISCUSSION

Plant morphology under LED light wavelengths. The spectral composition of LED radiation represents a key regulator of photomorphogenesis and metabolic activity in plants under controlled conditions, as different wavelengths of light induce specific morphological, anatomical, and biochemical responses (McAusland et al., 2020). In coriander, the quality and combination of light spectral components directly determine plant morphological traits, including plant height, the number of leaves, leaf area, and biomass accumulation (Wang et al., 2022).

Coriander plants grown under cool white LED light exhibit balanced growth characterized by proportional development of the aboveground and belowground parts of the plant (Picture 1CW). Cotyledons are properly oriented and symmetrically arranged, while leaves maintain

a typical intense green coloration, indicating the absence of pronounced light stress. Plants exposed to blue light (Picture 1B), compared to white light (Picture 1CW), show slightly increased vegetative activity, with well-developed roots and a mild stem elongation relative to cool white light. An increased compactness of the plants is observed, along with a regular arrangement of cotyledon leaves and the more intense green leaf coloration, indicating enhanced chlorophyll accumulation and improved photosynthetic efficiency.



Picture 1. Coriander grown under different LED lights are shown: CW-cool white, B-blue, R-red, and RB-a combination of red/blue light. (Author photo, 2026).

Exposure to red light (Picture 1R) leads to a pronounced stimulation of elongation growth, resulting in stem extension and a disruption of the balance between aboveground and belowground biomass. Leaves exhibit a lighter green shade compared to the cool white treatment, while the arrangement of cotyledon leaves remains regular. A balanced ratio of red and blue light (Picture 1RB) contributes to the harmonious development of both aboveground and belowground plant organs. Cotyledons are properly oriented, with a pronounced intense green leaf coloration that correlates with improved photosynthetic activity.

ATR-FTIR spectroscopy as a tool for investigating the impact of LED lighting on changes in coriander secondary metabolites. Methanol (polar solvent) is highly effective in isolating bioactive, polar compounds, producing higher yields compared to non-polar solvents. The methanol extract from the coriander herb is particularly rich in phenolic compounds, phenolic acids (vanillic, p-coumaric, and ferulic acids), flavonoids (quercetin, acacetin and kaempferol) (Scandar et al., 2023), and essential oils: monoterpene (linalool-tertiary alcohol), diterpene (phytol, primary alcohol) and monounsaturated fatty acid (oleic acid) (Nurzynska-Wierdak et al., 2013).

ATR-FTIR spectroscopy was used to gain deeper insight into the differences in chemical profiles of coriander plants grown in CW-control and LED light treatments (R, B, and RB) (Figure 1). FTIR analysis was performed in the range of 600–1800 cm^{-1} to identify functional groups present in the control and treated samples (RB, B, and R) and to evaluate possible changes after applied treatments. The preprocessed and averaged ATR-FTIR spectra of the coriander extracts are characterized by several transmission bands (Figure 1, Table 2), mainly assigned to vibrations of the essential oil and polyphenolic compounds.

At the first site, all analysed samples (Figure 1) showed a similar transmission-band profile, indicating that the basic chemical structure of the material was preserved under the treatments.

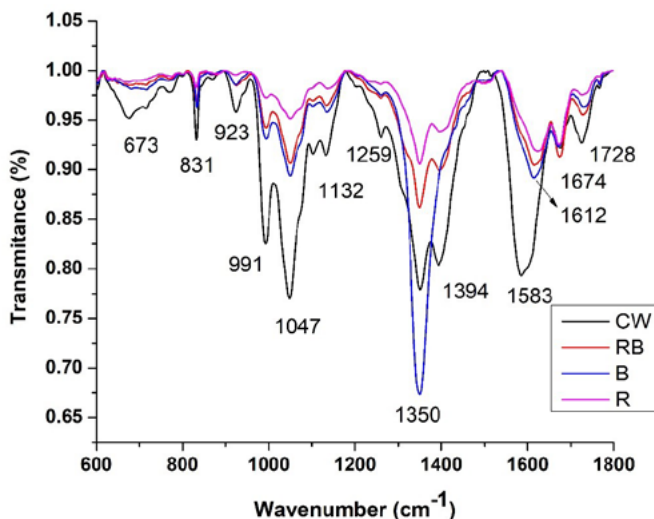


Figure 1. Baseline corrected and smoothed FTIR spectra of coriander extracts obtained under different LED light treatments (CW, R, B, and RB) in the range of 600–1800 cm^{-1} .

The peak at 1728 cm^{-1} may indicate the presence of carboxyl groups ($-\text{C}=\text{O}$) stretching modes, suggesting the occurrence of a dimer carboxylic acids or free esters. C–H scissoring and CH_3 bending vibrations of aliphatic groups are found in the band region of 1300–1480 cm^{-1} , with bands positioned at 1394 and 1350 cm^{-1} (Senrayan et al., 2019; Rahim et al., 2024). Peaks in the lower spectral region of 670–1250 cm^{-1} confirm the presence of ester groups through the stretching vibration of C–O in alcohols and CH_2 wagging vibrations (Ali et al., 2015). Additionally, C–H out-of-plane bending vibrations of aromatic rings can be found at these wavenumbers (Mahardika et al., 2023).

In all spectra of the analyzed samples, two very pronounced bands at around 1350 and 1583 cm^{-1} are observed. These can be attributed to C–H group scissoring and to symmetric and asymmetric C=C and C=O stretching vibrations of the RCOO^- ions (carboxylate ions) of fatty acids or organic acids, and/or C=C phenyl ring stretches, respectively (Luna et al., 2016; Mahardika et al., 2023). The band at 1394 cm^{-1} is due to the presence of the tertiary alcohol (C–OH) group linalool (Yashni et al., 2021). The weak peak at 1259 cm^{-1} could correspond to the C–H vibration of a methyl group and/or the C–O stretching band. Meanwhile, a higher intensity band at 1047 cm^{-1} , which could be related to the $-\text{C}-\text{O}$ vibration of alcoholic groups, is also observed (Luna et al., 2016; Mahardika et al., 2023).

Averaged spectra (Figure 1) showed a highly similar chemical composition among the investigated samples (CW, R, B, RB). Changes in the intensity of existing peaks suggest interactions or changes in the chemical environment of functional groups without significant alteration of the basic chemical structure of the extract. However, the differences could originate from peaks mainly associated with aromatic ring vibration and ester groups (831, 991

and 1047 cm^{-1} , respectively), essential oils (1350, 1394 cm^{-1}), and polyphenolic compounds (1583 cm^{-1}). These peaks show higher intensities for phenolic compounds in control plants than in other treatments, and a probably higher concentration of essential oils under blue light wavelengths than in other treatments.

Table 2. Wavenumbers and identified functional groups in coriander plant extract.

Wavenumber (cm^{-1})	Functional group / vibration	Chemical assignment	References
673	C–H out-of-plane bending	aromatic compounds	Mahardika et al. (2023)
831	C–H out-of-plane bending	substituted aromatic rings	Mahardika et al. (2023)
923	C–O stretching + CH_2 wagging (ester region)	ester groups	Ali et al. (2015)
991	=C–H bending	vinyl / unsaturated lipids	Rahim et al. (2024)
1047	C–O stretching	alcohols / esters / phenols	Ali et al. (2015), Luna et al. (2016), Mahardika et al. (2023)
1132	C–O stretching	esters / alcohol groups	Ali et al. (2015), Senrayan et al. (2019), Mahardika et al. (2023)
1259	C–O / C–H vibration	esters / methyl groups	Luna et al. (2016), Mahardika et al. (2023)
1350	CH_3 / CH_2 bending (scissoring)	aliphatic fatty acids	Ali et al. (2015), Senrayan et al. (2019), Rahim et al. (2024)
1394	CH_3 bending / C–OH (tertiary alcohol)	aliphatic alcohols (linalool)	Senrayan et al. (2019), Yashni et al. (2021), Rahim et al. (2024)
1583	C=C stretching	aromatic rings / phenolics	Luna et al. (2016), Mahardika et al. (2023)
1612	C=C stretching	conjugated/aromatic systems	Mahardika et al. (2023)
1674	C=O stretching (amide I / conjugated)	proteins / conjugated carbonyls	Mahardika et al. (2023)
1728	C=O stretching	esters / carboxylic acids	Ali et al. (2015), Senrayan et al. (2019)

PCA of the data obtained from FTIR spectra of coriander extracts. To identify the spectral regions that most strongly contribute to differences between samples, the FTIR data were combined with PCA. The PCA model obtained for the coriander samples resulted in two principal components, which together explained 99.42% of the original FTIR spectra (PC1-76.46%, PC2-22.96%). The scoreplot and loadings for the first two principal components are shown in Figure 2.

The score plot of PC1 versus PC2 (Figure 2A) clearly indicates the existence of two groups of objects along the PC1 axis; extract of RB and R lights differs clearly from blue and control samples. The loading plot (Figure 2B) shows that the variables with a positive influence along the PC1 axis correspond to the signals at 831, 991, 1047, 1350, and 1583 cm^{-1} .

The highest positive intensity loadings along PC1 at 991 and 1047 cm^{-1} are mostly responsible for the differentiation among samples from red-blue and red lights to all other samples, probably attributed to aromatic ring vibration and ester groups (Ali et al., 2015, Luna et al., 2016). Apparently, to a lesser extent, the observed differences were associated with fatty acids,

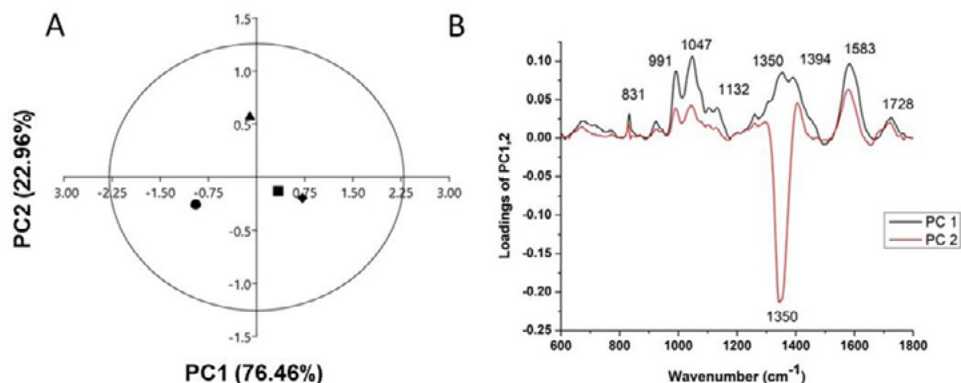


Figure 2. PCA applied to the averaged data obtained from FT-IR spectra of coriander extracts under different treatments, showing the most influential wavenumbers responsible for sample differentiation. a) score plot, b) loading plots, symbols indicated on the specified treatment (circle-CW, diamond-R, triangle-B, square-RB).

organic acids, and/or polyphenolic compounds, as suggested by the positive intensity loadings in the 1300–1600 cm^{-1} region (Senrayan et al., 2019, Rahim et al., 2024).

The second principal component (PC2) provides a clear separation of the investigated samples, with those samples exposed to blue light differing from all other samples. According to PC2, coriander extract from blue LED light treatment mainly differ in polyphenolic compounds (1583 cm^{-1}), followed by the ester groups of essential oils (Ali et al., 2015). PC2 also indicated that control samples form one cluster, while R and RB are grouped together, due to their similarities. The highest intensity loading at 1350 cm^{-1} indicated on the RCOO–ions of fatty acids or organic acids.

CONCLUSION

ATR-FTIR spectroscopic analysis combined with multivariate analysis based on PCA showed that LED light stress causes measurable changes in the chemical composition of coriander plant extracts, mainly seen in variations in the intensity of bands associated with phenolic compounds and aliphatic fatty acids. PCA confirmed that these functional groups act as key chemical markers for sample differentiation, showing a clear separation between the treated groups (R, B, RB) and the control based on polyphenolic and essential oil components. The results suggest activation of protective metabolic mechanisms and reorganization of cellular components as part of the plant's adaptation strategy.

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FTIR spektroskopija kao moćan alat za procenu razvoja korijandera pod različitim uslovima LED osvetljenja putem specifičnih hemijskih biomarkera

REZIME

Ova studija je istraživala efekte različitih talasnih dužina LED svetlosti na hemijski sastav i metaboličke odgovore korijandera (*Coriandrum sativum* L.) gajenog u kontrolisanim uslovima. Biljke korijandera uzgajane su pod različitim tretmanima LED osvetljenja (CW-kontrolna–be-

la, B–plava, R–crvena i RB-kombinacija crvene/plave svetlosti). Ekstrahovani nadzemni biljni materijal analiziran je primenom ATR-Furijske transformacione infracrvene spektroskopije (ATR-FTIR), nakon čega je sprovedena analiza glavnih komponenti (PCA). Najizraženije promene uočene su u spektralnom regionu od 600 do 1800 cm^{-1} , koji odgovara funkcionalnim grupama C=O, C=C, C–O, istezanju CH_2/CH_3 veza i aromatičnim C=C grupama u metanolnim ekstraktima korijandera; međutim, zabeležene su značajne varijacije u intenzitetu transmisionih pikova. PCA je potvrdila da je upravo ovaj region najviše doprineo razlikovanju CW i tretiranih uzoraka (B, R i RB). Uočene varijacije ukazuju na promene u sadržaju alifatičnih masnih kiselina i polifenolnih jedinjenja, što sugeriše aktivaciju antioksidativnih mehanizama odbrane kao odgovor na stres izazvan svetlošću. Ovi rezultati ističu potencijal LED tehnologije za optimizaciju uslova rasta biljaka i poboljšanje kvaliteta bioaktivnih jedinjenja, kao i FTIR metode kao odgovarajućeg alata za brzo utvrđivanje ovih promena.

Ključne reči: *Coriandrum sativum*, tretmani LED svetlom, stres svetlosti, ATR-FTIR, sekundarni metaboliti.