

Chemistry

Chemical constituents of extracts, circadian variation of essential oil chemical composition and antioxidant activity of *Plectranthus neochilus*

Constituintes químicos dos extratos, variação circadiana da composição química do óleo essencial e atividade antioxidante de *Plectranthus neochilus*

**Abraão José Silva Viana¹ , Alyson Tôrres de Barros¹ ,
Deilson de Almeida Alves¹ , Daniel José Silva Viana¹ ,
Paulo Henrique Fidêncio¹ , Patrícia Machado de Oliveira¹ **

¹ Universidade Federal dos Vales do Jequitinhonha e Mucuri, Diamantina, MG, Brazil

ABSTRACT

This work describes the phytochemical study of the extracts, the circadian variation of volatile compounds and the antioxidant activity of the leaves of the plant species *Plectranthus neochilus* Schltr. (Lamiaceae). The phytochemical study of the hexane extract provided two triterpenes: α -amyrin esterified and friedelin. A mixture of the steroids sitosterol and stigmasterol was also obtained from this extract. From the ethyl acetate extract, the methoxylated flavone at positions C-6 and C-7, cirsimaritin, was obtained. All the compounds obtained were described for the first time in the species, with the structural elucidation of the isolated compounds being based on spectroscopic analysis of 1D NMR, HPLC, ESI and comparison with data found in the literature. By evaluating the circadian variation in the composition of the essential oil, it was observed that the major compounds (*E*-caryophyllene (21.55%, 24.06% and 17.53%) and methyl communate (19.72%; 11.09% and 26.88%) showed significant variations in the three collection periods (8h, 13h and 18h), with the diterpene methyl communate identified for the first time in the essential oil of *Plectranthus*, as well as the species *P. neochilus*. The RSA of the essential oil at 13h showed the highest average among the three times evaluated (19.94%). Regarding the extracts, the extraction method with MeOH from the leaves (EMA) proved to be the most efficient in the RSA (10.46%) and RP (0.737) tests, confirmed by the greatest accumulation of total phenolics (466.67 mg.g⁻¹).

Keywords: Boldo; Flavonoid; Natural products

RESUMO

Este trabalho descreve o estudo fitoquímico dos extratos, a variação circadiana dos compostos voláteis e a atividade antioxidante das folhas da espécie vegetal *Plectranthus neochilus* Schltr. (Lamiaceae). O estudo fitoquímico do extrato hexânico forneceu dois triterpenos: α -amirina esterificada e friedelina. Deste extrato foi obtida também a mistura dos esteróides sitosterol e estigmasterol. A partir do extrato em acetato de etila obteve-se a flavona metoxilada nas posições C-6 e C-7, a cirsimarina. Todos os compostos obtidos foram descritos pela primeira vez na espécie, sendo a elucidação estrutural dos compostos isolados, baseada na análise espectroscópica de RMN 1D, CLAE, ESI e por comparação com dados encontrados na literatura. Através da avaliação da variação circadiana na composição do óleo essencial, observou-se que os compostos majoritários (*E*-carifoleno (21.55%, 24.06% e 17.53%) e comunato de metila (19.72%; 11.09% e 26.88%)) apresentaram variações significantes nos três períodos de coleta (8h, 13h e 18h), sendo que o diterpeno comunato de metila identificado pela primeira vez no óleo essencial de *Plectranthus*, bem como na espécie *P. neochilus*. O RSA do óleo essencial às 13h apresentou a maior média dentre os três tempos avaliados (19.94%). Quanto aos extratos, o método de extração com MeOH das folhas (EMA) se mostrou o mais eficiente nos testes de RSA (10.46%) e RP (0,737), confirmado pelo maior acúmulo de fenólicos totais (466,67 mg.g⁻¹).

Palavras-chave: Boldo; Flavonoide; Produtos naturais

1 INTRODUCTION

The genus *Plectranthus* belongs to the Lamiaceae family, composed of approximately 350 species of perennial herbs and shrubs native to tropical and subtropical regions of Africa, Asia, Oceania and South America (Sako et al., 2023; Rodriguez-Ferreiro et al., 2022). They are used as medicinal plants for infectious, dermatological and gastrointestinal diseases, and their pharmacological properties are often attributed to the presence of bioactive oxygenated diterpenes from abiethane, kaurane, phyllocladane, labdane, neoclerodane and halimane classes (Abdel-Mogib et al., 2002; Mesquita et al., 2021). Plants of the genus are also an important source of new bioactive compounds and potential medicines (Oliveira et al., 2007b).

Several species of *Plectranthus* have been shown to produce phenolic compounds and terpenes. Diterpenes of the abietane class are the most frequently found metabolites, therefore the most studied of the *Plectranthus* genus, characterized by a structural diversity resulting from oxygenation and rearrangement of the basic skeleton of tricyclic abietane (Gáborová et al., 2022).

Pharmacological studies of the genus *Plectranthus* have already demonstrated several biological activities, including embryotoxic activity, intestinal relaxant, antispasmodic (Câmara et al., 2003), repellent and fumigant (Luz et al., 2022; Albuquerque et al., 2024), antimicrobial (Oliveira et al., 2022; Antão et al., 2021), cytotoxic (Sako et al., 2023), nephroprotective (Basist et al., 2022), anti-inflammatory (Napagoda et al., 2022).

Among the medicinal species of the genus, *Plectranthus neochilus* Schltr. stands out, which is an aromatic herb used in folk medicine to treat liver failure and dyspepsia (Galbiatti et al., 2021; Lawal et al., 2010). In Brazil, the plant is popularly known as “boldo” or “boldo-gambá” and, like the species *P. barbatus* (“boldo-brasileiro”) and *P. ornatus* (“boldinho”), its leaves are used as tea *Peumus boldus* (“boldo-do-chile”) (Oliveira et al., 2007a). Its fresh leaves have a distinct odor and are used as an infusion or aqueous extract for curative purposes in its popular use (Lorenzi; Matos, 2002).

Studies have already demonstrated the pharmacological action of *P. neochilus*, with several biological activities already proven, such as antioxidant, diabetes control, cytotoxic (Borges et al., 2016; Mamoudou et al., 2025), but with great emphasis on antimicrobial activity (Oliveira et al., 2022). The study by Pereira et al. (2015) observed that the acetone extract obtained by the ultrasound technique showed activity against gram positive bacteria, while the study with the essential oil tested against bacteria that cause oral pathologies showed an MIC below 250 $\mu\text{g/mL}$, with activity against the pathogen *Streptococcus mutans* with an MIC of 3.9 $\mu\text{g/mL}$ (Crevelin et al., 2015).

The study of Brazilian biodiversity has been quite promising, since the abundance of natural reserves in Brazil represents a potential source of bioactive extracts and a possibility of discovering new therapies. This species under study was chosen due to its widespread use in worldwide folk medicine and its importance in traditional Brazilian medicine for treating various pathologies, which justifies its application in this study for the evaluation of this activity in vitro.

The present work describes the phytochemical study of the extracts, the circadian variation of volatile compounds and the antioxidant activity of the leaves of the plant species *Plectranthus neochilus*, identifying the volatile compounds present in the oil.

2 METHODOLOGY

2.1 Plant material

The species *P. neochilus* was cultivated on the JK Campus of the Federal University of Vales do Jequitinhonha and Mucuri – UFVJM, Diamantina, Minas Gerais, Brazil (Coordinates -18.12252; -43.56067), being planted through vegetative propagation using the plant's branches. The species was taxonomically identified and deposited in the DIA Herbarium at UFVJM, under registration number 1720.

The region is characterized by cultivating an average temperature of 19 °C in winter temperatures up to 10 °C, giving an altitude of 1370 meters. The plant showed flowering throughout the year, stopping only during the rainy season that lasts from November to February.

The leaves of the species *P. neochilus* were dried in an air circulation oven at a temperature of 55 °C until they maintained a constant weight. After the drying period, they were stored until the essential oils were extracted.

2.2 Foliar analysis

For leaf analysis was used Manual Chemical Analysis of Soils, Plants and Fertilizers from Embrapa (Silva, 2009), and quantified the levels of nutrients and heavy metals. We used the atomic absorption spectrometer (Varian Spectr AA 50) to the Ca, Mg, Fe, Cu, Mn, Zn, heavy metals Pb, Ni and Cd, UV-Vis spectrophotometer (Biospectro SP-22) for P, a flame photometer (Analyser 910M) to K. The analysis was performed in triplicate for all elements.

2.3 Phytochemistry of extracts

2.3.1 General experimental procedures

To isolate the compounds, glass columns of different diameters and sizes were used, eluted under atmospheric pressure and as stationary phase Merck silica gel 60 (70-230 Mesh) and Sephadex LH-20. The spectra in the infrared region were obtained using KBr or NaCl tablets, on SHIMADZU/IR-408 and Perkin-Elmer 283B equipment from the Department of Chemistry – ICEx/UFMG and the ^1H and ^{13}C RMN spectra and subspectra DEPT-135 were obtained on Bruker spectrometers models DX-200 (200 MHz) and DRX-400 (400 MHz) from the Department of Chemistry – ICEx/UFMG.

The chemical shifts were recorded in δ units and the coupling constants were given in Hz. As an internal reference standard for the RMN spectra, tetramethylsilane was used. The solvents used were deuterated chloroform and pyridine (CDCl_3 and $\text{C}_5\text{D}_5\text{N}$). High-resolution mass spectra were obtained from samples dissolved in 0.2 mol L^{-1} of NH_4OH in methanol (negative mode) and injected directly into the Q-ToF MicroTM equipment (Micromass, Manchester, UK) of the Department of Chemistry – ICEx/UFMG.

2.3.2 Extraction and isolation of chemical constituents

Leaves of *P. neochilus* were dried in an air circulation oven at a temperature of 55°C until maintaining a constant mass and subsequently ground in knife mills. The ground material (550 g) was subjected to exhaustive extractions by maceration, successively with Hexane and EtOAc, obtaining the respective extracts of Hexane (33 g) and EtOAc (45 g). The extracts were subjected to filtration in a silica gel column using the solvents hexane, CHCl_3 , EtOAc and EtOH as eluents, as well as a mixture of these providing a polarity gradient, starting from pure hexane to pure EtOH. Three compounds were obtained from the hexane extract. Compound (1) appeared as a white solid (101.1 mg), isolated from the Hexane:EtOAc fraction (9.5:0.5). When subjected to the Liebermann-Burchard test, it showed a pink color,

a positive result for triterpenes. Another identified compound (2) was isolated from the fraction eluted with Hexane: CHCl_3 (7:3), where it was washed extensively with ethyl ether, providing a white crystalline solid (33.5 mg). Compound (2) appeared as a white solid and, when subjected to the Lieberman-Burchard test, it presented a pink color, a positive result for pentacyclic triterpenes. A mixture of two compounds (3) was obtained from the fraction eluted with Hexane: CHCl_3 (3:7) and subsequently washed twice with ethyl ether until it appeared as a white crystalline solid (96.8 mg) and when subjected to the test of Liebermam-Burchard, showed a green color, indicative of the steroidal nature of the sample. Through the EtOAc extract, after filtration, the fraction eluted in CHCl_3 :EtOAc (7:3) obtained a material appearing as a reddish crystalline solid (40.0 mg), where it was subsequently subjected to two successive filtrations on a Sephadex column. LH-20, using a MeOH:EtOAc mixture (1:1) as solvent, thus obtaining compound (4), a light brown crystalline solid (20.0 mg).

2.3.3 Extractions and analysis of essential oil

For essential oil extraction, 500 g of fresh leaves were collected at three time intervals, at 8, 13 and 18 hours, to evaluate circadian variations in essential oil content. Essential oil extraction was performed by hydrodistillation for 3 hours, using a Clevenger apparatus. After extraction, the Clevenger apparatus column was washed with ethyl ether to collect all the essential oil, thus forming two phases. Using a separatory funnel, the organic phase containing the essential oil and ethyl ether was then separated from the aqueous phase, anhydrous calcium sulfate was added, filtered and then the ethyl ether was evaporated in a rotary evaporator at 40°C. Extractions were performed in triplicate. For the antioxidant test, the essential oil (0.3 mL) was dissolved in methanol until reaching 1 mL, from which aliquots of 200, 300 and 500 μL were removed and completed to 1 mL with methanol, thus obtaining a final concentration of 60, 90 and 150 ppm, all in triplicate.

2.4 Gas Chromatography-Mass spectrometry

The analysis was performed in a gas chromatograph Shimadzu GC-2010 equipped with DB-5 column (30 m x 0.25 mm, coating thickness 0.25 mm) and quadrupole mass detector GCMS-QP2010, belonging to the Núcleo de Pesquisas em Produtos Naturais e Sintéticos (NPPNS), Faculdade de Ciências Farmacêuticas de Ribeirão Preto, Universidade de São Paulo (USP). The conditions of analysis were the following: injector temperature 250°C, column temperature 60°C to 240°C at 3°C/min; helium to 1:33 mL/min.

2.5 Identification of essential oil constituents

The identification of individual constituents was performed by comparing the acquired mass spectra with those stored in the NIST12, NIST62, FFNSC1.3 and WILEY7 mass spectral libraries of the GC/MS data system. In addition, the retention index for each constituent was calculated according to Van der Dool and Kratz (1963) relative to a homologous series of hydrocarbons (C_9H_{20} - $C_{25}H_{52}$) and compared to retention indices from the literature Adams (2007).

2.6 Determination of antioxidant activity

The essential oil and extracts were checked for antioxidant activity. Using the method described by Singh et al. (2002) and Blois (1958) the DPPH radical scavenging activity (RSA) of both the essential oil and the hexane (EHA), ethyl acetate (EAA) and methanolic (EMA) extracts of the leaves and the methanolic extract of the flowers were evaluated (EMF). For the essential oil, 0.1 mL aliquots dissolved in methanol at concentrations 60, 90 and 150 ppm were placed in test tubes with 3.9 mL of 0.06 mM DPPH (2,2-diphenyl-1-picrylhydrazyl radical) and homogenized, while the extracts evaluated at concentrations of 200, 300 and 400 ppm. Readings were taken after 30 minutes of incubation at 25°C and a wavelength of 515 nm. 0.1 mL of 100 ppm alcoholic gallic acid solution was used as a positive control. A control tube containing the above mixture, without oil, was used as a blank and methanol was used as baseline compensation. All tests were performed in triplicate and DPPH

radical scavenging activity, expressed as the percentage of inhibition was calculated using the formula: %RSA = [(Control Abs - Sample Abs) / Control Abs] x 100.

The extracts were also subjected to quantification of Total Phenolics Contents (TPCs) and determination of Reducing Power (RP). For TPC quantification, the extracts were analyzed according to the methodology described by Singh et al. (2002), with the EAA, EMA and EMF extracts dissolved in methanol and the EHA extract dissolved in chloroform. In the TPC test, extract concentrations were 300 ppm and a calibration curve with gallic acid was used according to the methodology described by Bonoli et al. (2004). The TPC results found were expressed in gallic acid equivalents (GAE). To determine the amount of AG in the solution, the equation was used: mg AG in 10 mL = (10 x ppm AG)/1000 and subsequently, to find the value in mgGAE/g of extract, the equation was used mgGAE/g of extract = (1000 x mg AG in 10 mL)/3. To determine the RP, the extracts were evaluated at 50, 100, 200 and 300 ppm and analyzed according to the methodology described by Yildirim et al. (2001). Absorbance was measured at 700 nm. The increase in reducing power was evaluated with the increase in absorbance.

2.7 Statistical analysis

The major compounds of essential oils obtained by circadian variation and antioxidant activity were subjected to analysis of variance, where the means were compared using the Scott-Knott test, with a significance level of 5%, using the R software.

3 RESULTS AND DISCUSSIONS

3.1 Isolation and identification of chemical constituents

The chromatographic fractionation of the extracts from the leaves of *P. neochilus* led to the isolation of five substances (figure 1), four of which came from the hexane extract, the triterpenes esterified α -amyrin (1), friedelan-3-one (2) and the mixture of the steroids sitosterol and stigmasterol (3). From the ethyl acetate extract, the flavonoid

5,4"-dihydroxy-6,7-dimethoxyflavone (cirsimaritin) (4) belonging to the flavone class was obtained. The structural elucidation of these compounds consisted of the analysis of spectral data and comparison with data from the literature.

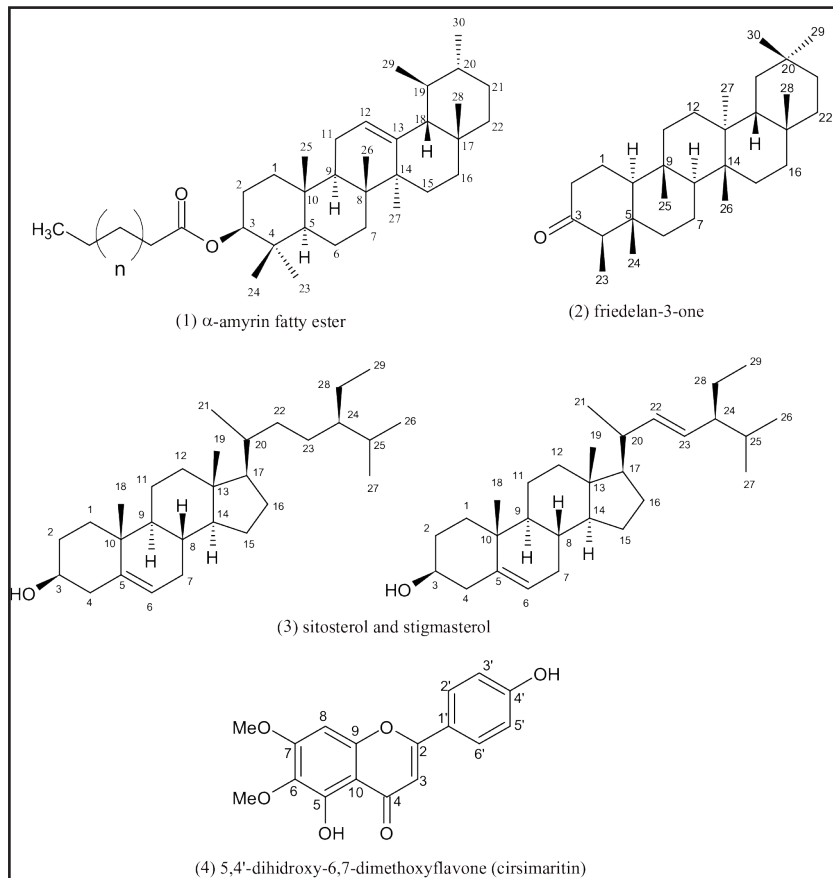
The review work by Benali et al. (2022) demonstrated the biological properties of cirsimaritin, including anticancer, antimicrobial, antidiabetic, antiparasitic, antioxidant and anti-inflammatory effects, in which the mechanisms involved in the multiple activities of this molecule are diverse and encompass subcellular, cellular and molecular levels. Studies have found that this bioactive induces anti-inflammatory and antiproliferative effects through the inhibition of cell membrane receptors, interference in signaling pathways and inhibition of transcriptional factors, such as $\text{Nf-}\kappa\text{B}$, involved in cell promotion and proliferation.

1. α -amyrin esterified. White crystalline solid. RMN ^1H [400MHz, CDCl_3 , δ (ppm), J (Hz)]: 0.80; 0.87; 0.98; 1.01 and 1.07 (s, 5 CH_3), 0.83 and 0.91 (s, C-29 and C-30), 4.51 (H-C-O, C-3), 2.29 (t, $J = 7.4$ and 7.6 Hz) and 1.25 (side chain linked to the ester group). RMN ^{13}C [400MHz, CDCl_3 , δ (ppm), J (Hz)]: 38.5 (CH_2 -1); 23.6 (CH_2 -2); 80.6 (CH-3); 37.8 (C-4); 55.3 (CH-5); 18.3 (CH_2 -6); 32.8 (CH_2 -7); 40.1 (C-8); 47.6 (CH-9); 36.8 (C-10); 23.4 (CH_2 -11); 124.3 (CH-12); 139.6 (C-13); 42.1 (C-14); 26.6 (CH_2 -15); 28.4 (CH_2 -16); 33.8 (C-17); 59.1 (CH-18); 39.4 (CH-19); 39.7 (CH-20); 31.3 (CH_2 -21); 41.5 (CH_2 -22); 28.1 (CH_3 -23); 16.9 (CH_3 -24); 15.7 (CH_3 -25); 16.9 (CH_3 -26); 23.2 (CH_3 -27); 28.8 (CH_3 -28); 17.5 (CH_3 -29); 21.4 (CH_3 -30).

2. friedelan-3-one. White solid in the shape of needles. RMN ^1H [400MHz, CDCl_3 , δ (ppm), J (Hz)]: 0.73; 0.87; 0.95; 1.00; 1.01; 1.05; 1.18 (s, 7 CH_3), 0.87 (d, C-23, $J = 6.50$ Hz), 1.97 (m, H-1), 2.23 (q, H-4, $J = 6.50$ Hz), 2.30 (m, H-2), 2.40 (dd, H-2, $J = 13.80$; 5.10; 1.90 Hz). RMN ^{13}C [400MHz, CDCl_3 , δ (ppm), J (Hz)]: 22.3 (CH_2 -1); 41.5 (CH_2 -2); 213.3 (C-3); 58.2 (CH-4); 42.2 (C-5); 41.3 (CH_2 -6); 18.2 (CH_2 -7); 53.1 (CH-8); 37.4 (C-9); 59.5 (CH-10); 35.6 (CH_2 -11); 30.5 (CH_2 -12); 39.7 (C-13); 38.3 (C-14); 32.8 (CH_2 -15); 36.0 (CH_2 -16); 29.7 (C-17); 42.8 (CH-18); 35.3 (C-19); 28.2 (C-20); 32.4 (CH_2 -21); 39.3 (CH_2 -22); 6.8 (CH_3 -23); 14.7 (CH_3 -24); 17.9 (CH_3 -25); 20.3 (CH_3 -26); 18.7 (CH_3 -27); 32.1 (CH_3 -28); 31.8 (CH_3 -29); 35.0 (CH_3 -30).

3. Sitosterol and Stigmasterol. White crystalline solid. RMN ^1H [400MHz, CDCl_3 , δ (ppm), J (Hz)]: 5.35 (d , H-6), 3.52 (H-3, CH-OH), 5.16 (dd , H-22, $J_{22-23} = 5.0$ Hz e $J_{22-20} = 4.4$ Hz), 5.03 (dd , H-23, $J_{23-22} = 4.4$ Hz e $J_{23-24} = 4.4$ Hz), 0.6 - 2.3 (CH_3 , CH_2 and CH). RMN ^{13}C [400MHz, CDCl_3 , δ (ppm), J (Hz)]: **Sitosterol**: 37.3 (CH_2 -1); 31.7 (CH_2 -2); 71.8 (CH-3); 42.3 (CH_2 -4); 140.8 (C-5); 121.7 (CH-6); 31.9 (CH_2 -7); 31.9 (CH-8); 50.2 (CH-9); 36.5 (C-10); 21.1 (CH_2 -11); 39.8 (CH_2 -12); 42.3 (C-13); 56.8 (CH-14); 24.3 (CH_2 -15); 28.3 (CH_2 -16); 56.1 (CH-17); 11.9 (CH_3 -18); 19.4 (CH_3 -19); 36.2 (CH-20); 19.0 (CH_3 -21); 34.0 (CH_2 -22); 26.1 (CH_2 -23); 45.5 (CH-24); 28.9 (CH-25); 19.8 (CH_3 -26); 18.8 (CH_3 -27); 23.1 (CH_2 -28); 12.1 (CH_3 -29). **Stigmasterol**: 37.3 (CH_2 -1); 31.7 (CH_2 -2); 71.8 (CH-3); 42.3 (CH_2 -4); 140.8 (C-5); 121.7 (CH-6); 31.9 (CH_2 -7); 31.9 (CH-8); 50.2 (CH-9); 36.5 (C-10); 21.1 (CH_2 -11); 39.7 (CH_2 -12); 42.3 (C-13); 56.9 (CH-14); 24.4 (CH_2 -15); 28.3 (CH_2 -16); 56.0 (CH-17); 12.0 (CH_3 -18); 19.4 (CH_3 -19); 40.5 (CH-20); 21.2 (CH_3 -21); 138.3 (CH-22); 129.3 (CH-23); 51.3 (CH-24); 31.9 (CH-25); 19.1 (CH_3 -26); 18.7 (CH_3 -27); 25.4 (CH_2 -28); 12.3 (CH_3 -29).

Figure 1 – Structure of compounds isolated from the leaves of *Plectranthus neochilus*



Source: Authors

4. 5,4"-dihydroxy-6,7-dimethoxyflavone (cirsimaritin). Light brown solid. RMN ^1H [400MHz, $\text{C}_5\text{D}_5\text{N}$, δ (ppm), J (Hz)]: 3.91; 4.02; 6.83; 6.98 (*s*, H-7, H-6, H-3, H-8); 7.31 (*d*, H-3'5', $J_{(3',5')} = 10$ Hz); 7.98 (*d*, H-2'6', $J_{(2',6')} = 10$ Hz). RMN ^{13}C [400MHz, $\text{C}_5\text{D}_5\text{N}$, δ (ppm), J (Hz)]: 183.5 (C-4); 165.2 (C-2); 163.2 (C-4'); 159.7 (C-7); 154.0 (C-5); 153.8 (C-9); 133.5 (C-6); 129.3 (CH-6'); 129.3 (CH-2'); 122.5 (C-1'); 117.3 (CH-5'); 117.3 (CH-3'); 106.7 (C-10); 104.1 (CH-3); 91.9 (CH-8); 60.9 (OMe); 56.8 (OMe).

3.2 Leaf Analysis

The levels of macro and micronutrients (table 1) found in *P. neochilus* are within the nutritional levels found for other cultivated plants (Malavolta, 2006). No traces of the heavy metals Ni, Pb and Cd were detected.

Table 1 – Analysis of the nutrition foliate of *Plectranthus neochilus*

Element	Content	Element	Content
	g kg^{-1}		mg kg^{-1}
Nitrogen (N)	12.68	Iron (Fe)	191.85
Calcium (Ca)	9.62	Copper (Cu)	3.79
Magnesium (Mg)	0.87	Manganese (Mn)	21.78
Potassium (K)	12.83	Zinc (Zn)	43.03
Phosphorus (P)	1.15	Nickel (Ni), Lead (Pb), Cadmium (Cd)*	ND

Source: Authors

*Heavy metals analyzed in the leaves. ND = Not detect

3.3 Essential oil constituents

The essential oil content from collection at different times of the day is presented in table 2. Through the circadian variation of the oils, 36 compounds were identified, with sesquiterpenes being the most abundant. At the three essential oil collection times, the presence of two major compounds, (*E*)-caryophyllene and methyl communate (figure 2), was observed, confirmed by fragments of the mass spectrum (m/z) (table 3). The times of 8h and 13h accumulated the highest content of the compound (*E*)-caryophyllene (21.55% and 24.06%, respectively) significantly reducing the biosynthesis of this compound at the

time of 18h (17.53%). On the contrary, we observed that methyl communate has the highest content at 18h (26.88%), showing that while there is a decrease in the production of (*E*)-caryophyllene, it favors the production of the methyl communate metabolite. This fact can also be observed at 13h when there was the highest accumulation of (*E*)-caryophyllene (24.06%) and the lowest concentration of methyl communate (11.09%). The other compounds in lower concentrations were also identified and totaled. Studies carried out by Lawal et al. (2010) with *P. neochilus* cultivated in South Africa differed in terms of the main compounds of the essential oil found in this work, while the studies carried out by Bandeira et al. (2011) and Galbiatti et al. (2021) found (*E*)-caryophyllene as the main compound in common, the same as that found by Mota et al. (2014) in *P. neochilus* cultivated in Portugal.

Table 2 – Volatile compounds identified in the leaf essential oils of *Plectranthus neochilus* in three different times of day

(Continue)

IR ¹ cal.	Compounds ²	Time of collection		
		8:00 h	13:00 h	18:00 h
		%		
869	(Z)-3-Hexenol	1.20	1.19	0.54
924	α-Thujene	0.73	1.94	0.69
932	α-Pinene	0.80	2.05	0.64
971	Sabinene	0.27	0.68	0.23
976	Octen-3-ol-1	6.72	8.08	2.75
1056	γ-Terpinene	0.09	0.09	-
1099	Linalool	0.23	0.11	-
1123	<i>cis-p</i> -Menth-2-en-1-ol	0.12	0.09	-
1141	<i>trans-p</i> -Menth-2-en-1-ol	0.10	0.07	-
1179	Terpin-4-ol	2.81	1.96	0.81
1194	α-Terpineol	0.49	0.26	0.10
1205	Decanal (N)	0.08	-	-
1344	α-Cubebene	0.78	0.83	0.54
1372	α-Copaene	1.36	1.51	1.02
1380	β-Bourbonene	1.66	2.14	1.47
1384	β-Cubebene	1.17	1.40	-
1400	(Z)-Caryophyllene	0.13	0.16	0.09
1416	(E)-Caryophyllene	21.55	24.06	17.53
1451	α-Humulene	1.18	1.39	-
1476	Germacrene D	4.21	4.84	3.48
1494	α-Muurolene	0.16	0.20	0.18

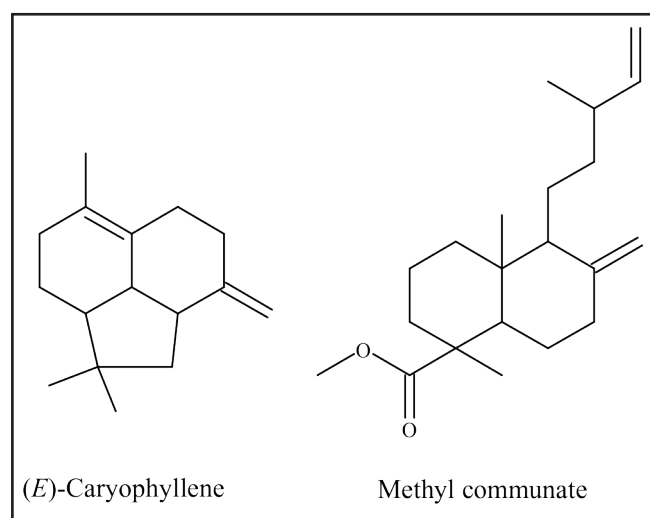
Table 2 – Volatile compounds identified in the leaf essential oils of *Plectranthus neochilus* in three different times of day (Conclusion)

IR ¹ cal.	Compounds ²	Time of collection		
		8:00 h	13:00 h	18:00 h
		%		
1507	γ-Cadinene	5.73	7.00	5.10
1514	δ-Cadinene	2.76	3.10	2.66
1558	(<i>E</i>)-Nerolidol	1.25	1.15	1.10
1576	Caryophyllene oxide	4.68	5.80	4.08
1597	β-Oplophenone	0.34	0.43	0.47
1603	Humulene epoxide II	0.19	0.21	0.15
1610	Cubenol 1,10-DI-EPI	0.22	0.24	0.25
1623	Cubenol 1-EPI	0.67	0.66	0.80
1637	Muurolol epi-alpha	4.74	4.67	5.90
1642	α-Muurolol	0.06	0.33	0.40
1651	α-Cadinol	3.54	3.21	5.04
2211	(<i>E</i>)-Phytol acetato	0.34	0.10	0.10
2507	Methyl communate	19.72	11.09	26.88
	Monoterpenes	13.64	16.52	5.76
	Sesquiterpenes	57.45	64.20	50.99
	Diterpenes	20.06	11.19	26.98
	Total identified	91.15	91.91	83.73

Source: Authors

¹IR = Retention index according index n-alkanes. ²Constituents listed in order of elution on DB-5 column

Figure 2 – Chemical structures of the major chemical constituents identified in the leaf essential oil of *Plectranthus neochilus*



Source: Authors

Table 3 – Fragments obtained from the mass spectrum of the main compounds of *Plectranthus neochilus* essential oil

Compounds	RT (min)	(m/z)
(E)-Caryophyllene	24.8	204, 189, 175, 161, 147, 133, 120, 105, 93, 79, 69, 55, 41
Methyl communate	61.1	344, 316, 301, 284, 269, 256, 241, 215, 191, 175, 161, 135, 121, 107, 95, 81, 67, 43

Source: Authors
RT = Retention time

3.4 Determination of antioxidant activity

The DPPH radical scavenging activity (RSA) was used to evaluate the antioxidant activity of *P. neochilus* essential oil and extracts. DPPH is a radical capable of reducing in the presence of electron-donating compounds (Abdallah et al., 2025). Evidence of the reaction occurs when the violet color of the methanolic DPPH solution disappears, therefore becoming colorless, when it reacts with substances that donate radicals (Bakhtiar et al., 2025). When evaluating the RSA of the essential oil (table 4), it was observed that the concentration of 150 ppm presented the highest averages at the three times evaluated, since at 13h (19.94%) it was significantly higher than at 8h (16.83%) and 18h (16.57%). At a concentration of 60 ppm, it was also observed that the 13h time (9.54%) had a significantly higher average than the other times, while at a concentration of 90 ppm there was no significant difference. The RSA of the positive control, gallic acid, was 67.0% at a concentration of 100 ppm. Through the circadian assessment of the essential oil content, it was observed that between the two major compounds there was a proportional relationship between the content of the compound (E)-caryophyllene and RSA, unlike the methyl communate compound, where as its content reduces RSA increases, being observed in the three collection periods, demonstrating that the major compound (E)-caryophyllene has a significant impact on the neutralization of DPPH through the donation of electrons. Studies have already demonstrated that (E)-caryophyllene has high pharmaceutical

potential due to its analgesic, antioxidant, antimicrobial and anti-inflammatory activities (Gushiken et al., 2022). The antioxidant activity of *P. neochilus* essential oil is probably due to the presence of antioxidant compounds found in different species of the genus (Oliveira et al., 2007b). The antioxidant activities of plant extracts, edible vegetables, fruits, and essential oils have been reported in several studies (Alara et al., 2021; Sun et al 2023).

Table 4 – DPPH radical scavenging activity (RSA) at different concentrations in the circadian evaluation of *Plectranthus neochilus* essential oil

Time of collection (hour)	Concentrations (ppm)		
	60	90	150
	%RSA		
8:00	8.69	12.51	16.83
13:00	9.54	13.11	19.94
18:00	8.29	11.65	16.57
Coefficient of variation (%)	3.64	5.38	6.56

Source: Authors

%RSA = DPPH radical scavenging activity. Means followed by the same letter in the column, in each concentration, do not differ from each other using the Scott-Knott test ($p < 0.05$)

The values found in the RSA test of *P. neochilus* extracts are presented in table 5. According to the results obtained, the EHA extract presented the lowest antioxidant activity among the extracts evaluated. It can be observed that, in the antioxidant evaluation of leaf extracts, the EAA and EMA extracts were those that showed the highest activity, with the EMA extract at the concentrations evaluated presenting the highest RSA averages. The most interesting result was that of the EMA extract, which presented 10.46% and 10.69% of RSA for concentrations of 300 and 400 ppm, showing a significant difference between the other concentrations of the different extracts. The higher values presented by the EMA extract compared to those observed by EMF (4.71%) may be associated with the higher concentration of phenolic compounds, results shown in table 6.

The reducing power (RP) test assists in the results of antioxidant activity (Munteanu; Apetrei, 2021). In this way, RP tests were carried out with the extracts EHA, EAA, EMA and EMF at concentrations of 200 and 300 ppm. The RP of EHA, EAA and EMA extracts were concentration dependent (table 5) and demonstrated a positive response with increasing concentration. It is noted that the best results of the RSA and RP test were observed for EMA, a result consistent with the highest averages of total phenolics.

Phenolic compounds constitute a class of phytochemicals and present in their chemical structure at least one aromatic ring, which is linked to one or more hydroxyls and, depending on the number and position of these hydroxyls in the structure, these compounds have different complexing properties with free radicals, neutralizing them (Alara et al., 2021). Phenolic compounds present in vegetables are mainly responsible for antioxidant activity (Zhang et al., 2023).

The total phenolic content (TPC) results were obtained through linear regression with the gallic acid curve and the results expressed in gallic acid equivalent (GAE) and presented in table 6. The results showed that the more polar extracts have higher TPCs values, with EMA presenting 466.67 mg GAE per gram of extract, followed by the EAA extract (235.42 mgGAE/g) and the EMF extract (181.94 mgGAE/g). EHA presented the lowest TPC value (35.42 mgGAE/g), since the hexane solvent has a low polarity index (0.1), however the presence of phenolic compounds in this extract may be related to the carryover of phenolic compounds during extraction with hexane.

Taking into account the TPC, RSA and RP results, it can be concluded that the methanol extraction method proved to be more efficient with regard to the efficiency of antioxidant activity, due to the extraction of polar compounds, responsible for the greater RSA through neutralization of the DPPH free radical. The greater activity is related to the higher concentration of determined phenolic compounds.

Table 5 – DPPH radical scavenging activity (RSA) and reducing power (RP) of *Plectranthus neochilus* extracts

Concentration (ppm)	Extract			
	EHA	EAA	EMA	EMF
%RSA				
200	3.71	6.32	6.03	4.71
300	3.86	7.31	10.46	4.53
400	3.76	7.39	10.69	4.18
RP (Abs. At 700 nm)				
200	0.137	0.218	0.495	0.246
300	0.176	0.314	0.737	0.329
400	NR	NR	NR	NR

Source: Authors

%RSA = DPPH radical scavenging activity. RP = Reducing Power. NR = Not registered. EHA = hexane leaf extract; EAA = ethyl acetate extract from the leaves; EMA = methanolic extract of leaves; EMF = methanolic extract of flowers. ND = Not registered

Table 6 – Total phenolic contents (TPC) in *Plectranthus neochilus* extracts

Extracts	GAE (mg g ⁻¹)
EHA	35.42 c
EAA	235.42 b
EMA	466.67 a
EMF	181.94 b
Coefficient of variation (%)	30.76

Source: Authors

GAE = Gallic acid equivalents. Means followed by the same letter do not differ from each other using the Scott-Knott test ($p < 0.05$). EHA = hexane leaf extract; EAA = ethyl acetate extract from the leaves; EMA = methanolic extract of leaves; EMF = methanolic extract of flowers

4 CONCLUSIONS

The study of the circadian evaluation of the essential oil of *Plectranthus neochilus* allowed us to verify that throughout the day the content of the major compounds (*E*-caryophyllene and methyl communate present variations. This result directly impacted the antioxidant activity of the essential oil, demonstrating that there was a direct relationship between the increase in the content of the compound (*E*-caryophyllene and

the DPPH radical scavenging activity, unlike the compound methyl communate, which as its content decreases, the DPPH radical scavenging activity increases. These results suggest that the time of collection of the plant influences the obtaining of metabolites of greater interest. The isolation, identification and elucidation of the compounds of the extracts of *P. neochilus* are described for the first time in the species, especially the flavonoid cirsimaritin, a class of compounds with diverse biological activities already recorded in the literature. Since this is an extremely versatile botanical family, more studies on its compounds should be carried out, since it has great pharmacological potential, with a promising future. Therefore, this work contributes to future studies on the species *P. neochilus*. Although this work shows the chemical constituents of the extracts, the circadian variation and the antioxidant activity of the essential oil, their individual and relative contributions to the pharmacological effects need to be further investigated. This approach corroborates efforts to apply the species in folk medicine and contribute to new discoveries of pharmacological activities, mainly for the elucidation of the mechanisms underlying the effects of the action and signaling pathways in the pathogenesis of *Plectranthus* species in inflammatory and painful responses, which can be performed in antimicrobial and antifungal assays, due to the high growth of drug-resistant pathogens.

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Authorship contributions

1 – Abraão José Silva Viana (Corresponding Author)

Federal University of the Jequitinhonha and Mucuri Valleys, PhD in Medicinal, Aromatic and Condiment Plants

<https://orcid.org/0000-0002-3140-859X> • abraao.viana@ufvjm.edu.br

Contribution: Data curation, Formal Analysis, Investigation, Methodology, Software, Visualization, Writing - original draft, Writing - review & editing

2 – Alyson Tôrres de Barros

Federal University of the Jequitinhonha and Mucuri Valleys, Master's Degree in Chemistry

<https://orcid.org/0000-0001-5896-6834> • alyson.torres@ufvjm.edu.br

Contribution: Investigation

3 – Deilson de Almeida Alves

Federal University of Jequitinhonha and Mucuri Valleys, PhD in Plant Production

<https://orcid.org/0000-0002-8524-9010> • deilson.alves@ufvjm.edu.br

Contribution: Conceptualization, Data curation, Formal Analysis, Writing - review & editing

4 – Daniel José Silva Viana

Federal University of Jequitinhonha and Mucuri Valleys, PhD in Biofuels

<https://orcid.org/0000-0003-1867-6845> • daniel.silva@ufvjm.edu.br

Contribution: Data curation, Formal Analysis, Writing - review & editing

5 – Paulo Henrique Fidêncio

Federal University of Jequitinhonha and Mucuri Valleys, PhD in Chemistry

<https://orcid.org/0000-0003-3108-9661> • paulo.fidencio@ufvjm.edu.br

Contribution: Data curation, Formal Analysis, Writing - review & editing

6 – Patrícia Machado de Oliveira

Federal University of Jequitinhonha and Mucuri Valleys, PhD in Chemistry

<https://orcid.org/0000-0003-3829-6751> • patricia.oliveira@ufvjm.edu.br

Contribution: Conceptualization, Data curation, Funding acquisition, Investigation, Methodology, Project administration, Resources, Software, Supervision, Validation, Visualization, Writing - original draft, Writing - review & editing

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