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Chemical characterization of *Lavandula dentata* L. essential oils grown in Uberaba-MG

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ABSTRACT: The essential oils of the different parts of Lavandula dentata L. (inflorescences and aerial part without inflorescences) collected in the city of Uberaba (minas Gerais State)were obtained by hydro distillation, and their chemical composition was determined by gas chromatography coupled to mass spectrometry and compared to the chemical composition of essential oil of Lavandula hybrida and Lavandula officinalis. It was observed that the essential oils of the studied species have varied chemical composition and are composed mainly of monoterpenes. The essential oils of L. hybrida and L. officinalis showed a higher concentration of linalool and linaline acetate, while L. dentata L. presented higher concentration of fenchone, eucalyptol and camphor. Results indicate that the essential oil composition of L dentata L. grown in Uberaba is similar to those produced in Curitiba – PR, providing a promising perspective for the cultivation and extraction of essential oils of this species in Minas Gerais.

Key words: Lavandula dentata, Fenchone, Eucalyptol.

Caracterização química de óleos essenciais de Lavandula dentata L. cultivados em Uberaba-MG

RESUMO: Os óleos essenciais das diferentes partes de Lavandula dentata L. (inflorescências e parte aérea sem inflorescência) coletados em Uberaba - MG foram obtidos por hidrodestilação, e sua composição química foi determinada por cromatografia gasosa acoplada a espectrometria de massas e comparada à composição química de óleo essencial de Lavandula hybrida e Lavandula officinalis. Observou-se que os óleos essenciais das espécies estudadas possuem composição química variada e são compostos, principalmente, por monoterpenos. Os óleos essenciais de L. hybrida e L. officinalis apresentaram maior concentração de linalol e acetato de linalina, enquanto L. dentata L. apresentou maior concentração de fenchona, eucaliptol e cânfora. Os resultados indicam que os óleos essenciais de L. dentata L. cultivada em Uberaba são semelhantes aos produzidos em Curitiba - PR, tornando-se uma perspectiva promissora para o cultivo e extração de óleos essenciais desta espécie em Minas Gerais.

Palavras-chave: Lavandula dentata, Fenchona, Eucaliptol.

INTRODUCTION

The *Lamiaceae* family is composed of approximately 300 genera and 7,500 species, of which 28 genera with about 350 species reported in Brazil (LORENZI & SOUZA, 2012). Part of this family are *Lavandula* plants known as lavenders or lavender, originating in the Mediterranean region of Europe, usually grown in mountainous regions and open savannas of tropical and subtropical climate. The genus presents about 25-30 different species of lavenders (BIASI & DESCHAMPS, 2009).

Lavandula dentata L. is a perennial, aromatic, erect sub-bush with great branching (BIASI

& DESCHAMPS, 2009). HANAMANTHAGOUDA

et al., (2010), complement that the bluish flowers in the peaks, the base of lignified stem and the opposing leaves and edges with contoured "teeth", are the main visual characteristic of identification. The medicinal and therapeutic properties of this plant are related to the presence of the oxygenated monoterpenes, 1,8-cineol and camphor, assigning to it antispasmodic, antifungal and bactericidal action (CHU & KEMPER, 2005; MOON et al, 2006).

Plants have some mechanisms to attract pollinators and repel pathogens, innate immunity is one such mechanism. These mechanisms involve different defense responses, such as cell

Received 11.21.18 Approved 05.31.19 Returned by the author 07.12.19 CR-2018-0964.R2 wall enhancement, lytic enzyme biosynthesis and production of secondary metabolites, such as essential oils or volatile oils. These pathogens may be, among others, microorganisms and, in response to these invasions, plants acquire biotechnical values with antimicrobial potential (JONES & DANGL, 2006).

Secondary metabolites play an important role in the interaction of plants with the environment, such as against herbivores, pathogen attack, competition between plants and attraction of pollinators (DUDAREVA et al., 2006). There are three major groups of secondary metabolites: terpenes, phenolic compounds and alkaloids. The essential oil constituents vary from terpenes, alcohols, aldehydes, ketones, phenols, esters, ethers, oxides, peroxides, furans, organic acids, lactones, coumarins, and even sulfur compounds. In the plant, these compounds are present at different concentrations, usually being the major compounds, while other compounds exist in lower concentrations or traces (SIMÕES et al., 2002).

The biodiversity of plant species of the Cerrado region of Brazil is enormous and the potential for scientific research is also vast (SAAD et al., 2013). This was the bioma in which the plant studied in research was obtained. In this context, this research had the objective of extracting the essential oil of *Lavandula dentata* L. grown in the countryside in Uberaba - MG, chemical characterization of these essential oils and the comparison with essential oils of two other *Lavandula* species, *L. hybrida* and *L. officinalis*.

MATERIALS AND METHODS

Preparation of plant material

The plant, cultivated in the countryside was obtained from a site located in Uberaba-MG (Latitude S 19° 61'92 " Longitude: W 47° 88'27 " Altitude: 823 m). The region of Uberaba, according to Köppen climatological classification, was codified as (Cwa) as a subtropical/tropical climate of altitude, where there are humid temperate climate characteristics, with dry winter and hot summer (ALVARES et al., 2014). The climatic data of the collection period were obtained from the database of the meteorological station located in Uberaba-MG city. Plant collections were made from February to May 2017, in the morning, period of the day in which the plants are richer in oil (RIBEIRO and DINIZ, 2008). Samples were separated according to 2 groups: Group 1 -Inflorescence (pre-anthesis/anthesis/senescent) and Group 2 - Aerial part without inflorescence (leaves and stems). These groups originated OE1 and OE2, respectively. For the comparative study the essential oils of *L. officinalis* and *L. hybrida* were acquired from Ferquima[®] O.E and were labelled OE3 and OE4, respectively.

Extraction and chemical analysis of essential oil

The extraction of the essential oils from the different groups of samples was carried out by water vapor dragging technique, where each extraction cycle had an average duration of 50 minutes for +/-200 g fresh plant.

The referred system is consisted of two stainless steel chambers (pressure cookers) with a measured volume of 4.5L each. Exhaust valves from both pressure cookers were removed and an access hose was installed between the chambers to enable water vapor exchange. In addition to that, there is an access hose connecting the second chamber and the condenser. The first chamber is dedicated to heat water, in a cycle of 500 mL each period, using a Bunsen burner. The second chamber contains plant matter. Vapor flowing through the hose installed in the security valve is directed to the Liebig condenser (450 mm), which is constantly cooled by current water. Saturated vapor produced in the first chamber flows to the second chamber, which contains plant matter and, doing so, carries the essential oil present in the plants. Vapor and essential oil are directed to the condenser, where they are liquefied and finally assembled in a collecting tube. Extracted essential oil is hydrophobic and presents lower density compared to water. Due to that, a two-phase system is created and the essential oil can be separated from water.

After extraction the essential oils were stored in glass vials at -20 °C until analysis. The efficiency (percentage yield) was calculated according to ZENEBON et al. (2008). The chemical characterization of essential oils was performed in the Chromatography Laboratory of the Department of Chemistry of Universidade Federal de Minas Gerais (UFMG) by GCMS-QP2010 ULTRA Chromatograph (Shimadzu) with mass detector Detector MS (Electronic Impact at 70eV) at 220 °C. The column used was Rxi-1MS with 30 m length, internal diameter of 0.25 mm and film with thickness of 0.25 µm (Restek). The conditions were: Initial temperature: 50 °C, Final temperature: 200 °C, and Ramp: 3 °C/min, Injector: 200 °C Detector: 220 °C, Carrier gas: Helium, Flow: 3.0 mL/min and the Injection volume 1.0 µL. The total run time was 50 minutes. In GC - FID, the conditions and equipment employed to analyze the essential oil were a gaseous chromatography HP 7820^a (Agilent) with a FID detector, under 220 °C. A HP5 column with 30 m

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of length, intern diameter of 0.32 mm and an Agilent film with 0.25 μ m thicknesses. Conditions involved initial and final temperatures of 50 °C and 200 °C respectively, ramp rate 3 °C/min, Split injector (1:50) 200 °C, carrier gas helium in a 3.0 mL/min flow, injection volume of 1.0 uL and the sample diluted in chloroform 1%. The mass spectrum and the linear retention index were compared to those reported in the literature NIST 11.

RESULTS AND DISCUSSION

Cultivation and preparation of plant material

The exsiccate of the botanical material was deposited in the Herbarium of the Biology Department of the Universidade Federal de Uberlândia, Uberlândia-MG, under registration HUFU 74.050. The climatic characteristics of the cultivation region, soil type, collection season, fertilization, irrigation, among others, may influence the chemical composition of essential oils (SEFIDKON et al., 2007). In table 1, the amount of precipitation, insolation and temperature from December 2016 to June 2017 can be visualized. In this period, there was a decrease in the amount of precipitation and the average temperature when compared to the two months of the first quarter of 2017 and the two months of the second quarter of the same year. The average of insolation remained stable in the months of the collections, not being observed any great oscillation.

Extraction Efficiency of essential oils

The efficiency of the *L. dentata* L essential oils, based on the mass of wet matter, extracted by hydro distillation of inflorescences was 0.44% and aerial part was 0.40%. Results of the average efficiencies obtained in this study corroborates with the results of SILVA (2015). The authors studied *L. dentata* species cultivated in Uberlândia-MG region and obtained averages of efficiency of

0.56% and 0,40% for essential oils from leaves and flowers, respectively (SILVA, 2015). However, the inflorescences obtained in this study were inferior to those reported by VERMA et al. (2010) in Kumaon, a sub-temperate region located in the western Himalayas. Where a content of 2.8% of essential oil of L. angustifolia was found and when using different extraction methodologies presented 0.80 to 1.3% efficiency of O.E in the inflorescences. The Kumaon region according to the climatological classification of Köppen is a region (Cwa), being this the same classification of the region of Uberaba, MG. Although these regions have the same climatic classification it was not possible to compare climatic data, since the research does not present the same. The O.E of the aerial parts obtained in this study are in agreement with those reported for plants of the L. genus, in which the leaves showed the lowest yield (PORTER, et al 1982). The efficiency (percentage yield) obtained can be justified by the methodology applied for this calculation, not taking into account the exact consideration of the amount of water present in the plant material at the time of extraction. According to SANGWAN et al. (2001), climatic factors such as, long period of sunshine favors flowering, but rainy and overcast periods during flowering, reduce the essential oil accumulation. This may have occurred in the present study, since the collections with higher efficiency were obtained in the periods of lower precipitation. According to NALEPA & CARVALHO, (2007) another efficiency impairment may be the genotype. However, as in the present study the seedlings were acquired from a nursery and from these were made vegetative propagations of the other plants that were used as object of study, the authors do not believe this occurred. The luminous intensity influences the concentration, as well as, the chemical composition of the essential oils. In the development of glandular trichomes, plant structures that biosynthesize and also store the essential oil, the presence of light is necessary (MORAIS, 2009). The greater biossynthesis

Table 1 - Climatic data of Uberaba-MG (December 2016 to June 2017).

Variables	Dec	Jan	Feb	Mar	Apr	Mai	Jun
Accumulated rainfall	248 mm	275 mm	140 mm	127 mm	82 mm	42 mm	25 mm
Average Temperature	25.90 °C	25.40 °C	27.16 °C	26.70 °C	25.05 °C	24.00 °C	22.1 °C
Minimum temperature	20 °C	20 °C	21 °C	21 °C	19 °C	17 °C	12 °C
Maximum Temperature	34 °C	33 °C	33 °C	33 °C	32 °C	30 °C	31 °C
Average insolation (Hours/Day)	4.48	4.23	7.58	7.13	7.07	7.39	8.60

Fonte: Instituto Nacional de Meteorologia, 2017.

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of secondary metabolites under high levels of insolation is explained by the fact that biosynthetic reactions are dependent on the supply of carbon skeletons, performed by photosynthetic processes and compounds that participate in the regulation of these reactions (TAIZ & ZEIGER, 2009).

Chemical characterization of essential oils

The GC-FID and GC-MS analyzes of OE1 and OE2 identified more than 23 compounds which have concentrations ranging from major to trace constituents, which can be seen in table 2. No significant differences were reported in the O.Es composition of the inflorescence (OE1) and aerial part (OE2) distillate material reinforcing the results of BOUSMAHA et al. (2005), which also did not observe large variations in composition of inflorescence oils and aerial part of *L. dentata* L. From table 3, which summarizes the major compounds of OE1, OE2 and the compounds present in OE3 and OE4, it is possible to observe that the aerial parts of *L. dentata* L. (OE1) presents higher concentrations of eucalyptol than the inflorescences (OE2), whereas the inflorescences presented higher concentrations of camphor than the aerial parts. Conversely, OE3 and OE4 present different major compounds, which are linalol and linaline acetate, thus OE3 presents the higher concentration of both compounds. The presence of eucalyptol and camphor may confer medicinal properties to the L. dentata L. essential oil, due to the antifungal and bactericidal action of these components, respectively. In addition, there are studies proving the antimalarial effect and the mitigation of hyperglycemia of fenchone, the third major constituent of OE1 and OE2 (CAMPBELL et al., 1997; SEBAI et al, 2013.). Linalol is the only compound present in all the essential oils study and this compound has a concentration 110 times greater in OE3 and OE4 than in the other oils. The presence of linalool in OE1 and OE2 (L. dentata L.) thus demonstrating that it is possible to use the whole plant to obtain essential oil, since the species of Lamiaceae family have glandular trichomes in every

Table 2 - Chemica	l composition of	essential oil 1	l and 2 of <i>l</i>	Lavandula dentata L.
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Peak	RT (min)	OE1 Area	OE2 Area	OE1 Conc (%)*	OE2 Conc (%)*	RI **	Probable Substance***
1	3.228	798154	746425	3.7	3.7	980	α-pinene
2	3.488	289624	242946	1.3	1.2	987	Camphene
3	4.008	153655	168236	0.7	0.8	1001	Sabinene
4	4.048	1149573	1242308	5.3	6.1	1002	β-pinene
5	4.440	129105	233452	0.6	1.1	1013	Mircene
6	5.225	105963	99752	0.5	0.5	1034	p-Cymene
7	5.320	684378	1067675	3.2	5.2	1037	Limonene
8	5.393	9957552	8235335	46.3	40.4	1039	Eucalyptol
9	7.043	3404876	2735814	15.8	13.4	1083	Fenchone
10	8.318	69502	64742	0.3	0.3	1117	Linalool
11	8.858	3229925	3468923	15.0	17.0	1132	Camphor
12	9.525	143015	133131	0.7	0.7	1150	Pinocarvone
13	10.428	90636	96904	0.4	0.5	1174	a-terpineol
14	10.753	187129	167106	0.9	0.8	1183	Mirtenol
15	12.432	63811	70558	0.3	0.3	1228	Citronelol
16	12.624	69147	67864	0.3	0.3	1234	Methyl citronelate
17	19.133	66519	138681	0.3	0.7	1409	β-Caryophyllene
18	20.008	73399	147057	0.3	0.7	1433	α-bisabolene
19	21.655	185081	198638	0.9	1.0	1477	β-selinene
20	22.845	129911	248834	0.6	1.2	1509	a-selinene
21	24.143	195943	479303	0.9	2.4	1544	germacrene
22	25.188	135610	182865	0.6	0.9	1572	β-Caryophyllene oxide
		188203	157977	0.9	0.8		Others

*Results obtained through the GC-FID;

**Retention index or Kovats index calculated through a series of linear hydrocarbons C12 to C18;

****Identificated by CG-MS. Spectral ibrary NIST11.

	L. dentata L. (OE1)	L. dentata L. (OE2)	L. officinalis (OE3)	L. hybrida (OE4)
Origem	Uberaba	Uberaba France		France
Main Compounds	Linalol 0,3%	Linalol 0,3%	Linalol 34%	Linalol 33%
	Camphor 15%	Camphor 17%	Cis-beta-ocimene 1,5%	Camphor 7%
	Limonene 3,2%	Limonene 5,2%	Linalyl acetate 38%	Linalyl acetate 28%
	Eucalyptol 46,3%	Eucalyptol 40,4%	Trans-beta-ocimene 2%	Eucalyptol 6%
	Fenchone 15,8%	Fenchone 13,4%	Lavandulyl acetate 1%	Borneol 3%
Extraction method	Steam distillation of aerial parts	Steam distillation of inflorescences	Steam distillation of flowers	Steam distillation of flowers

Table 3 - Concentration of the main chemical compounds of the L. dentata L., L. officinalis e L. hybrida essential oils.

plant (TURNER et al, 2000). The major constituents identified in the OE1 and OE2 were the oxygenated monoterpenes 1,8-cineol, fenchona, and camphor, in the following concentrations: OE1 (46.3%, 15.8%, 15.0%) and OE2 (40.0%, 13.4%, 17.0%), respectively. These results corroborated MASETTO (2011), in which the authors studied plants cultivated in the region of Curitiba-PR, a region according to the climatic classification of Köppen (Cfb), humid marine temperate climate, and obtained practically the same concentrations of camphor and fenchona. For the 1,8-cineol, the concentration in the present study is the double of the reported by MASETTO et al. (2011). SILVA (2015) obtained similar results to the present study, the same major compounds were reported in the flowers and leaves with similar concentration. These results reinforce the influence of climatic, localization and relief characteristics on the cultivation, yield and chemical composition of L. dentata L. The contents of the constituents observed in the present study differed from some previous reports for L. dentata L. essential oil, mainly in relation to the constituents such as canphor and fenchona. According to BOUSMAHA et al. (2005), these constituents were not identified in the essential oil of L. dentata L. cultivated in Algeria. There are studies showing the bactericidal activity β -pinene (CHU & KEMPER, 2005; LEITE et al., 2007) and limonene (VUUREN VAN & VILJOEN, 2007) and also the use of linalool as a non-steroidal anti-inflammatory agent (CHU & KEMPER, 2005). All these authors worked testing isolated compounds and in some cases combinations of more than one compound.

CONCLUSION

From this study is possible to conclude that there are variations of the concentrations and

the chemical components in the essential oils of the different species of Lavandulas, but no significant difference in the chemical composition between the essential oils from the different parts of the same plant (*L. dentata* L.). Results obtained in this study indicated that the essential oils of *L. dentata* L. cultivated in Uberaba-MG have similar chemical compounds to those obtained from this plant cultivated in Curitiba-PR. This is promising when considering the possibility of the cultivation and essential oil extraction of this plant in Minas Gerais.

ACKNOLDGEMENTS

The authors would like to thank Fundação de Amparo à Pesquisa do Estado de Minas Gerais (FAPEMIG), Conselho Nacional de Desenvolvimento Científico e Tecnológico (CNPq), Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES) and Laboratório de Cromatografia Departamento de Química da Universidade Federal de Minas Gerais (UFMG).

DECLARATION OF CONFLICT OF INTERESTS

The authors declare no conflict of interest. The founding sponsors had no role in the design of the study; in the collection, analyses, or interpretation of data; in the writing of the manuscript, and in the decision to publish the results.

AUTHORS' CONTRIBUTIONS

All authors contributed equally for the conception and writing of the manuscript. All authors critically revised the manuscript and approved of the final version.

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