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Essential oil constituents of *Lavandula officinalis* Chaix. from Northwest Iran

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Lavandula officinalis Chaix. is a multidisciplinary medicinal and aromatic plant with special importance in pharmaceutical and fragrance industries as well as in herb garden design. The essential oil content in the inflorescences and leaves of lavender cultivated in Northwest Iran was found to be 6.25% and 0.64% based on dry weight, respectively. The oil was analysed by GC / MS. Thirty seven and thirty four components were identified, comprising 97.0% and 96.5% of inflorescence and leaf total oil, respectively. Oxygenated monoterpenes (86.4% versus 84.2%) were the predominant class of components in both organs studied. Linalool (33.7%), 1,8-cineole (17.1%), borneol (14.7%) and camphor (7.8%) were the highlighted constituents of inflorescence volatile oil. At the same time, 1,8-cineole (31.9%), borneol (24.0%) and camphor (16.1%) showed the greatest content in leaf essential oil. Cis- and trans-linalool oxide (3.5% and 3.3%) and terpinene-4-ol (3.5%) were other components with notable amounts in the inflorescence oil. Meanwhile, cryptone (3.5%) was another appreciable compound in leaf essential oil. A comparative overview of the essential oil profile of *Lavandula officinalis* Chaix. plants from Northwest Iran revealed prominent quantitative and qualitative differences from previous reports from other parts of the world. In conclusion, the chemical and percentage composition of the analysed oils from Northwest Iran were characterized by the high content of linalool, 1,8-cineole and borneol, potentiating their use in related industries and lavender as an ornamental and aromatic herb.

Key words: *Lavandula officinalis* Chaix., GC / MS, inflorescences, leaves, linalool, 1,8-cineole, borneol

INTRODUCTION

Aromatic and medicinal plants play a pivotal role in health care systems, pharmaceutical, food, fragrance and perfume industries as well as in landscape and aromatic garden design [1].

The genus *Lavandula* is divided into eight sections and comprises a total number of species up to 39 distributed universally [2, 3]. Lavender (*Lavandula officinalis* Chaix; *L. angustifolia* Mill or *L. vera* DC; Fam. Lamiaceae) [4] is an important multidisciplinary aromatic evergreen shrub with upright woody branches; the bottom of branches is leafless, with many herbaceous twigs arising from up-sections of the main branches. The leaves are opposite, characteristic of mint family, long narrow (lanceolate in shape) and grayish-green with a hairy appearance. Each slender branch ends in an inflorescence in which the packed flowers are arranged as dense spikes [5].

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L. officinalis is a native of Southern Europe and the Mediterranean region and is commercially cultivated in France, Spain, Portugal, Hungary, the UK, Bulgaria, Australia, China and the USA [6]. In Iranian flora, lavender is mainly distributed in the northern parts of the country [5]. The pleasant aroma of this plant is mainly due to the occurrence of low molecular weight terpenoids synthesized and accumulated in aerial parts, especially in inflorescences [6, 7]. The distilled volatile oil of this plant has gained great importance in aromatherapy and in perfume, cosmetic and flavoring industries since antiquity [7, 8]. Furthermore, the volatile constituents of lavender are of special significance in pharmaceutical and food industries [8].

Pharmaceutically, this plant and its preparations have long been used for carminative, antispasmodic, antidepressant, expectorant, anti-rheumatic, relaxant, sedative, anti-inflammatory and tonic properties [3, 6, 7, 9–11]. Moreover, its preparations are prescribed against flatulent dyspepsia, colic and depressive headache [9]. It was also found to be active against some bacterial and fungal species [6]. Traditionally, lavender has been used as an antiseptic agent in swabbing of wounds (wound healing), for burns and insect bites, and in veterinary medicine to kill lice and other animal parasites [7, 10].

L. officinalis Chaix herba contains a wide diversity of secondary metabolites from which essential oils are the most appreciated biomolecules. Other compounds with documented bioactivities are coumarins, flavonoids and sterols [3, 11, 12].

From the agronomical point of view, lavender prefers arid and semi-arid climate for its best growth and productivity. During the growing season, lavender needs high light intensity, warm weather and relatively low moisture. Warm climate and ample light accelerate flowering and hence intensify volatile oil biosynthesis. The optimum pH range for this plant has been defined as 6.4 to 8.2 [3, 9, 11, 12].

The compositional analysis of *L. officinalis* Chaix. volatile oil has been the object of several studies. Evandri et al. reported that linalyl acetate (43.1%) and linalool (32.7%) were the major volatile oil components of *L. officinalis* plants from Italy [7]. In a previous study from the Isfahan province in middle parts of Iran, Afsharypour and Azarbayejany noted that the predominant constituents of *Lavandula officinalis* Chaix. inflorescense volatile oil were linalool (34.1%), 1,8-cineole (18.5%), borneol (14.5%) and camphor (10.2%) [9]. Linalyl acetate (47.6%), linalool (28.1%) and lavandulyl acetate (4.4%) have been characterized as the main inflorescence volatile oil components of lavender from India [6]. Furthermore, linalool (44.6%), geraniol (11.1%) and lavandulyl acetate (10.8%) were the major chemical constituents of *L. angustifolia* plants cultivated in Xinjiang, China [8]. Despite these reports on different wild and cultivated plants from diverse regions of the world, there is no documented research on the chemical composition of *L. officinalis* aerial part volatile oil from Northwest Iran. Therefore, owing to the multi-purpose usage of *L. officinalis* plants and as an ornamental plant for aromatic parks and garden design as well as the wide application of lavender essential oil in pharmaceutical and fragrance industries, the present study was conducted to characterize the volatile oil components of cultivated *L. officinalis* plants from Northwest Iran for the first time.

EXPERIMENTAL

Plant material. Aerial parts including leaves and inflorescences (spikes) of *L. officinalis* Chaix. were collected from different sites of the Maragheh municipality district in Northwest Iran. Leaves and inflorescence samples were separately mixed to obtain a homogeneous material representing a true sample of lavender population from the study region. Plants were at the full-bloom growth stage during harvesting representing the commercial harvest time of this plant. The Maragheh district is located in Northwest Iran at an altitude of 1476 m, where temperate semi-cool climate is common. The voucher specimen of the plant was submitted and archived in the Herbarium of the University of Maragheh. The harvested materials were air-dried in a shaded place at a convenient temperature and in an air-flow during 4–5 days. The air-dried organs were ground to a homogeneous fine-grade powder.

Volatile oil extraction. Air-dried powdered plant materials (50 g) were separately subjected to hydrodistillation by an all-glass Clevenger-type extraction apparatus for 3 hours. The oil fraction was dried and dehydrated over anhydrous sodium sulphate and stored in a refrigerator in sealed dark glass flasks prior to compositional analysis. Essential oil content as ml/100 g was evaluated based on the dry weight of plant material.

GC / MS analysis. The compositional analysis of the volatile oil was carried out by a GC (Agilent Technologies 6890N) interfaced with a mass selective detector (MSD, Agilent 5973B) equipped with an apolar Agilent HP-5ms (5%-phenyl methyl poly siloxane) capillary column (30 m × 0.25 mm i. d. and 0.25 μm film thickness). The carrier gas was helium with a constant flow rate of 1 ml/min. The oven temperature was set at 50 °C for 2 min, then programmed until 110 °C at the rate of 10 °C/min, then heated to 200 °C at the 20 °C/min rate and finally increased to 280 °C at the rate of 10 °C/min, isothermal at the temperature for 2 min. The injector and detector temperatures were 300 °C and 200 °C, respectively. Injection mode, split; split ratio 1 : 100, volume injected, 4 μl of the oil. The MS operating parameters were as follows: ionization potential 70 eV, interface temperature 200 °C, and acquisition mass range 50–800 m/z.

Identification and quantification of constituents. The relative percentage of the volatile oil components was evaluated from the total peak area (TIC) by apparatus software. Identification of components in the volatile oil was based on a comparison of their mass spectra and retention time with those of the authentic compounds and by computer matching with NIST and WILEY library as well as by comparison of the mass spectral data with those reported in the literature [13, 14].

RESULTS AND DISCUSSION

Water distillation of the inflorescences and leaves of *Lavandula officinalis* gave a pale yellow bright liquid with a yield of 6.25% and 0.64% (v/w) based on dry weight, respectively. Several authors [2, 6, 7, 8, 10] have reported that the majority of lavender essential oil is accumulated in the floral parts of a plant and that this organ is frequently harvested for oil extraction and further processing. Meanwhile, lavender is a perennial woody plant producing huge amounts of herbaceous shoots worthy of evaluation for volatile oil content and composition. Despite the low amounts of volatile oil in leaves versus inflorescence, it is surprising that volatile oil content in lavender leaves is comparable with many other volatile oil bearing plants and may be a good source of volatile constituents worth of attention in case of industrial use. The results obtained from the GC/MS analysis of volatile oils, i. e. the chemical components of oil, their elution order on an apolar column, retention indices, percentage as well as the main classes, subclasses and chemical groups of identified components are presented in Tables 1 and 2. In total, 37 and 34 components were quantified and characterized in the inflorescence and leaf essential oils of *L. officinalis* plants from Northwest Iran, accounting for 97.0% and 96.5% of total oils (Tables 1 and 2). Monoterpenoids (91.0% versus 89.7%) were characterized as the main class of components, followed by a minor share of sesquiterpens (1.2% versus 2.9%) in floral parts and leaves of lavender, respectively. Considering the proportional amounts of the main classes, there was no difference between the two organs. Monoterpenoids, oxygenated monoterpenes (86.4% versus 84.2%) contained the major subclass of compounds in floral tissues and leaves (Table 2). Monoterpene hydrocarbons (4.6% versus 5.6%) obtained proportional amounts much lower than that of their oxygenated counterparts. Higher amounts of oxygen-containing monoterpenes in both oils strongly support the dynamic pool of plastidal hydroxylases and dehydrogenases involved in the post-modification of the initial hydrocarbonic compounds [15]. Sesquiterpenoidal subclasses had a minor share in the component classification, and the role of oxygenated C_{15} compounds (0.8% versus 2.6%) was higher than that of hydrocarbonic sesquiterpenes (0.4% versus 0.3%). At a glance, it is worth noting that the lavender plant studied in the present investigation was potentiated in the biosynthesis and accumulation of plastidal volatile compounds (monoterpenes) rather than cytosolic sesquiterpene ones. Linalool (33.7%), 1,8-cineole (17.1%), borneol (14.7%) and camphor (7.8%) were the predominant components of inflorescence oil (Table 1). In contrast, 1,8-cineole (31.9%), borneol (24.0%) and camphor (16.1%) ranked as the major components of leaf volatile oil. Terpinene-4-ol (3.5%), cis-linalool oxide (3.5%) and translinalool oxide (3.3%) were the other constituents with a notable content in floral tissue oil (Table 1). Concomitantly, cryptone (3.5%) and cumin aldehyde (2.2%) attained appreciable quantities in leaf-extracted oil (Table 1).

Table 1. **Essential oil composition (%) of aerial parts of *Lavandula officinalis* Chaix. from Northwest Iran**

Compound	RI	%	
		Inflorescence	Leaves
Hexanol	0871	0.3	–
Tricyclene	0927	0.1	0.1
α-Thujene	0930	0.1	0.1
α-Pinene	0939	0.6	1.6
Camphene	0954	0.5	1.1
Sabinene	0975	0.3	0.2
β-Pinene	0979	1.2	1.4
Myrcene	0991	0.5	–
δ-2-Carene	1002	–	0.2
α-Terpinene	1017	0.2	–
p-Cymene	1025	0.4	0.1
δ-3-Carene	1031	0.1	–
1,8-Cineole	**1031**	**17.1**	**31.9**
β-Ocimene	1038	0.3	–
γ-Terpinene	1060	0.5	0.4
cis-Sabinene hydrate	1070	0.2	0.5
trans-Linalool oxide	**1073**	**3.3**	–
cis-Linalool oxide	**1087**	**3.5**	–
p-Cymenene	1091	–	0.5
Linalool	**1097**	**33.7**	**0.7**
α-Campholenal	1126	–	1.3
Camphor	**1146**	**7.8**	**16.1**
Pinocarvone	1165	–	0.9
Borneol	**1169**	**14.7**	**24**
Terpinene-4-ol	1177	**3.5**	1.3
Cryptone	1186	0.8	**3.5**
α-Terpineol	1189	1.5	1.1
Myrtenal	1196	0.4	1.3
trans-(+)-Carveol	1217	0.2	0.7
Cumin aldehyde	1242	0.3	**2.2**
Carvone	1243	0.2	0.9
Piperitone	1253	–	0.3
Linalyl acetate	1257	2.2	–
Lavandulyl acetate	1290	0.9	–
Cumin alcohol	1291	–	1.2
Hexyl tiglate	1333	0.1	0.1
α-Cubebene	1351	–	0.1
Neryl acetate	1362	0.1	0.1
Geranyl acetate	1381	0.2	–
trans-Caryophyllene	1419	0.1	–
Linalyl butyrate	1423	0.2	–
trans-(β)-Farnesene	1457	0.2	–
γ-Cadinene	1539	–	0.2
Ledol	1569	–	0.1
Caryophyllene oxide	1583	0.3	1.3
α-Cadinol	1654	–	1.1
α-Bisabolol	1686	0.5	–
Total identified		97.0	96.5

Note. Compounds are reported according to their elution order on apolar column.

Table 2. **Main classes, subclasses and chemical groups of volatile oil constituents of *Lavandula officinalis* Chaix. from Iran**

Class, subclass and chemical group of compounds		%	
		Inflorescence	Leaves
Monoterpenes		90.1	89.7
	Monoterpene hydrocarbons	4.6	5.6
	Oxygenated monoterpenes	86.4	84.2
Sesquiterpenes		1.2	2.9
	Sesquiterpene hydrocarbons	0.4	0.3
	Oxygenated sesquiterpenes	0.8	2.6
Others		4.8	3.7
Total identified chemical groups		97.0	96.5
	Alcohols	54.4	30.7
	Oxides	20.6	33.2
	Ketones	8.7	21.7
	Esters	3.4	0.1
	Aldehydes	0.7	4.8

Based on the major chemical components, it seems likely that there is a meaningful quantitative and qualitative difference between the two organs. Linalool as the major component (comprising one third of all identified components) of floral parts comprised negligible (0.7%) amounts in leaves. As previously understood [16], linalool content has been defined as one of the quality characteristics of lavender and other plants commonly used in flavour and fragrance industry. At the same time, 1,8-cineole, borneol and camphor content of leaf essential oil were about two times higher than that of inflorescence. Linalool oxide isomers (sum 6.8%), the other notable compounds of inflorescence oil, were completely missing in leaf essential oil. Moreover, linalyl acetate as the major constituent of lavender essential oil from some previous studies [6, 7, 10] was absent in leaf oil but had low amounts (0.9%) in floral organs. Cryptone – a characteristic C_9 compound – had considerable amounts (3.5%) in leaf oil compared to inflorescence (0.8%). From the chemical point of view, alcohols (54.4% versus 30.7%) were the principal components of both oils studied. Linalool, borneol and terpinen-4-ol had the major hydroxyl-containing constituents of inflorescence oil. Contrarily, borneol was the only principal alcoholic compound in leaf volatile oil. Oxides (20.7% versus 33.2%) comprised the second chemical group of components (Table 2). 1,8-Cineol was characterized as the most important oxidized compound in both oils. Camphor and cryptone were the chief ketonic compounds of leaf essential oil versus camphor as the only member of this group of compounds in inflorescence oil. Linalyl acetate and lavandulyl acetate (0.9%) were the principal members of this group in the essential oil of floral parts. In contrast, cumin aldehyde, myrtenal (1.3%) and α-compholenal (1.3%) had the highest quantity of aldehyde constituents in essential oil extracted from leaves. Overall, considering the oil content, its chemical components and groups, there was a significant difference between oils of two plant tissues. These differences might be due to a different occurrence of glandular trichomes in surface and unit areas of two organs, as well as they may be related to different potentials of these organs for the biosynthesis and accumulation of volatile constituents. Furthermore, the varying intrinsic biochemical and physiological potentials of different plant organs for the utilization of growth resources (light, water, nutrients, etc.) are another possible criterion for the abovementioned great discrepances in volatile oil profile. In total, taking into consideration the volatile oil profile (main classes, subclasses and major compounds) of *L. officinalis* plants cultivated in Northwest Iran and reports of other scientists from other parts of the world [2, 6–8, 10], it seems likely that here are huge quantitative and qualitative differences in the chemical profile of essential oils. Finally, the chemical profile of the volatile oil of lavender was drastically different from that of the previously reported plants and showed a high content of linalool, eucalyptol and borneol in inflorescence and 1,8-cineole, borneol and camphor in leaf essential oils. Nevertheless, some compositional similarity was recorded between our study and the previous report from Iran [9]. Furthermore, to our knowledge, the information on the leaf volatile oil content and composition of lavender is scarce; the present experiment reports and compares for the first time leaf volatile oil constituents of this plant from Northwest Iran. A comparative overview of the present and past reports reveals that there might be different chemotypes of *L. officinalis* plants from different localities of the world. It is likely that these chemical variations might be a consequence of climatic and geographical differences of *L. officinalis* habitats from different regions as well as of a different genetic potential of plants for the compartmentalization of biochemical routes. Additionally, it is possible that different volatile oil extraction procedures as well as the analytical and instrumental parameters had unwanted impacts on the chemical profile of the volatile oil. In summary, the chemical composition of the volatile oil of *L. officinalis* plants cultivated in Northwest Iran was characterized by the occurrence of appreciable amounts of linalool, 1,8-cineole, borneol and camphor. In conclusion, it is

important to note that *L. officinalis* studied in the present investigation could be a hopeful pool of the above-mentioned volatile constituents for supplying the high demands of fragrance, pharmaceutical, hygienic, cosmetic and food industries for those components. Furthermore, the favourite scent and sweet aroma emitted from lavender inflorescences and leaves makes this plant an optional choice for pavement borders and planting design programs in aromatic gardens and parks. For this reason, lavender takes an irreversible place in herb garden design and indoor landscaping owing to the biosynthesis, accumulation and mild emission of low molecular weight scent compounds.

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ŠIAURĖS VAKARŲ IRANO *LAVANDULA OFFICINALIS* CHAIX. ETERINIŲ ALIEJŲ SUDĖTIS

S a n t r a u k a

Lavandula officinalis Chaix. yra vaistingasis aromatinis augalas, svarbus farmacijos ir kvepalų pramonei. Šiaurės vakarų Irane auginamų levandų eteriniai aliejai sudaro atitinkamai 6,25 ir 0,64 % žiedynų ir lapų sausos masės. Eteriniai aliejai buvo analizuojami dujų chromatografijos–masių spektrometrijos būdu. Žiedynuose ir lapuose rasti 37 ir 34 eterinių aliejų komponentai, sudarantys atitinkamai 97,0 ir 96,5 % šių aliejų.