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Geographical and Seasonal Differentiation Along with Quality Evaluation of Lavender Essential Oil Through Volatile Profiling

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Abstract

The study aimed to characterize Romanian lavender essential oils (LEOs) according to geographical regions and harvested years by combining gas chromatography–mass spectrometry (GC/MS) with chemometric analysis and quality evaluation. Sixty-four LEO samples were collected from three Romanian areas (Moldova, Transylvania, Muntenia) during three consecutive years (2023–2025). GC–MS profiling identified 45 volatile compounds, with linalool, linalyl acetate, 1,8-cineole as predominant constituents. Oil quality was assessed using both a quality scoring algorithm based on characteristic volatile compounds and compliance with the ISO 3515:2002 standard. Most samples were classified as very good quality according to the proposed quality score, whereas only three samples fully complied with all ISO requirements. Pearson correlation analysis revealed significant positive associations among several biosynthetically related compounds, indicating identical variation within the volatile fingerprint. Linear discriminant analysis (LDA) successfully discriminated samples according to both geographical origin and harvest year, identifying characteristic combinations of volatile compounds responsible for sample classification. The results demonstrate that the overall volatile fingerprint, rather than individual compounds, provides a reliable basis for the authentication and differentiation of Romanian lavender essential oils. The combined GC–MS and chemometric approach represents an effective tool for quality evaluation, geographical traceability and authenticity assessment of lavender essential oils.

Keywords: lavender essential oil; geographical origin; GS-MS; quality evaluation; chemometrics

1. Introduction

Lavender essential oil, derived primarily from *Lavandula angustifolia* Mill. (true lavender or English lavender), represents one of the most commercially valuable aromatic products worldwide, with global market values exceeding hundreds of millions of dollars annually [1]. The oil finds extensive applications in aromatherapy, cosmetics, perfumery, pharmaceutical formulations, and food flavoring industries [2]. The therapeutic properties of lavender oil [3], including anxiolytic, sedative, antimicrobial, and anti-inflammatory activities [4], have been extensively documented in scientific literature [5–11]. Recently, natural additives such essential oils (EOs) and plant extracts, have increasingly replaced synthetic preservatives to extend food shelf life. Although the U.S. Food and Drug Administration (FDA) designates certain EOs as "Generally Recognized as Safe" (GRAS) [12]

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this classification is restricted to specific species, notably *Lavandula latifolia* Vill. and *Lavandula officinalis* Chaix [13]. These lavender essential oils (LEO) along with other essential oils, rich in antimicrobial, anticholinesterase and antioxidant compounds, like linalool, linalyl acetate, 1,8-cineole, terpinen-4-ol [14,15] show significant potential as a sustainable preservative in dairy production. Consequently, its integration as a flavoring agent in milk for cheese manufacturing could inhibit lipolysis and prevent oxidative spoilage, thereby preserving the quality of the final product [16].

Although the *Lavandula genus* is one of the most well-known EO crops in the world, with its 40 species, numerous hybrids and about 400 officially registered cultivars, only three of these species have high commercial value. The principal cultivated species for aromatic oils are fine lavender (*Lavandula angustifolia* L.), spike lavender (*Lavandula latifolia*) and lavandin (*Lavandula intermedia*), a sterile hybrid of *L. angustifolia* × *L. latifolia* [17].

The essential oils of the *Lavandula* species have the same chemical composition, but they are distinguished by their extraction yields and the specific proportions of those components. The quality of lavender essential oil is typically assessed based on its concentrations of camphor, linalool, and linalyl acetate. Lavender essential oil consists of over 100 individual components that define its distinct chemical and sensory profile. While many of these are identified, the oil also contains numerous minor constituents that often remain unidentified or unquantified. The main active constituents in *L. angustifolia* flowers' EO are monoterpenes (linalool, linalyl acetate, lavandulol, geraniol, bornyl acetate, borneol, terpineol, eucalyptol (also known as 1,8-cineole) and lavandulyl acetate) in different percentages, according to the geographic area of origin [5,14,17–19]. Gas chromatography–mass spectrometry (GC/MS) remains the method of choice when volatile compounds need to be analyses, due to its highly separation efficiency, sensitivity and ability to provide reliable quantitative and qualitative results. GC/MS enables comprehensive profiles of volatile compounds, making it the perfect candidate for authenticity and traceability purposes of essential oils [15,18–21]. Recent studies have further demonstrated that coupling GC/MS with chemometric methods, such as principal component analysis (PCA) and linear discriminant analysis (LDA), enhances the discrimination of lavender oils according to geographical origin, cultivar, and harvest year by exploiting the entire volatile fingerprint rather than individual marker compounds [22].

Lavender is cultivated worldwide in a number of countries, and the leading lavender oil producers are Bulgaria, France, the UK, China, India, Italy, Spain, and others [14,23,24]. In Romania, it is cultivated since 1950, and in present times, due to the high demands of the market, large areas are occupied by lavender crops Romania has developed substantial lavender production, particularly in Transylvania, where cultivation benefits from suitable altitude and climate conditions. Romanian oils have been characterized as exhibiting distinct chemotypes, with some cultivars showing linalool dominance while others favor linalyl acetate [25].

Geographical origin constitutes a fundamental quality parameter for lavender essential oil, influencing both chemical composition and market value. Environmental factors including climate, soil composition, altitude, and solar radiation interact with genetic background to modulate secondary metabolite biosynthesis, resulting in region-specific chemical profile. In addition, the global lavender essential oil (LEO) market, valued at USD 138.2 million in 2024, is projected to reach USD 267.2 million by 2034, representing a compound annual growth rate (CAGR) of 6.3–6.8%. This expansion is fueled by an increasing consumer preference for organic, non-toxic products, positioning Generally Recognized as Safe (GRAS)-certified oils as viable natural substitutes for synthetic food additives. However, widespread use has led to frequent adulteration with Lavandin intermedia [26–28]. Consequently, the determination of authenticity and provenance is one

of the main issues in high-value natural products such as lavender (*L. angustifolia*) essential oil [29–32].

The authentication of geographical origin for essential oils requires sophisticated analytical methodologies capable of detecting subtle compositional differences and multivariate statistical approaches to extract meaningful patterns from complex chemical datasets. Gas chromatography coupled with mass spectrometry (GC-MS) has become the gold standard for essential oil analysis, providing both qualitative identification through mass spectral matching and quantitative determination of individual compounds. The high resolution and sensitivity of modern GC-MS systems enable detection of minor compounds present at trace levels, which often prove valuable for geographical differentiation [11,31,33].

The present study aimed to investigate the geographical differentiation of lavender essential oils through comprehensive organic compound profiling, employing advanced analytical techniques coupled with multivariate statistical methods to establish region-specific chemical fingerprints. Specifically, the following steps were performed: (i) GC-MS analysis of EOs chemical composition from different geographic regions; (ii); development of robust chemometric models for geographical origin and for inter-annual classification (iii) identify region-specific chemical markers and compound patterns that enable geographical and year-to-year differentiation.

2. Materials and Methods

2.1. Essential Oil Samples Collection

A total of 64 lavender essential oil samples were collected from local producers from various regions of Romania: from Moldova n = 14, Transylvania n = 22, and Muntenia n = 28, respectively. According to year of plant growing and oil production, the sample distribution was as follows: 2023 (n = 28), 2024 (n = 20) and 2025 (n = 16). The collected volume was 10 mL, the oil samples were stored in dark glass bottles supplied by each producer. According to their labels, all the oil samples used in this study were obtained from the flowers of *Lavandula angustifolia* through steam distillation. The distillation was made as soon as possible after plants were harvested. Collection took place during July and August of each production year, depending on harvest period of each region. No synthetic additives or other ingredients were reported by producers. The sample preparation supposes the successive dilution of oil with hexane (0.01%, v/v) and stored at 4 °C prior to GC/MS analysis.

2.2. Gas Chromatography–Mass Spectrometry Analysis

The GC/MS procedure was described in our previously study published by Marincas et al. [32]. Briefly, analyses were performed using a Trace GC 1610 gas chromatograph coupled with ISQ 7610 single quadrupole mass spectrometer (Thermo Scientific, Bremen, Germany). The separation of volatile organic compounds was performed with non-polar DB-5MS (30 m × 0.25 mm, 0.25 µm film thickness) capillary column (5% diphenyl, 95% dimethylpolysiloxane stationary phase). The injection volume of each oil sample was 2 µL. Oven temperature programmed from 40 °C (held 3 min) to 300 °C at 10 °C/min, and kept at 300 °C for 10 min. The injector and transfer line were 250 °C, and 300 °C, respectively. The helium carrier gas was set to the constant flow mode at 1.5 mL/min. Data were acquired using Thermo Scientific Chromeleon software (7.2). Compounds tentative identification involved a comparison of the mass spectra with the databases (NIST 2011) using a probability-based matching algorithm and also based on linear retention indices which were calculated in the previously study [32]. The volatile compounds were quantified using normalized peak area method, the relative percentage of each compound was calculated

from peak area as a percentage of the total area of all identified compounds. Therefore, the reported values represent relative percentages rather than absolute concentrations.

2.3. Statistical Analysis

The quality evaluation of analyzed LEOs was made base on an algorithm developed in our previously published study regarding the quality of lavender oil [32]. In this work, for the first time, an algorithm according to ISO 11024-1 (2013) and ISO 11024-2 (2013) was proposed [34,35]. Within this algorithm two main indices were proposed, I_1 and I_2. First, we took into consideration the percent of the most abundant monoterpene, linalool and linalyl acetate related to a mean percentage, calculated from the minimum and maximum values presented in the standard (range for linalool was 25–38%, while for linalyl acetate it was 25–45%). Moreover, the second indices, for a comprehensive evaluation of essential oil quality, the sum of all peak areas of volatile compounds was incorporated, and it represents a key indicator, as it reflects the overall concentration and distribution of volatile compounds, which are directly associated with the oil's aromatic profile. By integrating the aforementioned indices into an arithmetic mean, a comprehensive evaluation was conducted, thus allowing a more accurate and holistic interpretation of the overall quality of the LEO samples, and corresponding grade was assessed.

All chemometric models were developed using SPSS v.24 (IBM, New York, NY, USA) software. A working data matrix was constructed having each lavender oil sample (64 samples) as rows and volatile compound concentrations (45 compounds) as columns. Other volatile compounds, which had zero values for more than 60% cases, were removed prior any other pretreatment. For the remaining compounds, the relative abundances were used as the starting point for data pretreatment, Z-score normalization being applied, and these values were used for further chemometric models' development. Pearson correlation analysis was performed to evaluate the linear relationships between volatile organic compounds detected and quantified in all lavender oil samples. Generally, Pearson correlation coefficients (r) have values between -1 and +1, where values close to +1 indicate a strong positive correlation (the variables have similar trend), values close to -1 indicate a strong negative linear association (variables have opposite trend), and values near 0 suggest the absence of a linear relationship. The identification of highly correlated compounds might become very helpful, due to the fact that may reflect similar geographic influences or similar chemotypes. Moreover, by highlighting strong correlations is important prior to multivariate statistical approach, as highly collinear variables may increase model instability and contribute to overfitting phenomena. Therefore, Pearson correlation might be employed both as a preliminary test and also as a preprocessing tool for feature reduction, thus contributing to models optimization.

For development of chemometric models, linear discriminant analysis (LDA) was chosen, which is a widely employed supervised chemometric method used for different classification purposes. The model consists of a linear combination of original variables into discriminant functions (DFs). The performance of the LDA model is evaluated through the "leave-one-out cross-validation" method (LOOCV). In this step, the number of iterations is equal with the number of samples, and each sample is removed from the dataset, and the model is trained on the remaining data and then tested with the removed sample. The overall classification accuracy is expressed as percent of correctly classified samples.

3. Results and Discussion

3.1. Volatile Composition of the Lavender Essential Oils (LEO)

In total, 45 volatile compounds were identified in the 64 lavender essential oil samples analyzed from three different areas from Romania in three consecutive years. The

chemical composition of all LEOs, including ISO-specified compounds and additional major terpenoids, is detailed in Table 1. The values reported in Table 1 correspond to the non-transformed relative percentages. The major compound classes included oxygenated monoterpenes (75.74–85.09%), monoterpene hydrocarbons (7.52–13.73%), sesquiterpene hydrocarbons (5.19–9.74%), oxygenated aliphatic (0.01–0.63%), and oxygenated sesquiterpenes (0.00–0.61%). LEOs are characterized by high amount of linalool and linalyl acetate, together accounting over 80% of the total oil composition. Even though all the LEOs were similar in terms of linalool and linalyl acetate in Transylvania and Muntenia, differences were remarked regarding Moldova area, which is distinguished by higher amounts of linalool (32.71–43.92%) compared to linalyl acetate (23.12–35.57%). Eucalyptol (1,8-cineol) was the second most abundant oxygenated monoterpene for the Transylvania area (3.46–4.06%), while for the Moldova, the percentages varied between and 0.39% and 2.19% with a mean of 1.30%. The third major compound identified was lavandulyl acetate for LEOs from Transylvania (3.63%) and Muntenia (3.87%), while for Moldova was terpinen-4-ol (3.42%). Other significant compounds include camphor, where the highest range being detected in Transylvania (1.69–2.61%) and Muntenia (0.92–3.47%) and endo-borneol with higher values in LEOs samples from Transylvania (1.26–3.08%). Among the monoterpene hydrocarbons, the main components were cis-β-ocimene and trans-β-ocimene, where the highest values being found in Moldova (2.62–7.08% and 2.50–3.26% respectively), and allo-ocimene with higher values detected in Transylvania (0.66–4.58%). Regarding the sesquiterpene hydrocarbons contained, differences were also observed between the tested oils. The highest abundances were detected in LEOs from Moldova (7.63%) and the lowest in those from Transylvania (7.03%). From this class of terpenes, caryophyllene was the majority representative for all EOs. Also, santalene (0.99–1.37%) was detected in almost the same percentages as cis-β-farnesene (0.73–1.37%). Oxygenated sesquiterpenes (0.13–0.29%) were in the lower percentages in all of the analyzed LEOs. In order to sustain the previously remarks regarding the differences occurred among LEOs from different harvest years and different geographical areas, one-way ANOVA was applied for each criterion. Thus, for the geographical area (Moldova, Transylvania, Muntenia) only two compounds were statistically different, 1-hexen-3-ol ($p = 0.036$) and linalool oxide ($p = 0.040$). Regarding the harvest year almost all compounds presented statistically significant differences, except α-pinene, limonene, geranyl acetate, neryl acetate, camphor, trans-β-ocimene, cis-β-ocimene, eucalyptol and linalool.

The results obtained in this study are also in agreement with other studies performed for essential oils, in the same species (isolated from different subspecies and cultivars of *L. angustifolia*) but in specific pedo-climatic conditions [36]. Previously studied [37] found that LEO from southern Romania had a concentration of 47.55% linalool and 3.75% linalool acetate. In contrast, other studies [3] showed that lavender essential oils from western Romania are mainly composed of linalool (29.41–35.77%) and linalyl acetate, which occurs in comparable amounts, followed by eucalyptol (1,8-cineol) (8.50%), lavandulyl acetate (5.38%), trans-β-ocimene (6.90%), and camphor (7.7%). According to work reported by Marchidan et al. (2023) [7], LEOs from Muntenia contain linalool (39.10%), linalyl acetate (6.40%) and eucalyptol (1,8-cineol) (14.59%) as its major constituents, while those from Moldova contain 27.78% linalool, 22.66% linalyl acetate and 0.28% eucalyptol (1,8-cineol). Bogdan et al. (2021) [38] demonstrated that LEO from Moldova, northeastern part of Romania and harvested in three consecutive years (2017–2019) is characterized by the predominance of linalyl acetate (26.60–40.66%), with linalool being the second most abundant compound (3.5–27.39%), followed by terpinen-4-ol (3.06–7.70%), trans-β-ocimene (1.52–6.99%), cis-β-ocimene (0.43–2.70%), and caryophylene (3.55–5.39%), respectively. Oroian et al. (2019) [25] state that the volatile oil obtained from the Transylvania region,

contains linalool (18.46–39.5), linalyl acetate (25.64–29.86%), ocimene (1.63–14.39%) and eucalyptol (1,8-cineol) (0.16–0.74%). These changes in the essential oil composition may be attributed to a combination of environmental (climatic, seasonal, geographical) and genetic differences [39]. Moreover, in addition to the aforementioned factors, the differences in percentages of some volatile compounds may also arise from variations in extraction procedures, cultivar characteristics and post-harvest processing stages.

Table 1. Chemical composition of the LEOs detected through GC-MS obtained from 3 different regions during three consecutive years: 2023, 2024, 2025.

No.	Compounds	Relative Percentages (%)								
		Moldova			Transylvania			Muntenia		
		2023	2024	2025	2023	2024	2025	2023	2024	2025
1	α-thujene	0.13	0.07	0.05	0.14	0.06	0.04	0.10	0.02	0.05
2	α-pinene	0.90	0.20	0.11	1.11	0.35	0.65	0.57	0.08	0.27
3	Camphene	0.29	0.06	0.11	0.53	0.16	0.24	0.32	0.03	0.17
4	Sabinene	0.04	nd	nd	0.13	0.03	nd	0.03	nd	nd
5	β-pinene	0.18	nd	0.24	0.38	0.28	0.12	0.15	0.03	0.15
6	β-Myrcene	0.46	1.61	0.18	1.11	0.94	1.68	0.93	0.82	1.35
7	3-Carene	0.12	nd	0.21	0.36	0.11	0.06	0.19	nd	0.06
8	o-Cymene	0.12	0.12	nd	0.13	0.05	0.11	0.12	nd	0.05
9	p-cymene	0.26	nd	0.10	0.35	nd	0.05	0.34	nd	0.10
10	Limonene	0.25	0.31	0.73	0.46	0.30	0.63	0.24	0.31	0.88
11	cis-β-ocimene	2.62	3.74	7.08	2.15	2.52	2.23	4.14	1.81	3.11
12	trans-β-ocimene	2.50	3.26	2.78	1.80	2.08	1.54	2.92	1.49	2.30
13	γ-Terpinene	0.44	0.04	0.08	0.31	0.14	0.11	0.22	0.09	0.07
14	α-Terpinolene	0.29	0.11	0.08	0.24	0.16	0.05	0.23	nd	0.12
15	α-phellandrene	0.19	nd	nd	0.21	0.01	0.02	0.19	nd	0.01
16	Allo-ocimene	3.38	0.54	1.28	2.16	4.58	0.66	2.93	2.85	0.57
	Monoterpene hydrocarbons	12.17	10.06	13.00	11.56	11.76	8.19	13.63	7.52	9.28
17	1-Hexen-3-ol	nd	0.02	nd	nd	0.01	0.01	nd	0.17	0.07
18	3-Octanone	0.01	nd	nd	0.06	nd	nd	0.06	nd	nd
19	Octenyl-acetate	nd	0.08	0.33	0.07	0.61	0.19	0.02	0.24	0.23
	Oxygenated aliphatics	0.01	0.10	0.33	0.12	0.63	0.20	0.08	0.41	0.31
20	1,8-cineole	2.19	0.39	1.33	4.06	3.96	3.46	1.92	0.84	3.41
21	Linalool oxide	0.21	0.10	0.03	0.31	0.06	0.55	0.13	0.01	0.07
22	Linalool	32.71	43.92	36.44	28.29	30.10	30.68	27.02	36.68	33.71
23	Camphor	1.49	0.09	0.18	1.69	2.51	2.21	0.92	3.47	1.99
24	Lavandulol	nd	0.17	nd	0.04	0.83	0.19	nd	1.22	0.22
25	Endo-borneol	2.83	0.26	1.31	3.08	1.26	1.83	1.86	1.07	1.78
26	Terpinen-4-ol	0.94	4.08	5.23	1.37	5.19	2.85	1.52	3.97	3.80
27	α-Terpineol	0.14	0.42	2.50	0.64	1.97	1.63	0.33	1.33	1.27
28	Linalyl acetate	35.57	30.62	23.12	34.98	27.82	32.77	39.53	29.76	28.72
29	α-Terpinyl acetate	2.02	0.12	nd	1.87	0.38	nd	1.57	nd	nd
30	Lavandulyl acetate	nd	2.97	3.91	1.22	5.97	4.43	0.71	6.13	4.04
31	Neryl acetate	0.16	0.09	0.61	0.22	0.45	0.46	0.19	0.23	0.33
32	Geranyl acetate	0.24	0.03	1.11	0.33	0.74	0.64	0.30	0.38	0.54
	Oxygenated monoterpenes	78.52	83.26	75.74	78.09	81.24	81.70	76.00	85.09	79.89
33	α-Cedrene	4.12	nd	nd	nd	nd	nd	1.71	nd	nd
34	Santalene	1.89	0.73	0.50	2.29	0.23	0.45	3.62	0.13	0.34
35	Caryophyllene	0.21	2.49	6.27	1.30	3.09	3.42	0.88	2.09	4.16
36	trans-α-Bergamotene	0.19	0.06	0.19	0.13	0.05	0.11	0.15	0.04	0.13
37	cis-β-Farnesene	nd	1.36	1.93	0.30	0.47	1.43	0.30	0.58	3.22
38	trans-β-Farnesene	0.58	0.90	nd	1.05	2.16	0.23	1.12	2.17	0.16
39	β-Copaene	nd	0.13	nd	nd	0.10	nd	0.01	0.16	0.05
40	Germacrene D	0.30	0.04	0.51	0.57	0.12	0.37	0.45	nd	0.50
41	γ-Cadinene	0.16	nd	0.00	0.18	0.01	nd	0.12	nd	nd
42	γ-Muurolene	nd	nd	0.35	0.13	0.01	0.26	0.05	0.01	0.19
	Sesquiterpene hydrocarbons	7.45	5.70	9.74	8.60	6.24	6.26	8.40	5.19	8.74
43	Caryophyllene oxide	0.61	0.11	0.16	0.19	0.03	0.65	0.11	nd	0.30
	Oxygenated sesquiterpenes	0.61	0.11	0.16	0.19	0.03	0.65	0.11	nd	0.30
	Total identified	**98.76**	**99.23**	**98.96**	**98.56**	**99.90**	**97.00**	**98.22**	**98.21**	**98.51**

nd—not detected.

Also, the obtained results in this study are comparable with those found in other papers which investigated LEOs obtained from indigenous plants harvested from other EU countries (Figure 1). This comparation was based on relevant published studies, but without claiming to be an exhaustive one [17,33,40–45]. Based on these mentioned studies it was observed that the mean percentages of the principal components found in LEOs presented considerably variation among countries. For examples (Figure 1), linalool was the dominant compound in almost all samples, with the highest mean values in Spain (50.4%) and Hungary (38.6%), while the lowest values were presented for Bulgaria (24.2%) and France (28.9%) [46]. Linalyl acetate presented a distinct pattern, presented the maximum values being recorded in oil samples from France (39.2%) and Spain (35.6%), whereas the lowest values were detected in oil samples from Italy (13.1%). These two monoterpene compounds presented also very closed values in LEO samples from Romania and this tendency is confirmed by other studies [38], which reported the same conclusion regarding these two compounds. The same tendency was observed for samples from Ukraine and Bulgaria. It is interesting to note that lavender oil samples from Romania, analyzed in our previously study [32], presented very different percentages of linalool (20.8% vs. 31.7% in the preset study), while the values for linalyl acetate (32.8% and 32.6%) and terpinene-4-ol (3.4% and 2.9%) were comparable. The reason for these differences in percentages of linalool could be justified by higher temperatures and increased solar radiation, which may favor the accumulation of linalool.

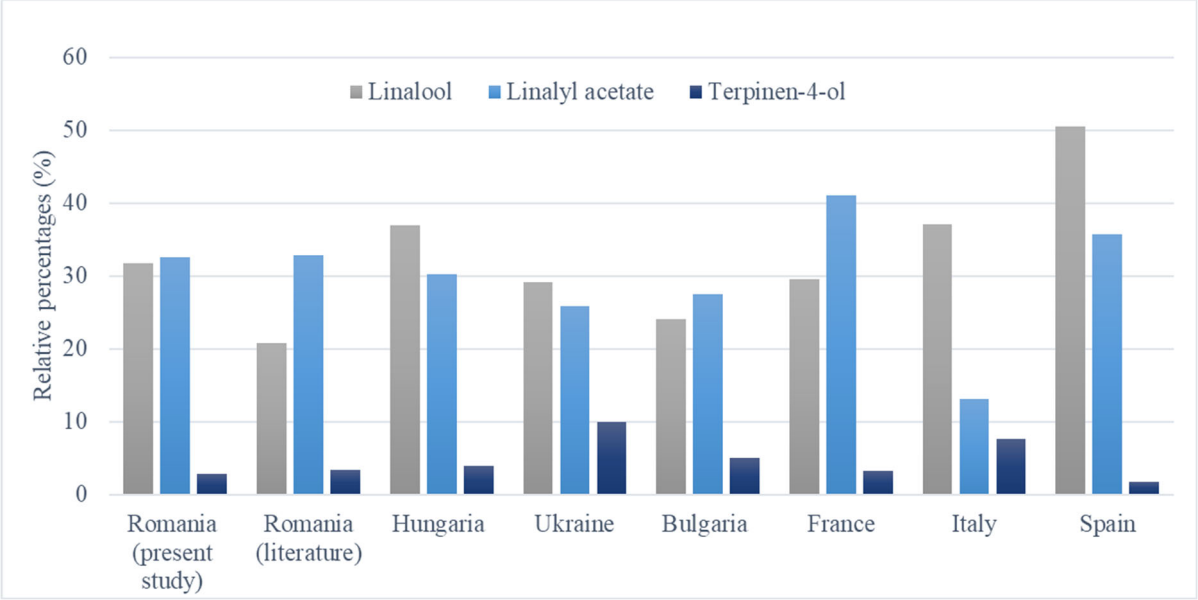

Figure 1. Variation in major compounds from LEOs in different European countries (the references which were used for these comparisons are the following: [17,32,40–44]).

The chemical profile of lavender essential oils is influenced by a variety of environmental, biological and technical factors. Variations in LEOs composition are largely attributed to cultivation practices and geographic regions, which have a significant impact on how the chemical compounds accumulate [47]. Specific external factors, such as light exposure and soil characteristics (including pH and nutrients) can increase terpene concentrations [36]. Meteorological conditions and plant development also play critical roles. Other studies [48] found that while higher temperatures and advanced flowering stage have a positive influence on the EO composition, rainfall during the flowering and harvest periods negatively impacts both overall oil content and linalool production. Beyond natural factors, the addition of synthetic compounds can affect the chemical composition and its concentrations [49].

Finally, the different isolation methods used to extract the essential oil can further lead to differences in composition [50].

With regard to the ISO regulation, Standard 3515:2002 (Other origins) [51] clarifies acceptable ranges for the major components of *L. angustifolia* essential oil: 1,8-cineole (eucalyptol), 0–3%; limonene, 0–1%; trans-β-ocimene, 0.5–6%; cis-β-ocimene, 1–10%; 3-octanone, 0–3%; camphor, 0–1.5%; linalool, 20–43%; linalyl acetate, 25–47%; terpinen-4-ol, 0–8%; lavandulol, 0.3–3%; lavandulyl acetate, 1–8%; α-terpineol, 0–2%. In our results, only three samples fully complied with requirements specified by the standard, whereas nine samples deviated from the recommended ranges for a single compound, and 22 samples missed two compounds. However, 11 out of 64 samples did not meet the requirements of ISO linalyl acetate content as this content was only 10.02–24.69%. Ten out of 64 samples contain more than 2% α-terpineol. Twelve samples are also characterized by a 1,8-cineole (eucalyptol) content that is too high (3.59–13.20%). Most of the samples (55 out of 64) conformed to the requirements of the ISO standard for the camphor content. All the samples contained the recommended amounts of linalool, trans-β-ocimene, cis-β-ocimene, terpinen-4-ol, lavandulyl acetate, lavandulol, limonene and 3-octanone [52]. Our results corroborate previous research suggest that many authentic lavender oils do no align with official specifications due to natural chemical variations. Despite their authenticity, studies show that various *L. angustifolia* oils from different cultivars and geographical origins do not meet these standards [42,53].

3.2. Quality Evaluation of Analyzed LEO

The LEOs distribution according to quality grade is presented in Figure 2. In order to provide a systematic interpretation of the results, the quality interval was split as follows: excellent quality (values exceeding 7.5), very good quality (ranging between 5.0 and 7.5) and good quality (values below 5.0). This classification framework enables a clearer differentiation between high-quality samples that meet superior standards, those that remain within acceptable limits of quality, and those that fall below the minimum threshold. Consequently, it supports a more consistent evaluation of sample variability and enhances the comparability of findings across the analyzed dataset. At the first visual inspection of the sample distribution, only two samples were classified as excellent quality, one originating from Transylvania and the other from Muntenia, both produced in 2025. The majority of the analyzed samples were categorized as very good quality, while a smaller proportion were placed into the good-quality group. Most samples from Muntenia were assigned to the very-good-quality category, whereas the good-quality group was predominantly composed by samples from Transylvania. With respect to the year of production, 2025 exhibited the most favorable profile, with all samples—except the two classified as excellent quality—falling within the very-good-quality category. The same tendency was followed by samples produced in 2023, where only seven samples were classified as good quality, while the rest were assigned to the very-good-quality group. As for the samples produced in 2024, most of them were also evaluated as very good quality, although seven samples were included in the good-quality group. In conclusion, the present quality assessment of lavender essential oil indicates that samples originating from the Muntenia region and produced in 2025 exhibit a comparatively higher abundance of organic compounds. This result may reflect favorable environmental conditions for lavender plants and suitable cultivation practices.

In order to statistically evaluate the quality grades of LEOs, a two-way ANOVA was performed considering the production year and geographical area as fixed factors. The returned results highlighted a significant effect for year of production ($F(2,55) = 8.263$, $p = 0.001$), indicating that quality varies among harvest years, but no significant effects

were observed for the geographical area (F (2,55) = 0.782, p = 0.462. The interaction between these two factors (harvest year and geographical areas) was not statistically significant (F (4,55) = 2.368, p = 0.064), suggesting that the influence upon quality of LEOs is mainly due to harvest year. The results are summarized in Table 2.

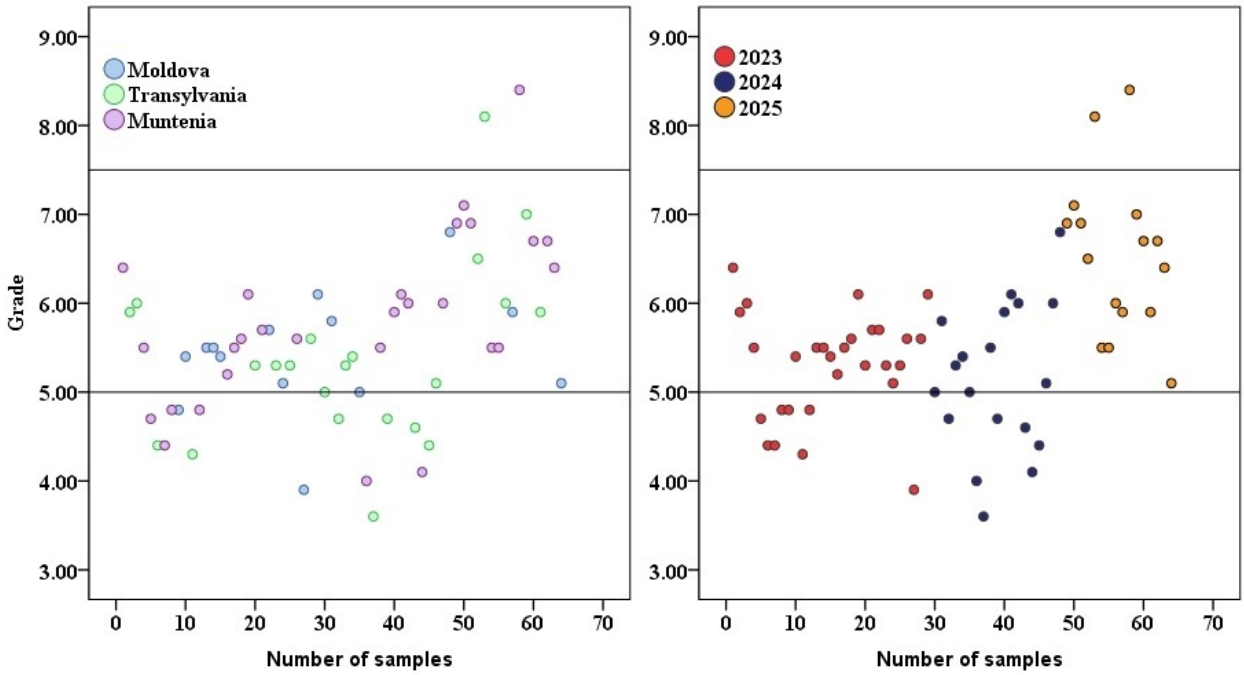

Figure 2. Distribution of lavender oil according geographical origin and year of production, based on calculated grade.

Table 2. Quality grades of LEOs expressed as mean and standard deviation, grouped according to geographical origin and harvest year.

Harvest Year	Geographical Areas	Mean Quality Grade	Standard Deviation
2023	Moldova	5.27	0.62
	Transylvania	5.26	0.63
	Muntenia	5.36	0.60
	Total	5.30	0.60
2024	Moldova	5.87	0.90
	Transylvania	4.76	0.55
	Muntenia	5.37	0.92
	Total	5.16	0.83
2025	Moldova	5.50	0.57
	Transylvania	6.70	0.90
	Muntenia	6.68	0.87
	Total	6.54	0.90
Total	Moldova	5.43	0.67
	Transylvania	5.38	0.99
	Muntenia	5.79	0.98
	Total	5.57	0.93

3.3. Development of Chemometric Models for Seasonal Variability and Geographical Classification

3.3.1. Pearson Correlation

The correlation with r values higher that 0.7 are considered strong, while moderate correlations have values between 0.5 and 0.7. All significant correlations ($p < 0.001$, 2-tailed) obtained in the present study had positive values. Thus, the following strong correlation were observed: camphene, sabinene with α-pinene (r = 0.827 and r = 0.709), α-phellandrene with camphene (r = 0.702), eucalyptol (1,8-cineol) with β-pinene (r = 0.829), camphor with eucalyptol (1,8-cineol) (r = 0.740), lavandulyl acetate with terpinene-4-ol (r = 0.737), α-terpineol with neryl acetate and geranyl acetate (r = 0.796 and r = 0.839), cis-β-farnesene with caryophyllene (r = 0.715). Most of the identified correlations were observed among monoterpenes compounds, fact might be due to their similar biosynthesis pathways. These low molecular weight molecules are derived from condensation of the universal terpene precursors isopentenyl diphosphate (IPP, C5) and dimethylallyl diphosphate (DMAPP, C5). The products of this condensation reactions are geranyl diphosphate (GPP) and farnesyl diphosphate (FPP), which represent important intermediates for further biosynthesis of terpenes. These precursors are transformed through enzymatic reaction into a wide range of monoterpenes, which are synthetized from GPP, and sesquiterpenes, which arise from FPP. Their chemical abundance in LEO reflects this biosynthetic activity, which is influenced by environmental and geographical factors [54].

3.3.2. Linear Discriminant Analysis (LDA)

The identification of several significant positive correlations among volatile compounds may indicate a degree of multicollinearity within dataset, such correlation being somehow expected since monoterpenes follow similar biosynthesis pathways. Although this aspect may have an influence upon discriminant coefficients, it does not necessary reduce the classification performance of LDA. Thus, the classification accuracies obtained in the present study demonstrated that the observed multicollinearity did not alter the robustness of LDA.

For the case of LDA a new dependent variable was made and the sample set was split according to collection years (code 1 for 2023, code 2 for 2024 and code 3 for 2025). After running stepwise LDA, the obtained model provided a very good classification, 85.9% for both initial classification and cross-validation step. It is interesting to observed that the same individual samples were misclassified in both initial and cross-validation procedure, namely, four samples from 2023 were placed in 2025 group, two samples from 2024 were reattributed to 2025 and three samples from 2025 were replaced to 2024 group. Two discriminant functions were obtained for this classification: DF1 with eigenvalues of 2.811 and 79.4% from total variance and DF2 with 0.727 eigenvalues and 20.6% variance. The organic compounds with the highest discriminant coefficients, that were included in the model are: α-phellandrene, α-terpinyl acetate, trans-β-farnesene, 3-octanone, γ-muurolene, cis-β-ocimene and terpinene-4-ol. The lavender oil samples distribution is presented in Figure 3, below.

In addition to overall classification accuracy, from the confusion matrix, sensitivity per each class was also calculated, and had the following values: 85.7% for 2023, 90.0% for 2024 and 81.3% for 2025, respectively, which indicated excellent performances for all harvested years.

Regarding the β-ocimene key discriminant compound, this was also a year of production marker, in another published study [22], where orthogonal partial least squares–discriminant analysis (PLS-DA) was applied for revealing the differences from year to year, in terms of volatile content. Differences observed in LEO yield have clear correspondence with the variation in rainfall between years. Some of the identified markers from this

study were reported also by other authors, for example, 1,8-cineole (eucalyptol) percentage showed remarkable increases in dryer years. In contrast, rainfall and temperature drops lead to a higher content of terpinen-4-ol [55].

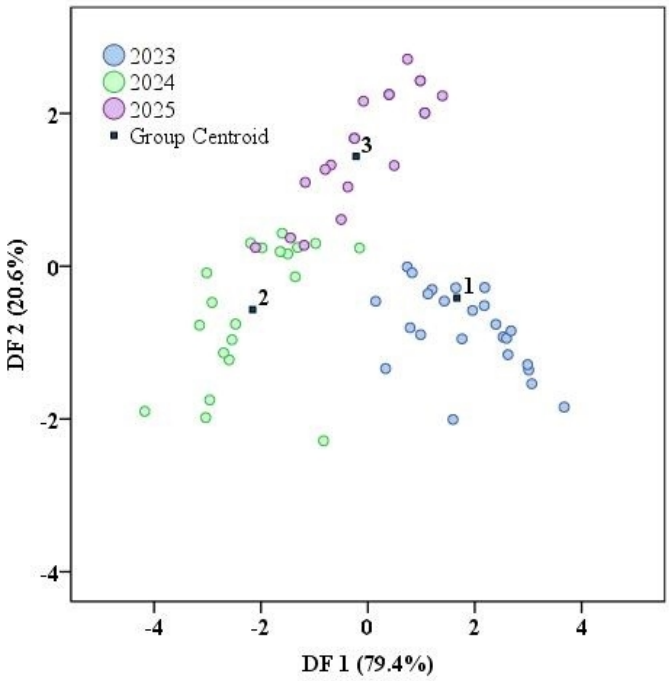

Figure 3. Lavender oil distribution obtained with stepwise LDA according to year of cultivar and oil production. The numbers from the figure correspond to harvest year, as follows: 1—2023, 2—2024 and 3—2025.

For the following classification, the initial data set was divided into three production areas as follows: area 1—Moldova, 2—Transylvania, 3—Muntenia. The significance of the discriminant model was assessed using Wilks' lambda and the associated F-test, indicating a statistically significant separation among the groups. The number of discriminant functions is lower with one than the number of compared groups, thus the two discriminant functions explained the total variance, accounting for 73.4% and 26.6%, respectively. The classification accuracy of the model was evaluated using leave-one-out cross-validation, yielding an overall correct classification rate of 95.2%, for both initial and cross-validation stages. The volatile compounds with the highest discriminant power were included β-pinene, eucalyptol (1,8-cineol), linalool, linalyl acetate, caryophyllene with high coefficients in DF1, and β-ocimene, α-thujene, p-cymene, β-myrcene with higher coefficients in DF2. The geographical separation is presented in Figure 4.

In addition to overall classification accuracy, from the confusion matrix, sensitivity per each class was also estimated, and had the following values: 92.3% for Moldova, 100% for Transylvania and 92.6% for Muntenia, respectively, indicating excellent performances for all regions.

Some of these compounds with a representative contribution in DF1 represent specific components of lavender oil and are associated with the monoterpene and oxygenated monoterpene biosynthetic pathways, which are strongly influenced by genetic and environmental factors [56]. Previously reported papers showed that linalool content of LEO is highly correlated with the age of plant, having an increasing trend between the first and fourth years. Moreover, weather conditions (precipitation) have a seriously influence upon linalool to linalyl acetate ratio [57–60]. Among the identified markers for geographical

origin and year of oil production differentiation, cis-β-ocimene seems to be powerful for both purposes.

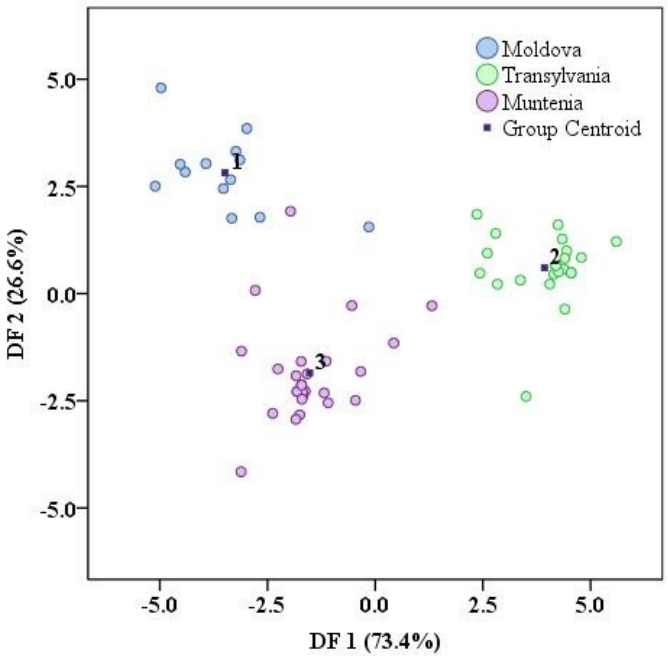

Figure 4. Lavender oil distribution after LDA, according to geographical origin. The numbers from the figure correspond to geographical area, as follows: 1—Moldova, 2—Transylvania, 3—Muntenia.

Although LDA provided high accuracy for geographical and harvest year classifications, several methodological limitations should be addressed. The number of variables included in the data matrix was high comparing with the number of LEO samples, and at the same time several volatile compounds exhibited high correlations among them, a fact that can affect the stability of the model and can introduce multicollinearity. Model performance was evaluated using a highly recognized cross-validation method, leave-one-out, which provides an estimation of the model robustness.

4. Conclusions

This study provided a detailed GC/MS along with chemometric evaluation of *Lavandula angustifolia* essential oils collected from different geographical regions of Romania. The GC–MS analysis revealed that the main compounds of the oils belonged to monoterpenes and oxygenated monoterpenes, and they included linalool, linalyl acetate, eucalyptol (1,8-cineol) and *β*-pinene. Positive significant correlations were identified among some of the compounds, especially among compounds from the same chemical class, confirming that geographical origin and production year are influenced by an overall fingerprint, rather than individual compounds. Linear discriminant analysis allowed a clear discrimination of the essential oil samples according to year of production and to geographical origin, highlighting the contribution of several key compounds to the separation of the groups. Compounds such *α*-phellandrene, *α*-terpinyl acetate, *trans*-*β*-farnesene, 3-octanone, *γ*-muurolene, *β*-ocimene and terpinene-4-ol showed strong contributions to essential oil classification according to year of production, while *β*-ocimene, *α*-thujene, *p*-cymene and *β*-myrcene were more strongly associated with the second classification, confirming their role in geographical differentiation of the samples.

Two-way ANOVA highlighted a significant effect for year of production indicating that quality varies among harvest years, but no significant effects were observed for

geographical area. The interaction between these two factors was not statistically significant, suggesting that the influence upon quality of LEOs is mainly due to harvest year.

Overall, the results obtained within this study demonstrate that volatile profile of Romanian lavender essential oils indicate a very good quality, assessed through a comprehensive algorithm and also by comparing with values from ISO 3515, only three LEO samples being totally aligned with recommended values. This result may reflect favorable environmental conditions for lavender plants and suitable cultivation practices.

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