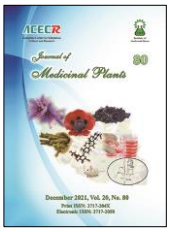
J. Med. Plants 2021; 20(80): 34-46

Institute of Medicinal Plants

Journal of Medicinal Plants

Journal homepage: www.jmp.ir



Research Article

Evaluation of adulteration in *Lavandula angustifolia* Mill. products using GC/MS combined with chemometric methods

Zahra Tarassoli[1], Hakim Faraji[1], Fateme Tajabadi[2,*], Mohsen Shabani[1], Hamidreza Shahbazi[1]

[1] *Department of Chemistry, Varamin-Pishva Branch, Islamic Azad University, Varamin, Iran*
[2] *Medicinal Plants Research Center, Institute of Medicinal Plants, ACECR, Karaj, Iran*

ARTICLE INFO

Keywords:
Lavandula angustifolia
Essential oil
Adulteration
Principal component analysis
Herbal medicine

ABSTRACT

Background: The essential oil of *Lavandula angustifolia* Mill. (*L. angustifolia*), a species from the Lamiaceae family, possesses several biological activities; therefore it is used in some herbal medicines. The lack of studies into identifying the essential oil of *L. angustifolia* and its similar appearance to *Nepeta menthoides* Boiss. & Buhse *(N. menthoides)* as "Ustukhuddoos" in Iranian traditional medicine, have caused misuse and adulteration in the products. **Objective:** In this study, the chemical compositions of *L. angustifolia* and *N. menthoides* essential oils, and three commercial herbal medicines of *L. angustifolia* essential oil in Iranian markets were evaluated and investigated as adulteration with the help of GC/MS analysis and chemometric methods. **Methods:** The essential oils of *L. angustifolia* and *N. menthoides*, and commercial samples were extracted by different extraction methods. Furthermore, their chemical compositions were evaluated by GC/MS analysis. After identification of components by GC/MS, the obtained results were assessed by principal component analysis (PCA, Unscrambler X version 10.4) for clustering. **Results:** Results showed that all three commercial herbal preparations matched with the manufacturer's claim about using *L. angustifolia* essential oil in the products. PCA distinguished two groups which were characterized based on different types and amounts of the components. **Conclusion:** GC/MS analysis with the help of chemometric methods is a powerful method to evaluate and discriminate between the essential oils and their products. In general, the combination of instrumental analysis and clustering chemometric analysis can provide an accurate tool for identifying misuse between plant species.

1. Introduction

Lavandula angustifolia Mill. known as medicinal, common, and true lavender is an evergreen perennial plant from the Lamiaceae family. Although lavender is grown in many countries, it is native to the Western Mediterranean [1, 2]. Its aerial parts, including flowers and leaves, are used as herbal medicine, especially in the form of essential oil [3, 4]. In addition, its essential oil is used in cosmetics,

Abbreviations: GC/MS, Gas Chromatography/Mass Spectrometry; HPLC, High Performance Liquid Chromatography; RT, Retention time; KI, Kovats index

*Corresponding author: tajabadi@imp.ac.ir

doi: 10.52547/jmp.20.80.34
Received 4 September 2021; Received in revised form 30 October 2021; Accepted 6 November 2021

perfumes, flavorings, and aromatherapy applications [5]. Previous studies have reported that lavender extracts have antioxidant and antibacterial activities [6]. Moreover, lavender essential oils and extracts have been used in Chinese traditional medicine for the treatment of ulcer, nerve ache, scald, rheumatism, and dermatosis [5].

The essential oil of *L. angustifolia* is seldom adulterated with synthetic oils and the essential oils of other species consist of linalool and linalyl acetate as major components (also the main components of *L. angustifolia*) [7]. There are two species in Iranian traditional medicine, *L. angustifolia* Mill. and *Nepeta menthoides* Boiss & Buhse, with similar local name "Ustukhuddoos"; therefore it can make a mistake in the process of producing herbal medicines from *L. angustifolia* [8]. *N. menthoides* is one of the 75 species of genus *Nepeta* L. from the Lamiaceae family which is wildly growing in Iran, and has similar appearance to *L. angustifolia* [9]. *N. menthoides* is easily found in the local herb shops with lower price than *L. angustifolia*. Due to the high cost of *L. angustifolia* and the similarity of these two plants, some *L. angustifolia* products in the local markets are adulterated. Unfortunately, in the context of essential oil usage, adulteration may occur to decrease manufacturing costs and increase sales revenue [10].

Lavender essential oil contains linalool and linalyl acetate [11] as main components, while the essential oil of *N. menthoides* is rich in 1,8-cineole and nepetalactone diastereoisomers [12]. Analysis of their essential oils has shown that their compositions have the same and different components which are related to the growing location and plant species [13].

Cluster analysis is a technique with the aim of dividing a set of data into groups. Observations in the same groups are similar to each other with dissimilarities between the different groups. Principal component analysis (PCA) is an important method for clustering and reducing the dimension of data sets to identify new, meaningful, and underlying variables. In the unsupervised learning method, PCA-variance is essentially used for data reduction by changing many variables into a much smaller number of components [14, 15].

Therefore, two plants' essential oils and their products were extracted and analyzed. Ultimately, the chemometric statistical data-analysis method was applied for essential oils discrimination based on GC/MS data. By applying this method to the cluster of essential oils samples, it was shown that interpreting the obtained results is not difficult.

2. Materials and Methods

2.1. Material

The aerial parts of *L. angustifolia* and *N. menthoides* were collected from the Institute of Medicinal Plants (ACECR, Alborz, Iran) and Tehran University (Herbarium of Faculty of Pharmacy, Tehran, Iran), respectively. These plants were identified and coded by herbarium as 100-IMPH for *L. angustifolia* and 6878-TEH for *N. menthoides*. Three commercial herbal medicines (HM1, HM2, and HM3) that had been claimed to contain *L. angustifolia* essential oil were purchased from local markets (Tehran, Iran) in the different dosage forms of oral drops (HM1 and HM2) and soft gel capsule (HM3). Solvents were supplied by Millipore Sigma Co. (Massachusetts, USA).

2.2. Essential oil extraction of the plants

The flowers and leaves of *L. angustifolia* and *N. menthoides* were air-dried at room temperature in the shadows. Then the dried plants

[DOR: 20.1001.1.2717204.2021.20.80.6.3]
[DOI: 10.52547/jmp.20.80.34]

were powdered and stored at 4 ºC for the next steps. Extraction of *L. angustifolia* and *N. menthoides* essential oils was performed using the hydro-distillation method by Clevenger apparatus [16]. For this purpose, 500 ml distilled water with 50 g of the plants' powder were placed in a flask and connected to Clevenger hydro-distillation apparatus. The round bottom flask was heated up to start distillation and consequently the distillate containing the essential oil and water was condensed and collected in a separating funnel. After about four hours, the essential oil was collected, dehydrated by anhydrous Na_2SO_4 and analyzed by GC-MS.

2.3. Essential oil Extraction of the commercial herbal preparations

Due to the HM1 and HM2 formulation containing the volatile emulsifying agents for dissolving essential oils, the extracted essential oils by Clevenger were not pure and mixed with an evaporated emulsifying agent. Thus the extracted essential oils of these two products were performed by solvent extraction with the help of a non-polar solvent such as n-pentane [17]. Using the solvent extraction method, emulsifier extraction with the essential oil was minimized and the purer essential oil was obtained. Briefly, 30 ml of the samples were placed in a separator funnel and 6 g salt (NaCl) was added to them. Then, 4 ml n-pentane was added to it and the mixtures were shaken vigorously to mix the two phases. Then, the lower aqueous layer was discarded, while the upper organic layer was collected and evaporated to remain the pure essential oil.

Due to the lack of other volatile agents in the soft gel product (HM3), extraction of the pure essential oil using Clevenger apparatus was obtained without the mentioned problems for HM1 and HM2. The percentages of the obtained essential oils of HM1, HM2, and HM3 products were 0.69, 0.64, and 0.28 (w/w), respectively.

2.4. GC/MS analysis

The chemical compositions of the essential oils were analyzed by GC/MS using an Agilent instrument model 6890 with a BPX5 column (30 m × 0.25 mm i.d., 0.25 μm film thickness, SGE, Australia) coupled to a Mass Spectrometer model 5973N. Following injection, 5 min after injection, the oven temperature was increased from 50 to 240 °C at a rate of 3 °C/min and then reached to 300 °C at the rate of 15 °C/min and held 3 min in this temperature. Other operating conditions were as follows: carrier gas, He (99.999 %), with a flow rate of 0.5 ml/min; injector temperature, 250 °C; and split ratio, 1:35. Mass spectra were taken at 70 eV a scan time of 1 s and a mass range of 40-500 amu [18].

2.5. Cluster Analysis

Cluster analysis is a statistical method for processing GC/MS data. It works by organizing samples into groups and clusters, based on how closely associated they are. The Unscrambler X version 10.4 was used for cluster analyses based on the principal component analysis (PCA) method [19].

3. Results

3.1. GC/MS analysis

As mentioned above, the essential oils of *L. angustifolia, N. menthoides* and HM3 product were collected by the hydro-distillation method and the essential oils of HM1 and HM2 products were collected by the solvent extraction method. The percentages of the obtained essential oils of *L. angustifolia, N. menthoides*, HM3, HM2, and HM1 have been 0.40 %, 0.30 %, 28.5 %, 2.1 %, and 2.0 % (w/w), respectively. All essential oils

[DOR: 20.1001.1.2717204.2021.20.80.6.3]
[DOI: 10.52547/jmp.20.80.34]

were analyzed using GC/MS. Chemical compositions of the essential oils were obtained by comparing their retention times and Kovats indices with the references of essential oils [20]. Total percentages of identified components for *L. angustifolia*, *N. menthoides*, HM3, HM2, and HM1 were 92.03 %, 94.47 %, 94.96 %, 89.46 %, and 91.34 %, respectively. The identified components are reported in Table 1 and their chromatograms are shown in Fig. 1.

Table 1. Chemical compositions of the origin plants and examined products essential oils

No.	Components	RT	KI	*Lavandula angustifolia*	*Nepetha menthenoides*	HM1	HM2	HM3	Type
1	*α*-Thujene	12.49	935	-	0.39	-	-	-	MH
2	*α*-Pinene	12.90	943	1.40	1.35	-	-	0.34	MH
3	Camphene	13.82	961	**3.59**	-	-	-	0.31	MH
4	*β*-Pinene	15.29	990	-	**3.40**	-	-	-	MH
5	1-Octen-3-ol	15.55	995	0.39	-	-	-	0.28	OT
6	*β*-Myrcene	15.82	1000	1.18	0.30	-	-	**2.03**	**MH**
7	3-Octanol	15.90	1003	-	-	-	-	0.23	OT
8	*α*-Terpinene	17.35	1030	0.57	1.46	-	-	-	MO
9	*o*-Cymene	17.57	1034	1.24	**4.58**	-	-	0.25	MH
10	*p*-Cymene	17.86	1040	-	0.99	-	-	-	MH
11	Limonene	18.02	1043	1.27	-	-	-	0.67	MH
12	1,8-Cineole	18.22	1046	**4.89**	**60.07**	0.86	0.29	**2.14**	**MO**
13	*trans*-*β*-Ocimene	18.86	1059	0.50	-	0.26	-	**3.66**	**MH**
14	*γ*-Terpinene	19.56	1072	-	**2.79**	-	-	0.26	MH
15	*cis*-Linalool oxide	19.66	1077	-	-	-	0.58	-	MO
16	*trans*-Linalool oxide	20.22	1085	0.47	-	-	0.73	-	MO
17	*trans*-Sabinene hydrate	20.31	1087	-	0.28	-	-	-	MO
18	Terpinolene	20.95	1099	-	0.48	-	-	0.23	MH
19	Linalool	21.87	1117	**32.11**	**4.02**	**35.38**	**43.84**	**30.23**	**MO**
20	*trans*-*p*-Menth-2-ene-1-ol	23.14	1143	-	0.22	-	-	-	MO
21	Camphor	24.47	1170	**4.07**	-	-	0.91	0.74	MO
22	2,6-Dimethyl-3,7-octadiene-2,6-diol	24.83	1175	-	-	-	0.37	-	MO
23	Lavandulol	25.02	1181	0.88	-	-	-	1.21	MO
24	Borneol	25.75	1195	**15.97**	-	-	0.78	1.12	MO
25	Terpinen-4-ol	26.02	1201	**2.89**	**2.82**	**3.51**	**2.63**	**4.30**	**MO**
26	*endo*-Borneol	26.13	1203	1.00	-	-	-	-	MO
27	*p*-Cymenol	26.47	1210	-	0.33	-	-	-	MO
28	*α*-Terpineol	26.80	1217	**2.61**	**3.79**	-	**8.56**	**2.41**	**MO**
29	Geraniol	27.64	1220	-	-	-	**2.85**	-	MO
30	*m*-Cresol	27.83	1239	-	1.81	-	-	0.96	OT
31	Nerol	27.97	1242	0.43	-	-	0.81	0.33	MO
32	Linalyl acetate	28.95	1263	**4.85**	-	-	**23.80**	**22.45**	**MO**
33	Cuminaldehyde	29.21	1268	-	0.46	-	-	-	MO
34	Lavandulyl acetate	30.54	1296	**3.07**	-	-	-	**4.62**	**MO**
35	*trans*-Bornyl acetate	30.77	1301	0.49	-	-	-	0.23	MO

[DOR: 20.1001.1.2717204.2021.20.80.6.3]
[DOI: 10.52547/jmp.20.80.34]

Table 1. Chemical composition essential oils of origin plants and examined products (Continued)

No.	Components	RT	KI	*Lavandula angustifolia*	*Nepetha menthenoides*	HM1	HM2	HM3	Type
36	Carvacrol	31.79	1325	-	0.21	-	-	-	MO
37	Neryl acetate	33.97	1374	0.57	-	**48.39**	1.18	0.63	MO
38	Nepetalactone	34.75	1391	-	**3.70**	-	-	-	MO
39	Geranyl acetate	34.85	1393	1.24	-	0.58	**2.13**	1.05	MO
40	*β*-bourbenene	35.16	1401	-	0.29		-	-	SH
41	*β-trans*-Farnesene	36.35	1428	-	-	0.45	-	4.38	SH
42	Santalen	36.59	1435	1.21	-		-	0.55	SO
43	Caryophyllene	36.77	1439	1.07	-	**5.53**	-	**4.94**	**SO**
44	Germacrene D	37.93	1491	-	-		-	0.56	SH
45	*γ*-Cadinene	40.71	1535	0.47	-		-	-	SH
46	Caryophyllene oxide	43.64	1609	**3.60**	-		-	0.23	SO
47	Hexahydrofarnesyl acetone	52.57	1857	-	0.24		-	-	DO
48	Manoyl oxide	58.09	2025	-	0.76		-	-	DO
	Total			**92.03**	**94.74**	**94.96**	**89.46**	**91.34**	
	Monoterpene Hydrocarbon			9.18	14.28	0.26	0	7.75	**MH**
	Oxygenated Monoterpene			76.11	77.36	88.72	89.46	71.46	**MO**
	Sesquiterpene Hydrocarbon			0.47	0.29	0.45	0	4.94	**SH**
	Oxygenated Sesquiterpenes			5.88	0	5.53	0	5.72	**SO**
	Other			0.39	1.81	0	0	1.47	**OT**
	Oxygenated Diterpene			0	1	0	0	0	**DO**

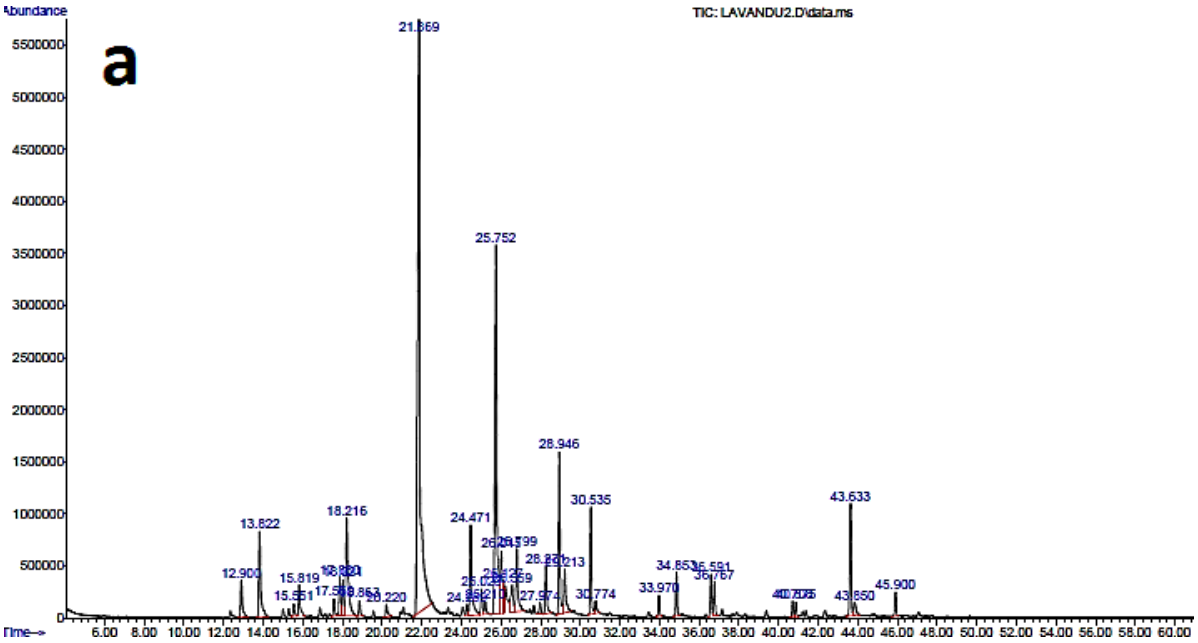


Fig. 1. GC/MS chromatograms obtained from a) *L. angustifolia, b) N. menthoides*, c) HM1, d) HM2 and e) HM3 samples

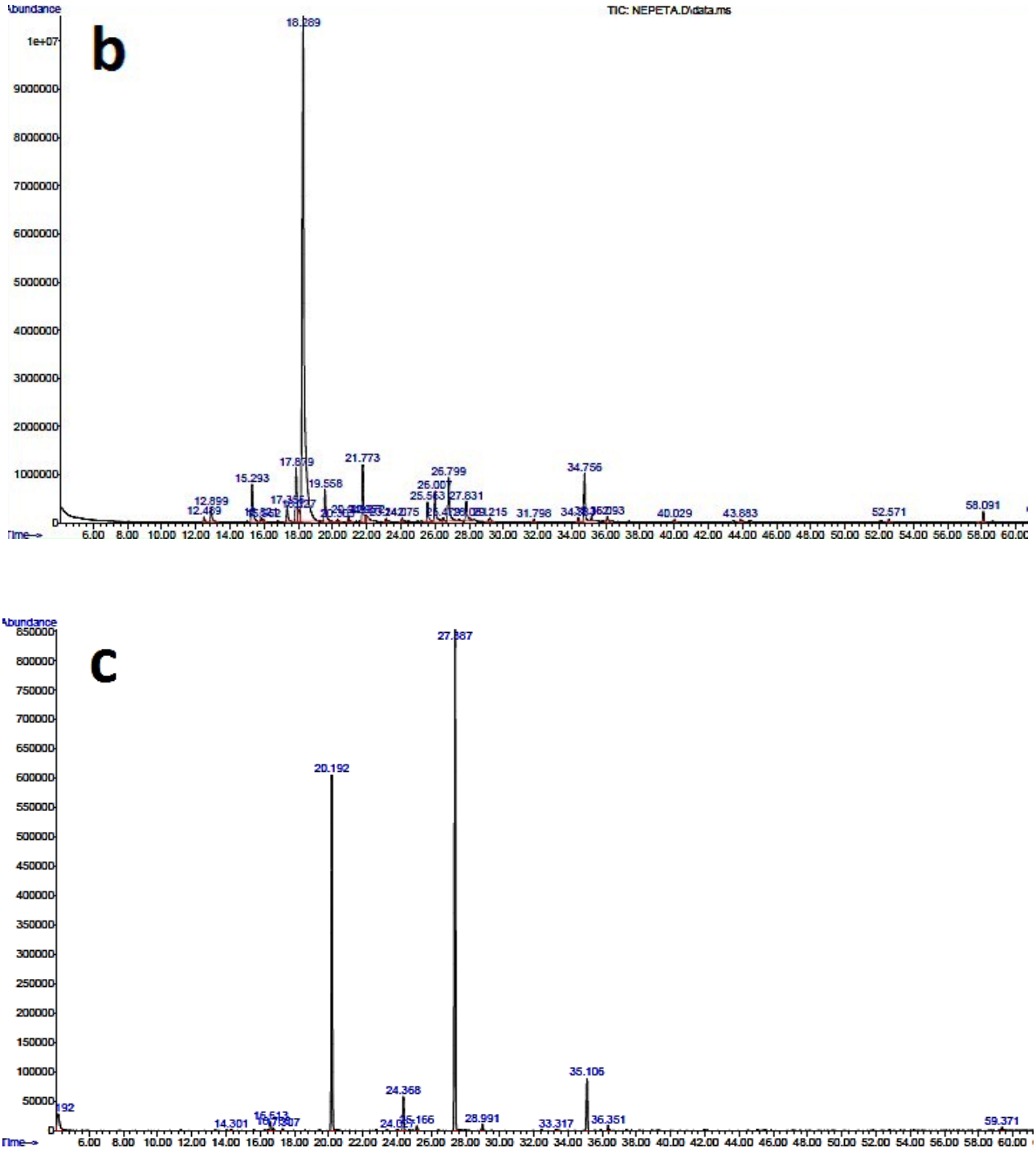


Fig. 1. GC/MS chromatograms obtained from a) *L. angustifolia*, *b) N. menthoides*, c) HM1, d) HM2 and e) HM3 samples (Continued)

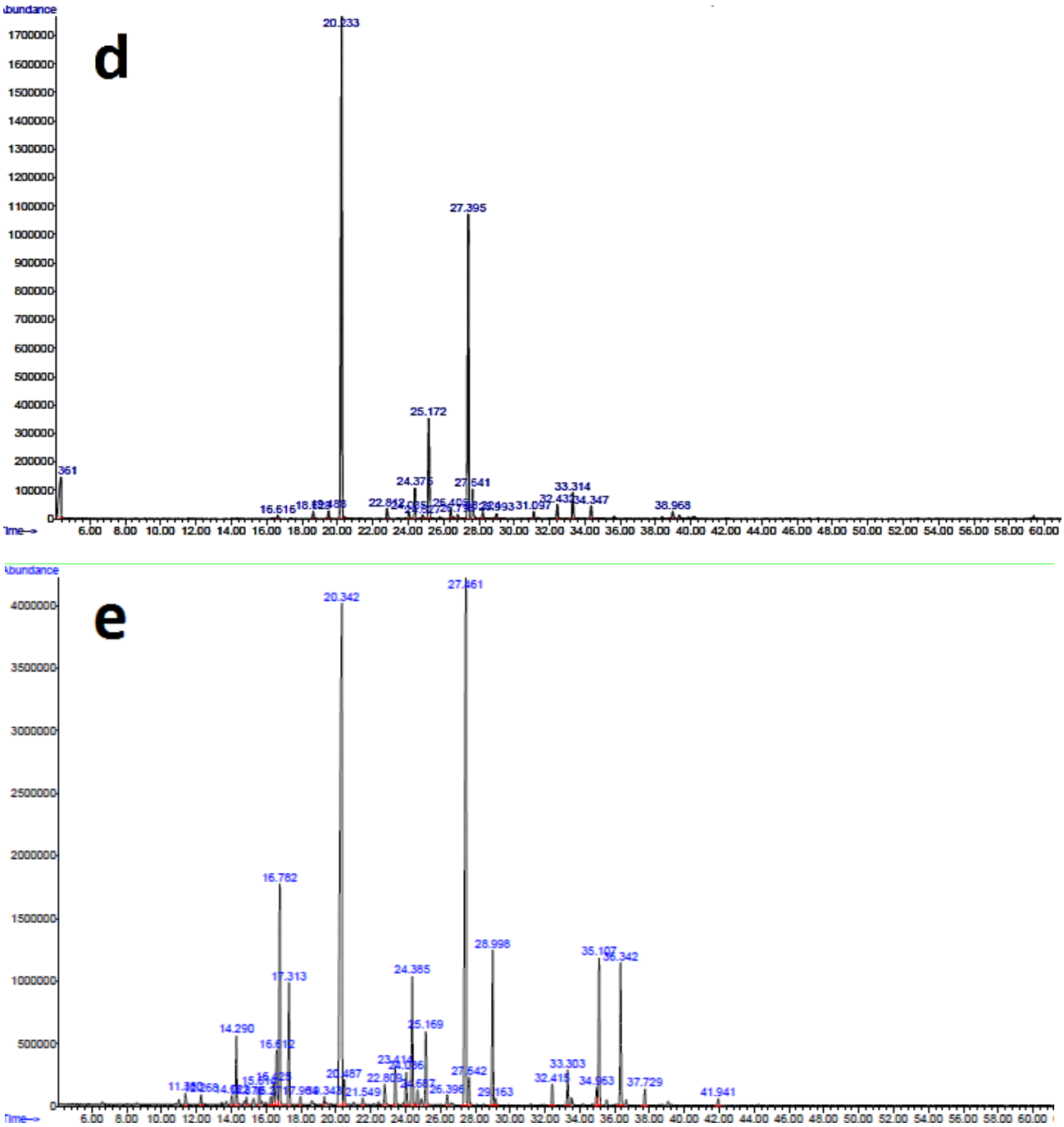


Fig. 1. GC/MS chromatograms obtained from a) *L. angustifolia, b) N. menthoides,* c) HM1, d) HM2 and e) HM3 samples (Continued)

The major components of *L. angustifolia* essential oil were linalool, borneol, 1,8-cineol, and linalyl acetate, respectively. Also the major components of *N. menthoides* essential oil were 1,8-cineol, *o*-cymene, linalool, and *α*-terpineol, respectively. Linalool and linalyl acetate were the major components of all three products.

3.2. Principal Component Analyses

The scoring diagram demonstrates the predicted positions of principal components (PCs) found among components of each sample and statistically determined the similarity between samples. Depending on the position of each group in the scoring diagram (position with positive or negative values on the 4-quadrat chart), it is possible to assign specific PC values for all samples. The PCA results of five essential oil sample types are presented in Fig. 2, based on components. The first two principal components should explain at least 60% of the correlation [21]. The first and second PCs accounted for 62 % and 30 % of the total sample variance, respectively. The sum of the first two PCs represents 92 % of the total sample variance, presenting sufficient information for explaining differences in the aromas of essential oils. There is a clear difference between the samples of *N. menthoides* and *L. angustifolia* essential oils.

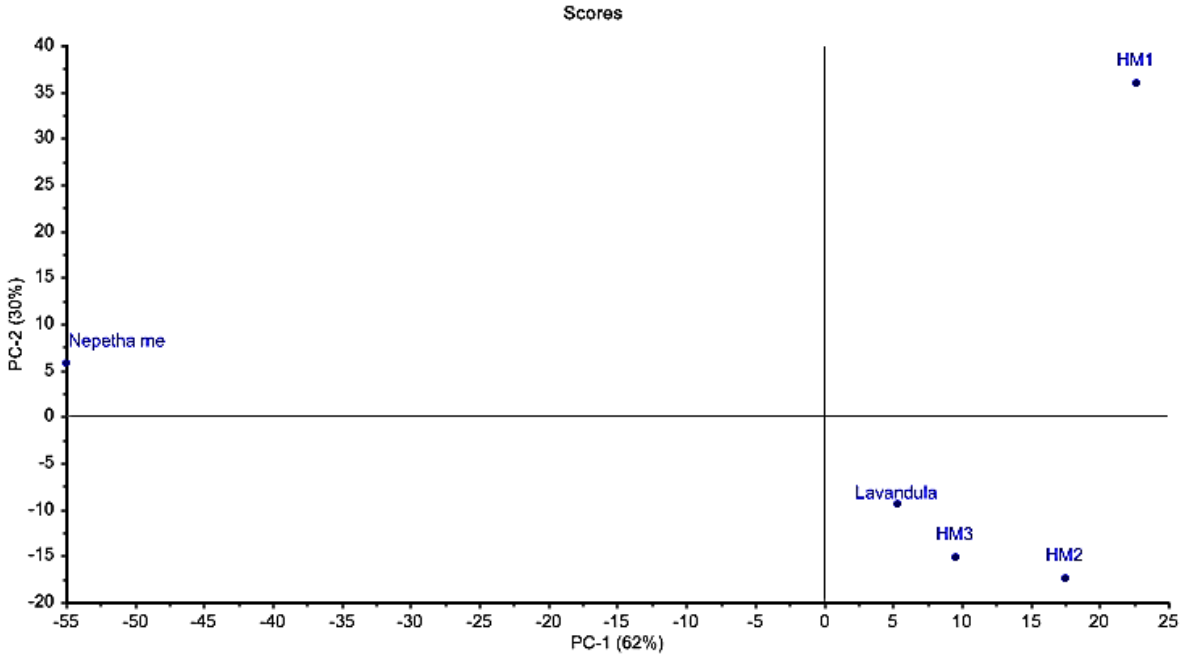


Fig. 2. Two-dimensional PCA plot performed on five purified essential oils based on data collected using GC/MS

The loading diagrams also demonstrate the relationship between independent variables (e.g., compounds) and clusters. These diagrams are produced by compound percentages using special vector equations. For each sample, a calculated high-loading value (for PCs) indicated that a larger share of the total percentages is derived (accounted for) from that samples. Fig. 3 shows the loading values of these samples in PCs. Therefore, *L. angustifolia*, HM1, HM2 and HM3 have the lowest loading coefficients and *N. menthoides* has the highest loading coefficient, so they play a more important role in the classification of the samples.

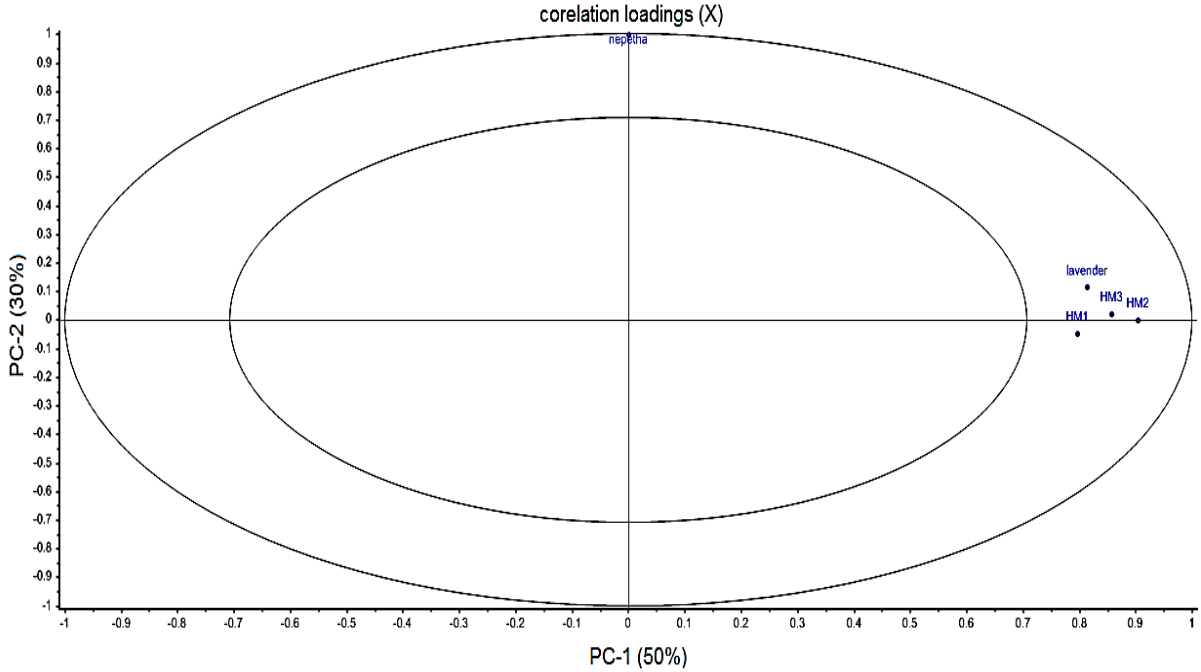


Fig. 3. Loading plot for 2-dimensional PCA analysis showing samples based component percentages-clustering distribution with associated principal components

4. Discussion

Based on the reported studies, location and season of sample collection, as well as extraction conditions, can affect the amounts and compositions of the obtained essential oils of *L. angustifolia* and *N. menthoides* [22-24]. For example, essential oil yields of *L. angustifolia* were reported in amounts of 0.2 to 1.1 % (w/w) by the hydro-distillation method in different months [24]. In another study, the hydro-distilled *N. menthoides* oil from its aerial parts has been reported in a yield of 0.85 % (w/w) [9].

As mentioned in the results section, and shown in Tables 1, the major components of *L. angustifolia and N. menthoides* were linalool (32.11 %) and 1,8-cineole (60.07 %), respectively. The percentages of the major components in the extracted essential oils of *L. angustifolia* [25] and *N. menthoides* [26] have been reported previously. The major components and the range of their percentages for *N. menthoides* have been reported as linalool (9.30 - 68.80 %), linalyl acetate (1.20 - 59.40 %), 1,8-cineole (41.10 - 70.06%), and nepetalactone (4.61 %) from Sabalan mountains (Ardabil, Iran), by Kahkeshani [27]. The study by Salata et al. [28] was investigated the quality and quantity of the essential oils of *L. angustifolia* samples that have been cultivated in different situations and collected in different seasons. The main reported constituents of the monoterpene group found in lavender essential oil were (in decreasing order): borneol (9.77 - 13.90 %), linalyl acetate (0.59 - 15.76 %), linalool (1.17 - 7.87 %), and 1.8-cineole (1.97 - 5.90 %); the percentage of cryptone, β-pinene, limonene, camphor, and neryl formate were in the range 1.17 - 4.57 %. As regards the sesquiterpene group, α-muurolol had the highest percentage (10.36 - 19.67 %), followed by caryophyllene oxide (5.50 - 9.08 %) and γ-cadinene (4.43 - 8.66 %).

As the result summarized in Table 3, three major components of *L. angustifolia* (linalool, borneol, and linalyl acetate) and *N. menthoides*

[DOR: 20.1001.1.2717204.2021.20.80.6.3]
[DOI: 10.52547/jmp.20.80.34]

(1,8-cineol, β-pinene, and nepetalactone) with their percentages are shown for better comparing with the products. All three components of *L. angustifolia* were found in the commercial products with agreeable percentages. Also as shown in Fig. 2, based on the location and spatial distribution of data clusters (represented by each sample type), *N. menthoides* essential oil (left) was well differentiated from samples of *L. angustifolia* (right), indicating significant differences in the chemical compositions from these two groups based on their corresponding volatile essential oil analytes. The relatively tight data clusters, derived from multiple sample replications of each sample type, indicate that instrument precision was good for all five samples.

Therefore, based on the obtained results of the origin plants in this study and cluster analysis, the existence of *L. angustifolia* essential oil in three commercial products is confirmed. This conclusion is due to the greater agreement of compounds' type and amount observed in three products with *L. angustifolia* compared to *N. menthoides*. However, based on the data which was shown in Fig. 2 and Table 2, the essential oil of HM2 and HM3 samples had higher compatibility in components with *L. angustifolia* essential oil. This observation showed that the extraction method for essential oils of *L. angustifolia* and HM3 was the same as hydro-distillation method.

Table 2. Correlation index between samples

Pair	Pearson's r	95 % CI		0		p-value
Lavandula angustifolia, Nepeta menthoides	0.090	-0.279	to 0.436	0.27892371	0.43648147	0.6346
***Lavandula angustifolia*, HM1**	0.461	0.121	to 0.705	0	0.58326387	0.0103
***Lavandula angustifolia*, HM2**	0.803	0.622	to 0.902	0	0.27976171	<0.0001
***Lavandula angustifolia*, HM3**	0.741	0.520	to 0.869	0	0.34975583	<0.0001
***Nepeta menthoides*, HM1**	-0.025	-0.382	to 0.338	0.38180494	0.33834252	0.8958
***Nepeta menthoides*, HM2**	-0.018	-0.376	to 0.344	0.37609951	0.34422868	0.9235
***Nepeta menthoides*, HM3**	0.002	-0.358	to 0.362	0.3584672	0.36206856	0.9913
HM1, HM2	0.481	0.146	to 0.717	0	0.57112785	0.0072
HM1, HM3	0.420	0.071	to 0.678	0	0.60726639	0.0208
HM2, HM3	0.951	0.898	to 0.976	0	0.07857059	<0.0001

H0: $\rho = 0$, the correlation coefficient ρ of the bivariate population is equal to 0.
H1: $\rho \neq 0$, the correlation coefficient ρ of the bivariate population is not equal to 0.

Table 3. Comparing the major components, determined using GC/MS

Sample	Linalool	Linalyl acetate	Borneol	1,8-Cineole	Nepetalactone	β-Pinene
***L. angustifolia* Essential oil**	32.11	4.85	15.97	4.89	**N.D.**	--
***N. menthoides* Essential oil**	4.02	N.D.	-	60.07	**3.70**	3.40
HM1	35.38	48.39	-	0.86	**N.D.**	-
HM2	43.84	23.80	0.78	0.29	**N.D.**	-
HM3	30.23	22.45	1.12	2.14	**N.D.**	-

N.D.: Not Detected

5. Conclusion

In this study with the help of chemometric methods coupled with GC/MS, precise methods for monitoring the quality and quantity of the claimed essential oils in the herbal products were reported. Based on the obtained results, the greater agreement of the type and amount of compounds was observed in three products with *L. angustifolia* compared to *N. menthoides*. The GC/MS analysis and processing of its obtained data by chemometric analysis such as cluster analysis provide a powerful tool to identify various adulteration in essential oils or to verify their biological or geographic origins. There is a need to prove that principal components are the continuous solution of cluster membership. Moreover, dimension reduction automatically performs data clustering according to the analysis results.

Author contributions

Z. T.: Doing practical tests, writing the manuscript, F. T. & H. T.: Project administration, Supervision, Validation the original draft, M. S. & H. S.: Review & Editing the original draft.

Conflict of interest

The authors declare that they have no known competing financial interests or personal relationships that could appear to influence the work reported in this paper. The authors alone are responsible for the content of the paper.

Acknowledgement

The supports of the Varamin-Pishva branch, Islamic Azad University, and also Institute of Medicinal Plants Center, ACECR are greatly acknowledged.

References

1. Denner SS. Lavandula angustifolia miller: english lavender. *Holistic Nursing Practice* 2009; 23(1): 57-64. doi: 10.1097/01.HNP.0000343210.56710.fc.

2. Smigielski K, Raj A, Krosowiak K and Gruska R. Chemical composition of the essential oil of *Lavandula angustifolia* cultivated in Poland. *J. Essential Oil Bearing Plants* 2009; 12(3): 338-347. doi: 10.1080/ 0972060X.2009.10643729.

3. Nurzyńska-Wierdak R and Zawiślak G. Chemical composition and antioxidant activity of lavender (*Lavandula angustifolia* Mill.) aboveground parts. *Acta Sci. Pol. Hortorum Cultus* 2016; 15(5): 225-241.

4. Amin Gh, Bozorgi M, Hossein salari A, Khalaj A, Zolfaghari B, Rahimi R, Soleimani S, Shams Ardakani M, Shirzad M and Taleb T. Ostokhodus. *Teb sonati eslam & iran* 1398; 10: 89-96 [In Persian].

5. Cong Y, Abulizi P, Zhi L and Wang X. Chemical composition of the essential oil of *Lavandula angustifolia* from Xinjiang, China. *Chemistry of Natural Compounds* 2008; 44(6): 810-810. doi:10.1007/s10600-009-9210-8.

6. Prusinowska R, Śmigielski K, Stobiecka A and Kunicka-Styczyńska A. Hydrolates from lavender (*Lavandula angustifolia*)-their chemical composition as well as aromatic, antimicrobial and antioxidant properties. *Natural Product Res*. 2016; 30(4): 386-393. doi: 10.1080/14786419.2015.1016939.

7. Lis-Balchin M. Lavender: the genus Lavandula. CRC press; 2002.

8. Kahkeshani N, Hadjiakhoondi A and Khanavi M. Differentiation of *Lavandula angustifolia* Mill. and *Nepeta menthoides* Boiss & Buhse using microscopic and phytochemical evaluations. 3rd National Congress on Medicinal Plants. 2014, 341.

[DOR: 20.1001.1.2717204.2021.20.80.6.3]

[DOI: 10.52547/jmp.20.80.34]

9. Sonboli A, Gholipour A, Yousefzadi M and Mojarrad M. Antibacterial activity and composition of the essential oil of *Nepeta menthoides* from Iran. *Natural Product Communications* 2009; 4(2): 1934578X0900400224. doi: 10.1177/ 1934578X0900400224.

10. Tisserand R and Young R. Essential Oil Safety. 2nd ed., London: Churchill Livingstone; 2014: 187-482.

11. Budzyńska A, Wickowska-Szakiel M, Sadowska B, Kalemba D and RÓŻALSKA B. Antibiofilm activity of selected plant essential oils and their major components. *Polish J. Microbiol*. 2011; 60(1): 35-40. doi: 10.37134/ ejsmt.vol4.1.1.2017.

12. Formisano C, Rigano D and Senatore F. Chemical constituents and biological activities of *Nepeta* species. *Chemistry & Biodiversity* 2011; 8(10): 1783-1818. doi: 10.1002/cbdv. 201000191.

13. Almasa I, Innocenta E, Machumia F and Kisinzab W. Effect of Geographical location on yield and chemical composition of essential oils from three Eucalyptus species growing in Tanzania. *Asian Journal of Traditional Medicines* 2019; 14: 1-12.

14. Alzate C and Suykens, JAK. Image Segmentation using a Weighted Kernel PCA Approach to Spectral Clustering. Computational Intelligence in Image and Signal Processing. 2007, CISBN: 1-4244-0707-9: 208 - 213.

15. Chen XW and Huang T. Facial expression recognition: A clustering-based approach, *Pattern Recognition Letters* 2003; 24: 1295-1302.

16. Elyemni M, Louaste B, Nechad I, Elkamli T, Bouia A, Taleb M, Chaouch M and Eloutassi N. Extraction of essential oils of *Rosmarinus officinalis* L. by two different methods: Hydrodistillation and microwave assisted hydrodistillation. *The Scientific World J*. 2019; 2019: 1-6. doi: 10.1155/2019/3659432.

17. Organization INS. Rose water-Test methods. in 2nd.Revision. 2014.

18. Tajabadi F, Khalighi-Sigaroodi F and Rezazadeh S. Improving gas chromatography-mass spectrometry analysis of essential oils by multivariate curve resolution: full identification of co‐eluting compounds of *Dracocephalum moldavica* L. *Chromatographia* 2017; 80: 1069-1077. doi: 10.1007/s10337-017-3322-2.

19. Silva AFS, Martins LC, Moraes LMB, Gonçalves IC, de Godoy BBR, Erasmus SW, Ruth SV and Rocha FRP. Can Minerals Be Used as a Tool to Classify Cinnamon Samples? *Proceedings* 2021; 70: 22-28. doi: 10.3390/foods_2020-07652

20. Adams RP. Identification of essential oil components by gas chromatography/mass spectrometry. Vol. 456. Allured publishing corporation Carol Stream, IL; 2007.

21. Combes C and Azema J. Clustering using principal component analysis: Application of elderly people autonomy-disability. *Decision Support Systems* 2013; 55(2): 578-586. doi: 10.1016/j.dss.2012.10.016.

22. Dubnicka M, Cromwell B and Levine M. Investigation of the Adulteration of Essential Oils by GC-MS. Current Analytical Chemistry. 2020; 16(8): 965-969.

23. Hassiotis CN, Lazari DM and Vlachonasios KE. The effects of habitat type and diurnal harvest on essential oil yield and composition of *Lavandula angustifolia* Mill. *Fresenius Environmental Bulletin* 2010; 19(8): 1491-1498.

24. Lakušic B, Lakušic D, Ristic M, Marčetic M and Slavkovska V. Seasonal variations in the composition of the essential oils of *Lavandula angustifolia* (Lamiacae). *Natural Product Communications* 2014; 9(6): 859-862. doi: 10.1177/1934578X1400900635.

25. Prusinowska R and Śmigielski K. Composition, biological properties and therapeutic effects of lavender (*Lavandula angustifolia* L.). A review. *Herba Polonica* 2014; 60(2): 2014; 56-66. doi: 10.2478/hepo-2014-0010.

26. Salehi B, Valussi M, Jugran AK, Martorell M, Ramírez-Alarcón K, Stojanović-Radić ZZ, Antolak H, Kręgiel D, Mileski KS and Sharifi-Rad M. *Nepeta* species: From farm to food applications and phytotherapy. *Trends in Food Science & Technol*. 2018; 80: 104-122. doi: 10.3390/ijms19092843.

27. Kahkeshani N, Hadjiakhoondi A, Navidpour L, Akbarzadeh T, Safavi M, Karimpour-Razkenari E and Khanavi M. Chemodiversity of *Nepeta menthoides* Boiss. & Bohse. essential oil from Iran and antimicrobial, acetylcholinesterase inhibitory and cytotoxic properties of 1, 8-cineole chemotype. *Natural Product Res*. 2018; 32(22): 2745-2748. doi: 10.1080/ 14786419. 2017.1378202.

28. Sałata A, Buczkowska H and Nurzy´nska-Wierdak R. Yield, Essential Oil Content, and Quality Performance of *Lavandula angustifolia* Leaves, as A_ected by Supplementary Irrigation and Drying Methods. Agriculture 2020; 10(12): 590-602. doi: 10.3390/agriculture10120590.

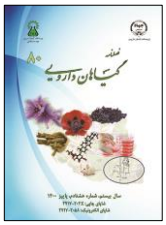
How to cite this article: Tarassoli Z, Faraji H, Tajabadi F, Shabani M, Shahbazi HR. Evaluation of adulteration in *Lavandula angustifolia* Mill. products using GC/MS combined with chemometric methods. ***Journal of Medicinal Plants*** 2021; 20(80): 34-46.
doi: 10.52547/jmp.20.80.34

فصلنامه گیاهان دارویی ۱۴۰۰؛ ۲۰(۸۰): ۳۴-۴۶

فصلنامه گیاهان دارویی

Journal homepage: www.jmp.ir

پژوهشکده گیاهان دارویی
جهاد دانشگاهی



مقاله تحقیقاتی

بررسی تقلبات گیاهی در محصولات اسطوخودوس توسط دستگاه کروماتوگرافی گازی متصل به طیف‌سنج جرمی به همراه روش‌های دسته‌بندی کمومتریک

زهرا ترسلی[۱]، حکیم فرجی[۱]، فاطمه تاج‌آبادی[۲،*]، محسن شعبانی[۱]، حمیدرضا شهبازی[۱]

[۱] گروه شیمی، شعبه ورامین- پیشوا، دانشگاه آزاد اسلامی، ورامین، ایران

[۲] مرکز تحقیقات گیاهان دارویی، پژوهشکده گیاهان دارویی، جهاد دانشگاهی، کرج، ایران

اطلاعات مقاله

گل‌واژگان:
اسطوخودوس
اسانس
تقلب در گیاه
آنالیز جزء اصلی
داروی گیاهی

چکیده

مقدمه: اسطوخودوس (*Lavandula angustifolia*)، گونه‌ای از خانواده نعناعیان بوده که اسانس آن دارای چندین فعالیت بیولوژیکی است؛ بنابراین در برخی از داروهای گیاهی مورد استفاده قرار می گیرد. فقدان مطالعه ای برای شناسایی اسانس اسطوخودوس و وجود شباهت در ویژگی های ظاهری آن با اسطوخودوس ایرانی (*Nepeta menthoides*) باعث سوء استفاده یا تقلب در محصولات آن شده است. **هدف:** در این مطالعه ترکیب شیمیایی اسانس اسطوخودوس و اسطوخودوس ایرانی مورد ارزیابی قرار گرفت و همچنین سه داروی گیاهی تجاری اسانس اسطوخودوس در بازارهای ایران به عنوان بررسی تقلبات در این حوزه مورد بررسی قرار گرفت. **روش بررسی:** اسانس‌های اسطوخودوس و اسطوخودوس ایرانی و نمونه‌های تجاری به روش تقطیر به دست آمد و ترکیب شیمیایی آنها توسط دستگاه کروماتوگرافی گازی متصل به طیف‌سنج جرمی مورد ارزیابی قرار گرفت. پس از آن با روش‌های کمومتریک جهت شباهت سنجی و دسته‌بندی با روش آنالیز جزء اصلی (PCA) مورد بررسی قرار گرفتند. **نتایج:** نتایج نشان داد که هر سه داروی گیاهی تجاری با ادعای سازنده در مورد استفاده از اسانس اسطوخودوس مطابقت دارد و دو گروه بین نمونه‌ها تشخیص داده شد. **نتیجه‌گیری:** تجزیه و تحلیل نتایج کروماتوگرافی گازی متصل به طیف‌سنج جرمی با روش‌های کمومتریک به عنوان روش مهمی برای ارزیابی اسانس اسطوخودوس و اسطوخودوس ایرانی بر اساس نتایج این مطالعه در نظر گرفته شده است. بنابراین تلفیق روش‌های دستگاهی با روش های آماری ابزار دقیق و قدرتمندی را جهت شناسایی و گروه‌بندی گونه‌های مختلف گیاهی و فرآورده‌های آنها ایجاد می‌کند.

مخففها: GC/MS، کروماتوگرافی گازی متصل به طیف‌سنج جرمی؛ HPLC، کروماتوگرافی مایع با کارایی بالا؛ RT، زمان بازداری؛ KI، شاخص بازداری

* نویسنده مسؤول: tajabadi@imp.ac.ir

تاریخ دریافت: ۱۳ شهریور ۱۴۰۰؛ **تاریخ دریافت اصلاحات:** ۸ آبان ۱۴۰۰؛ **تاریخ پذیرش:** ۱۵ آبان ۱۴۰۰

doi: 10.52547/jmp.20.80.34