GC-MS ANALYSIS OF ESSENTIAL OIL OF LAVANDULA ANGUSTIFOLIA

[1]MUKHAMADIEV ABDUKODIR, [2]NAYIMOVA BAKHORA, [3]MUKHAMADIEV NURALI, [4]FAZLIYEVA NIGINA, [5]MASAIDOVA MADINA

[1,2,3,4] Samarkand State University named after Sharof Rashidov, Uzbekistan
[5]Medical College named after Bobojon Gafurov, Khujand, Tajikistan
E-mail: [1]mqodir0808@gmail.com, [2]nayimovabahora@gmail.com, [3]nuralimukhamadiev@gmail.com, [4]niginafazliyevabonu@gmail.com, [5]muyassar.sobitova@mail.ru

Abstract - The paper presents a gas chromatographic analysis of Lavandula angustifolia essential oil, which allows to determine its chemical composition, classify its components by their nature, and evaluate potential areas of application. 34 compounds were identified, the majority of which were oxygen-containing monoterpenes, such as camphor (48.32%), linalool (9.34%), and endo-borneol (9.21%). The oil composition was analyzed by compound classes, optical isomers, and their functional purpose. It was shown that lavender oil has pronounced antiseptic, anti-inflammatory, sedative, and aromatic properties, which determines its demand in medicine, cosmetology, aromatherapy, and perfumery. The data obtained can be used for standardization and development of new products based on lavender oil.

I. INTRODUCTION

Lavender (Lavandula angustifolia) essential oil is one of the most popular and widely used natural products in medicine, cosmetology, perfumery and food industry [1-4]. Its unique properties are due to its chemical composition, including terpene and terpenoid compounds, such as linalool and linalyl acetate, which have antibacterial, anti-inflammatory, antiseptic and soothing effects [5-7]. In the context of growing interest in natural products, strict requirements for the quality of essential oils are becoming especially important [8-17]. The qualitative composition of the oil can vary significantly depending on the geographical origin, extraction methods and storage conditions. This makes quality control of lavender oil using modern analytical methods, such as gas chromatography combined with mass spectrometry (GC-MS), an important task. GC-MS allows not only to identify the main components of the oil, but also to accurately assess their concentration, which is crucial for product standardization [18-23]. Analysis of the composition of lavender essential oil also helps to reveal its potential therapeutic effect and application in various fields. The study of the chemical composition of lavender essential oil using high-precision analytical methods has both scientific and applied significance, contributing to the development of technologies for its use and improving product quality control.

Lavender essential oil, due to its unique properties, has become the object of numerous studies aimed at studying its chemical composition and biological activity [24-26]. The main components of the oil, such as linalool, linalyl acetate, camphor and geraniol, have been studied quite well in terms of their chemical structure, concentration and properties [27].

The literature contains extensive data on the composition of lavender oil of various species, including Lavandula angustifolia, Lavandula latifolia and Lavandula intermedia. The oil composition depends on the geographical region of growth, climatic conditions and extraction methods [28]. The researches devoted to the analysis of lavender oil are most often based on the use of gas chromatography (GC) and gas chromatography combined with mass spectrometry (GC-MS). These methods are the standard for the analysis of essential oils and allow obtaining detailed data on the composition and concentration of individual components [29].

Thus, the problem of studying lavender essential oil is at a high level of development, but requires further research in the field of the influence of various factors on the composition of the oil, its stability, biological activity and standardization of analytical methods. The purpose of this research is to analyze the chemical composition of lavender essential oil using the GC-MS method, identify the main components and assess their quantitative content.

II. MATERIALS AND METHODS OF THE RESEARCH

The analysis was performed on the essential oil obtained from the flowers of Lavandula angustifolia grown in the experimental plot of the Samarkand State University named after Sharof Rashidov (September-October, 2024). The oil was obtained by distillation with water vapor. The samples were stored in dark glass vials at a temperature of 4 ° C until analysis.

To study the chemical composition of the essential oil, gas chromatography combined with mass spectrometry (GC-MS) YL6900 and a chromatographic column HP-5MS (30 m × 0.25 mm × 0.25 μm) were used, where helium acted as a carrier gas with a flow rate of 1 ml / min. The temperature regime included an initial temperature of 60°C (5 min hold), a 4°C/min increase to 250°C, with a final hold at 250°C for 5 min; the injector temperature was 250°C, the samples were injected in splitless mode, and the mass spectrometer was operated in the 50–500 amu mass range using an electron impact (EI) ionization source with an energy of 70 eV.

The essential oil was diluted in hexane at a ratio of 1:100 before injection into the system. The injection volume of the sample was 1 μl.

The components of the essential oil were identified by comparing the mass spectra with the NIST (National Institute of Standards and Technology) library and literature data [30]. Retention indices (RI) calculated on the basis of the analysis of alkanes standard (C8–C20) injected under similar conditions were used for confirmation.

For quantitative determination of the components, peak areas on chromatograms were used. The concentrations were expressed as percentages of the total peak area (relative content). All experiments were performed in five replicates. The resulting chromatogram of the essential oil isolated from Lavandula angustifolia plant is shown in Fig. 1.

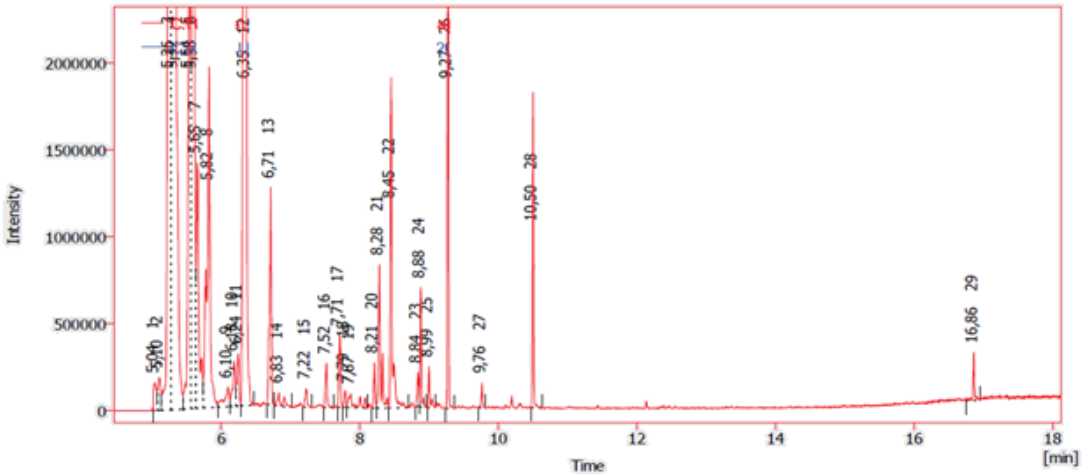

Figure 1. Chromatogram of the essential oil isolated from Lavandula angustifolia plant

III. RESULTS AND DISCUSSION

The results were processed using Agilent MassHunter software. Standard statistical methods were used to analyze the data variations using the OriginPro software package. The results of GC-MS analysis of Lavandula angustifolia essential oil are shown in Table 1.

Name	Chemical formula	Retention time, min	Percentage content %
(E)-p-2,8-Menthadien-1-ol	$C_{10}H_{16}O$	5,038	0,26
Hexyl isobutyrate	$C_{10}H_{20}O_2$	5,099	0,26
L-camphor	$C_{10}H_{16}O$	5,257	13,08
L-camphor	$C_{10}H_{16}O$	5,318	48,32
endo-Borneol	$C_{10}H_{18}O$	5,536	3,63
endo-Borneol	$C_{10}H_{18}O$	5,583	9,21
3-Hydroxydecanoic acid	$C_{11}H_{22}O_3$	5,651	2,08
a-Terpineol	$C_{10}H_{18}O$	5,823	3,18
Isopulegol	$C_{10}H_{18}O$	6,099	0,31
Hexyl 2-methylbutyrate	$C_{11}H_{22}O_2$	6,185	0,38
Isobornyl thiocyanoacetate	$C_{13}H_{19}NO_2S$	6,242	0,37
Linalool, formate	$C_{11}H_{18}O_2$	6,35	9,34
(R)-Lavandulol	$C_{10}H_{18}O$	6,712	1,20

Bornyl acetate	$C_{12}H_{20}O_2$	6,83	0,09
p-Cymen-7-ol	$C_{10}H_{14}O$	6,909	0,08
n-Butyl tiglate	$C_9H_{16}O_2$	7,224	0,12
Neryl propionate	$C_{13}H_{22}O_2$	7,518	0,23
Nerol acetate	$C_{12}H_{20}O_2$	7,708	0,39
Hexyl caproate	$C_{12}H_{24}O_2$	7,787	0,09
α-Zingiberene	$C_{15}H_{24}$	7,865	0,12
β-Curcumene	$C_{15}H_{24}$	8,005	0,09
Linalool, formate	$C_{11}H_{18}O_2$	8,077	0,05
α-Santalene	$C_{15}H_{24}$	8,206	0,20
(Z)-β-Caryophyllene	$C_{15}H_{24}$	8,281	0,69
trans-α-Bergamotene	$C_{15}H_{24}$	8,328	0,28
(E)-б-Famesene	$C_{15}H_{24}$	8,45	1,75
Germacrene D	$C_{15}H_{24}$	8,84	0,23
Linalyl iso-valerate	$C_{15}H_{26}O_2$	8,88	0,47
α-Himachalene	$C_{15}H_{24}$	8,994	0,26
Humulene	$C_{15}H_{24}$	9,27	1,82
Caryophyllene oxide	$C_{15}H_{24}O$	9,761	0,09
trans-Cadinol	$C_{15}H_{26}O$	10,191	0,05
a-Bisabolol	$C_{15}H_{26}O$	10,499	1,05
Di(2-ethylhexyl) terephthalate	$C_{16}H_{22}O_4$	16,863	0,20

Table 1. The results of GC-MS analysis of Lavandula angustifolia essential oil

As is shown in Table 1 the gas chromatographic analysis of the essential oil of Lavandula angustifolia allowed us to identify 34 compounds that varied in content and retention time. The largest part in the oil composition is occupied by camphor (48.32%) and linalool in the form of linalool-formate (9.34%). The high content of camphor and linalool indicates the potential antibacterial and anti-inflammatory activity of the oil. The presence of terpenoids, such as α-terpineol and (R)-lavandulol causes a pleasant aroma, which makes the oil in demand in perfumery.

Although some components, such as humulene (1.82%) and α-bisabolol (1.05%), are present in smaller quantities, they can play a synergistic role in the biological activity of the oil.Thus, the obtained data confirm that the essential oil of Lavandula angustifolia is characterized by a high content of biologically active components, such as camphor and linalool. GC-MS analysis allows to accurately determine the composition of the oil, which is important for its standardization and quality assessment.

As can be seen from the data in Table 1, the terpenoids make up the bulk of the essential oil, including monoterpenes and their oxygen-containing derivatives, which largely determine the aromatic and biological properties of the oil. Total content of oxygen-containing monoterpenes (71.36%): L-camphor (48.32%), endo-Borneol (9.21%), α-Terpineol (3.18%), Linalool, formate (9.34%), Isopulegol (0.31%), (R)-Lavandulol (1.20%), which are responsible for the antibacterial, anti-inflammatory and sedative properties of the oil. The content of hydrocarbon monoterpenes (1.17%) consists of α-Santalene (0.20%), (Z)-β-Caryophyllene (0.69%) and trans-α-Bergamotene (0.28%).

The oil contains hydrocarbon sesquiterpenes such as α-Zingiberene (0.12%), β-Curcumene (0.09%), Humulene (1.82%) and their oxygen-containing derivatives: Caryophyllene oxide (0.09%), trans-Cadinol (0.05%), α-Bisabolol (1.05%). These compounds enhance the antibacterial activity of the oil. The presence of such simple and complex esters as Hexyl isobutyrate (0.26%), Hexyl 2-methylbutyrate (0.38%), Bornyl acetate (0.09%), Nerol acetate (0.39%), Linalyl iso-valerate (0.47%) contribute to the aromatic properties of the oil and its stability. Also in the oil there is 3-Hydroxydecanoic acid (2.08%), which can contribute to the stability of the oil and its biological properties. Of the other compounds, Di(2-ethylhexyl) terephthalate (0.20%) was detected as an impurity.

The analysis of the composition of the essential oil of Lavandula angustifolia taking into account optical isomers is important, since the biological properties and aromatic characteristics of many compounds depend on their stereochemistry. Several compounds characterized by optical activity have been identified in the essential oil of lavender. These compounds include L-Camphor, Endo-Borneol, α-Terpineol, (R)-Lavandulol, Linalool, Isopulegol. The optically active components identified make up a significant portion of the Lavandula essential oil and determine its main properties.

Thus, as a result of the GC-MS study, the chemical composition of lavender essential oil (Lavandula

angustifolia) was studied in detail. The analysis revealed 34 components that were classified by their chemical nature, biological activity, and possible areas of application.

IV. CONCLUSION

It was revealed that the basis of the oil is oxygen-containing monoterpenes, such as camphor (48.32%), endo-borneol (9.21%), linalool (in the form of linalool-formate, 9.34%) and α-terpineol (3.18%). Among the minor components, terpenes (72.53%), simple and complex esters (1.59%), organic acids (2.08%) and sesquiterpenes (3.22%) were identified, which contribute to the aromatic profile and biological properties of the oil. It was shown that the oil contains cheral compounds, including L-Camphor, Endo-Borneol, α-Terpineol, (R)-Lavandulol, Linalool, Isopulegol.

REFERENCES

[1] Lawrence BM. Progress in Essential Oils. Perfumer and flavorist. 2009 Jan 1;18(6):43–6. https://img.perfumerflavorist.com/files/base/allured/all/document/2016/02/pf.PF_26_01_036_15.pdf

[2] Basch E, Foppa I, Liebowitz R, Nelson J, Smith M, Sollars D, et al. Lavender (Lavandula angustifolia Miller). Journal of Herbal Pharmacotherapy. 2004 Jan;4(2):63–78. https://doi.org/10.1080/J157v04n02_07

[3] Baser KHC, Buchbauer G, editors. Handbook of Essential Oils. CRC Press; 2009. https://doi.org/10.1201/9781420063165

[4] Renaud ENC, Charles DJ, Simon JE. Essential Oil Quantity and Composition from 10 Cultivars of Organically Grown Lavender and Lavandin. Journal of Essential Oil Research. 2001 Jul;13(4):269–73. https://doi.org/10.1080/10412905.2001.9699691

[5] Şahin F, Karaman İ, Güllüce M, Öğütçü H, Şengül M, Adıgüzel A, et al. Evaluation of antimicrobial activities of Satureja hortensis L. Journal of Ethnopharmacology. 2003 Jul;87(1):61–5. https://doi.org/10.1016/S0378-8741(03)00110-7

[6] Lis-Balchin M, Hart S. Studies on the mode of action of the essential oil of LavenderLavandula angustifolia P. Miller). Phytotherapy Research. 1999 Sep;13(6):540–2. https://doi.org/10.1002/(SICI)1099-1573(199909)13:6%3C540::AID-PTR523%3E3.0.CO;2-I

[7] C. Jianu, Pop G, Gruia AT, Horhat FG. Chemical composition and antimicrobial activity of essential oils of lavender (Lavendula angustifolia) and lavandin (Lavandula intermedia) grown in western Romania. International Journal of Agriculture and Biology. 2013 Jan 1;15(4):772–6. http://www.fspublishers.org

[8] Shapoval OG, Sheremetyeva AS, Dumova NA, Mukhamadiev NQ, Rabbimova GT, Nazirbekov MH. Antimicrobial Activity of Thymus serpyllum L. and Thymus marschallianus Willd. Essential Oils Against Candida albicans. Pharmaceutical Chemistry Journal. 2023 Dec 1;57(9):1449–53. https://doi.org/10.1007/s11094-023-03009-6

[9] Shapoval O, Sheremetyeva A, Durnova N, Mukhamadiev N, Rabbimova G, Nazirbekov M. Screening assessment of antibacterial activity of Thymus serpyllum L., Thymus marschallianus Willd. and Pimpinella anisum L. essential oils against uropathogens, isolated from pregnant women. Vestnik of Saint Petersburg University Medicine. 2023;18(2):167–75. https://doi.org/10.21638/spbu11.2023.205

[10] Shapoval OG, Sheremetyeva AS, Durnova NA, Mukhamadiev NQ, Rabbimova GT, Nazirbekov MK, et al. Antibacterial Activity of Essential Oils of Thymus serpyllum L. and Thymus marschallianus Willd.. Drug development & registration. 2023 Aug 31;12(3):143–50. https://doi.org/10.33380/2305-2066-2023-12-3-143-150

[11] Shapoval OG, Sheremetyeva AS, Durnova NA, Mukhamadiev NK, Rabbimova GT, Nazirbekov MKh. Antimicrobial activity of essential oils of Thymus serpyllum L. and Thymus marschallianus Willd. against Candida albicans. Chemical-pharmaceutical journal. 2023 Oct 7;57(9):26–31. https://doi.org/10.30906/0023-1134-2023-57-9-26-31

[12] Sheremetyeva AS, Karavaeva LV, Durnova NA, Shapoval OG, Mukhamadiev NQ, Rabbimova GT, et al. Comparative analysis of chemical composition of Thymus Serpyllum L. and Thymus Marschallianus Willd. Essential oils by gas-liquid chromatography with mass spectrometry detection. Problems of Biological, Medical and Pharmaceutical Chemistry. 2024 Feb 2;27(2):47–54. https://doi.org/10.29296/25877313-2024-02-06

[13] Shapoval O, Sheremetyeva A, Durnova N, Mukhamadiev N, Rabbimova G, Nazirbekov M. Comparative assessment of antibacterial activity of essential oils of Thymus serpyllum L., Thymus Marshallianus Willd. and Pimpinella Anisum L. against gram-negative bacteria causing urinary infections in pregnant women. Ovchinnikov Bulletin of Biotechnology and Physical-Chemical Biology, 2022. 18(3), 63. https://biorosinfo.ru/upload/file/journal_v18_no3.pdf#page=63

[14] Muhamadiev AN, Rabbimova GT, Nurmurodova SA, Muhamadiev NK. Possibilities of using essential oils in obstetric and gynecological practice. Central Asian Journal of Medical and Natural Sciences. 2020 Jun 22;1(2):31–43. https://doi.org/10.17605/cajmns.v1i2.46

[15] Nayimova BK, Mukhamadiev AN, Mukhamadiev NK. Modeling the process of chromatographic separation of melissa essential oil components on a capillary column using a cross-diffusion model. Central Asian journal of medical and natural science. 2024:5:1119-1125. https://doi.org/10.17605/cajmns.v5i4.2669

[16] Muxamadiev AN, Nayimova BK, Muxamadiev NK. Optimization of separation technological process of essential oils from "Pimpinella anisum L.". Scientific Journal: Exact and Natural Sciences Series. 2016:1(95):131-134. https://axborotnoma.uz/research/173/

[17] Nayimova BK, Muhamadiyev AN, Muhamadiyev NQ. Optimization of the essential oil selection from pimpinella anisum l. with the use of multifactor planning of the experiment. Scientific Journal: Exact and Natural Sciences Series. 2017:3(103/2):76-79. https://axborotnoma.uz/research/596/

[18] Muxamadiev AN, Nayimova BK, Muxamadiev NK. Kinetics of accumulation of components of melissa essential oil. Scientific Journal: Exact and Natural Sciences Series. 2024: 5(147/1):158-162. https://axborotnoma.uz/en/research/2997/

[19] Mukhamadiev NQ, Sayitkulov ShM, Ergashev IM, Khafizov KhF, Fayzullaev NI. Optimization of separation on the basis of unifac parameters and evaluation of the composition of the stationary phase in gas-liquid chromatography. Chromatographia. 2003 Jun;57(11-12):831–3. https://doi.org/10.1007/BF02491773

[20] Nayimova BK, Mukhamadiev AN, Mukhamadiev NK. GC-MS analysis of the chemical composition of the hydrodistillate of the above-ground part of Melissa Officinalis L. Central Asian journal of medical and natural science. 2024:5:1025-1031. https://doi.org/10.17605/cajmns.v5i4.2654

[21] Muhamadiev, A. N., Khalilov, K. F., Nayimova, B. K., & Muhamadiev, N. Q. GC-MS Investigation of Composition of Essential Oils, Extracted from Mentha Piperita and Pelargonium Roseum. International Journal of Applied Chemistry. 2019 May 25;6(2):31–4. https://doi.org/10.14445/23939133/IJAC-V6I2P105

[22] Karabaev HE, Mamatova ShR, Muhamadiev NK, Nayimova BK. Determination of microorganisms markers by the

method GC-MS and efficacy evaluation of rhinosinusitis. Central Asian Journal of medical and natural Science.2022:4(3):384-393. https://doi.org/10.17605/cajmns.v3i4.729.

[23] Nayimova BK, Fazlieva NT, Ergashova ShI, Mukhamadiev AN, Mukhamadiev NK. Gas chromatography-mass spectrometric analysis of methanol extract of Ferula sumbula. Proceedings of the IV-international conference on integrated innovative development of Zarafshan region: Achievements, challenges and prospects dedicated to the 65th Anniversary of Navoi Mining and Metallurgical Company.2023 Nov:1:305-306.

[24] Nayimova BK, Mukhamadiev AN, Mukhamadiev NK. GC-MS analysis of chemical composition melissa officinalis essential oil. XXII Mendeleev Congress on General and Applied Chemistry, October 7-12, 2024, Federal Territory "Sirius", Russia. 2024: 7:165. https://mendeleevcongress.ru/en/home/

[25] Topcu G, Ulubelen A. Structure elucidation of organic compounds from natural sources using 1D and 2D NMR techniques. Journal of Molecular Structure. 2007 May;834-836:57–73. https://doi.org/10.1016/j.molstruc.2006.12.001

[26] Cavanagh HMA, Wilkinson JM. Biological activities of Lavender essential oil. Phytotherapy Research. 2002;16(4):301–8. https://doi.org/10.1002/ptr.1103

[27] Zheljazkov VD, Astatkie T, Hristov AN. Lavender and hyssop productivity, oil content, and bioactivity as a function of harvest time and drying. Industrial Crops and Products. 2012 Mar 1;36(1):222–8. Available from: https://www.sciencedirect.com/science/article/abs/pii/S0926669011003852

[28] Kamatou GP, Vermaak I, Viljoen AM. Eugenol--from the remote Maluku Islands to the international market place: a review of a remarkable and versatile molecule. Molecules (Basel, Switzerland). 2012 Jun 6;17(6):6953–81. Available from: https://www.ncbi.nlm.nih.gov/pubmed/22728369

[29] ISO 3515:2002. ISO. Available from: https://www.iso.org/standard/36253.html

[30] Adams R. Identification of Essential Oil Components by Gas Chromatography/ Mass Spectrometry, 5th Ed. (online). 2017. Available from: http://www.juniperus.org/uploads/2/2/6/3/22639912/bk4frontisbnpreface-contents5thedonline2017.pdf

★★★