

Article

GC-MS Analysis of The Chemical Composition of The Hydrodistillate of The Above-Ground Part of Melissa Officinalis L

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Abstract: In this paper, a detailed chemical analysis of the hydrodistillate of the above-ground part of the plant *Melissa officinalis* L. using gas chromatography with mass spectrometry (GC-MS) was carried out. The study showed that the hydrodistillate obtained from the above-ground part of *Melissa officinalis* contains a rich complex of bioactive compounds including terpenes, flavonoids, phenolic acids and other volatile substances. The major components identified include 1,4-Dioxaspiro[4.5]decane-7-butanoic acid, 6-methyl-, 2-(methylsulfonyloxy)ethyl ester (12.59%) and 2-octadeca-9,12-dienoxyethanol (8.59%). Analysis of the hydrodistillate composition also revealed the presence of compounds such as Dipalmitin, Ethyliso-allocholate and Glycine, N-[(3 α ,5 β)-24-oxo-3-[(trimethylsilyl)oxy]cholan-24-yl]-, methyl ester. These data are important for standardisation and quality control of melissa-based phytopreparations and for the development of new therapeutic and cosmetic products

Keywords: *Melissa Officinalis* L., Hydrodistillate, GC-MS, Chemical Composition, Steam Distillation

1. Introduction

Melissa officinalis L. (*Melissa officinalis* L.) is a perennial herbaceous plant in the clematis family (Lamiaceae), widely distributed in Europe, Asia and North America [1]. It has long been used in folk medicine for its diverse therapeutic properties such as sedative, antispasmodic, antioxidant and antimicrobial effects [2-11]. The essential oil and hydrodistillate obtained from the above-ground part of melissa contain a rich complex of bioactive compounds including terpenes, flavonoids, phenolic acids and other volatile substances, making them the subject of numerous scientific studies [12-15].

In recent years, interest in natural sources of bioactive substances has increased significantly. This is due to the search for new effective and safe medicines based on plant extracts [16-23]. In this context, melissa is of particular interest due to its wide range of therapeutic properties and availability of raw materials [24]. One of the most effective methods for analyzing the chemical composition of plant extracts is gas chromatography with mass spectrometry (GC-MS) [25-26]. This method allows for a detailed study of the composition of essential oils and hydrodistillates, identification and quantification of key components, and assessment of their biological activity [27-28].

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The relevance of the research topic is due to several factors. Firstly, melissa is traditionally used in folk medicine in many countries due to its soothing, antispasmodic, antioxidant and antimicrobial properties. Secondly, standardization and quality control of melissa-based phytopreparations require accurate determination of their chemical composition. Third, the study of the chemical composition of melissa hydrodistillate contributes to the discovery of new bioactive compounds and understanding of their mechanisms of action, which is important for the development of effective medicinal and cosmetic products. Finally, the use of modern methods of analysis, such as GC-MS, allows to optimize the processes of extraction and processing of plant raw materials, which is of great importance for the development of agriculture and processing industry.

Thus, carrying out a comprehensive analysis of the chemical composition of the hydrodistillate of the above-ground part of the melissa plant using the GC-MS method is an urgent task aimed at improving the efficiency of the use of this valuable natural resource in various fields.

The purpose of this work is to conduct a comprehensive analysis of the chemical composition of the hydrodistillate of the above-ground part of the melissa plant using GC-MS to identify the key components.

2. Materials and Methods

Research material

Above-ground parts of melissa plant (*Melissa officinalis* L.) including leaves, stems and flowers were used as the object under study. Plant material was collected in July 2023 in Urgut and Pasdargom districts of Samarkand region.

Hydrodistillate was obtained from fresh above-ground parts of the plant by steam distillation [29].

Research Methods

Above-ground parts of melissa were placed in a distillation unit, where the process of steam distillation takes place. Steam passing through the plant material captures volatile components, which were then condensed and collected in the form of hydrodistillate.

Gas chromatography with mass spectrometry (GC-MS) was used to analyze the chemical composition. Sample preparation was carried out by extraction of the hydrodistillate with hexane, which was used for analysis.

Analyses were performed on a GC-MS YL6900 chromatograph using an HP5 stationary phase capillary column with a length of 30 m, an inner diameter of 0.32 mm and a thickness of 0.25 μm .

Chromatography conditions: column thermostat temperature - initial - 60°C for 3 minutes (isothermal conditions); Hold at 15°C/min (temperature programming condition) to 250°C and 250°C (isothermal condition) for 3 minutes. Injector temperature is 250°C, carrier helium flow rate is 1 mL/min, and separation factor is 1/100. Mass detector parameters - solvent delay - 3 minutes, emission current - 50 mA, scanning interval - 30-350 a.m.n., scanning speed - 1600 a.m.n./s, ion source temperature - 230°C, transfer temperature - 280°C. The analysis time was 22 minutes.

The components were identified by comparison of the mass spectra obtained with the NIST mass spectra library and retention times [30]. The internal normalization method was used for quantitative analysis [31]. The chromatogram of the hydrodistillate of the above ground part of *Melissa* plant is shown in Fig.1 and the composition and content in Table 1. Table 1 presents the chemical composition data of the hydrodistillate of the above-ground part of *Melissa* plant obtained by gas chromatography-mass spectrometry (GC-MS), in which 20 components are listed with their chemical formula and percentage content.

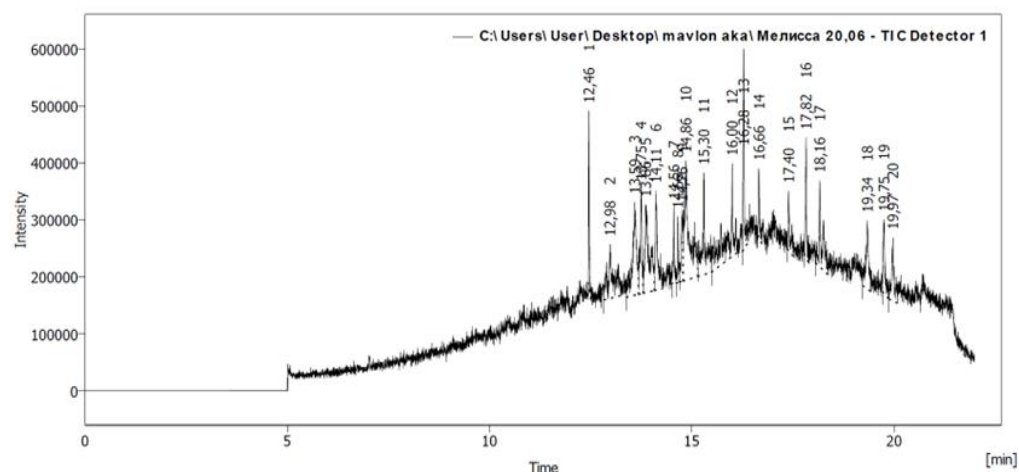
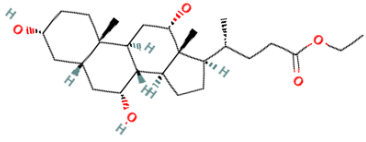
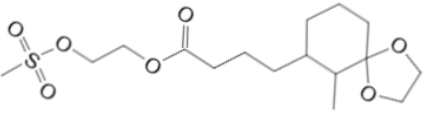
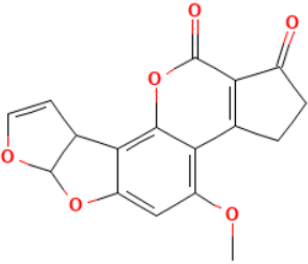
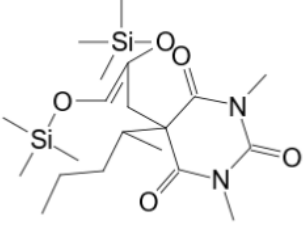
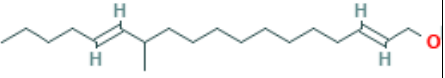
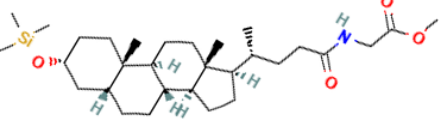
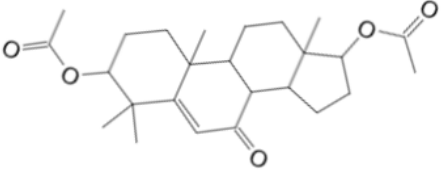
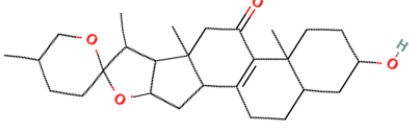
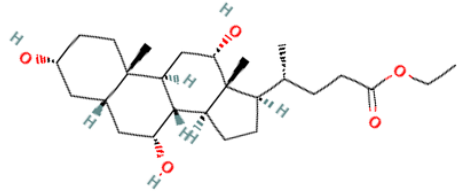
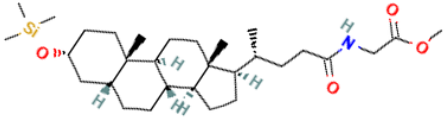
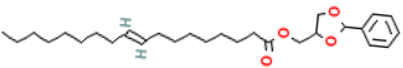
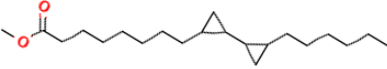


Fig.1. Chromatogram of hydrodistillate above ground parts of the plant *Melissa officinalis* L.

Table 1. Chemical composition of the hydrodistillate of the above-ground part of *Melissa officinalis* L.

№	Compound Name	Chemical formula	Structure	Content, %
1	Dipalmitin	$C_{70}H_{136}O_{10}$		2.87
2	Ethyliso-allocholeate	$C_{26}H_{44}O_5$		6.67
3	12-Methyl-E,E-2,13-octadecadien-1-ol	$C_{19}H_{36}O$		8.26
4	1,2-Dipalmitin	$C_{35}H_{68}O_5$		4.43
5	2-octadeca-9,12-dienoxyethanol	$C_{20}H_{38}O_2$		8.59
6	unknown	-		5.17
7	Glycine, N-[(3 α ,5 β)-24-oxo-3-[(trimethylsilyl)oxy]cholan-24-yl]-, methyl ester	$C_{30}H_{53}NO_4Si$		1.81
8	Pregn-5-ene-3,11-dione, 17,20:20,21-bis[methylenebis(oxy)]-, cyclic 3-(1,2-ethanediyl acetal)	$C_{25}H_{34}O_7$		1.47

9	Ethyl iso-allocholate	$C_{26}H_{44}O_5$		2.54
10	1,4-Dioxaspiro[4.5]decane-7-butanoic acid, 6-methyl-, 2-(methylsulfonyloxy)ethyl ester	$C_{16}H_{28}O_7S$		12.59
11	4H,5aH,9H-Furo[2,3-b]furo[3',2':2,3]cyclopenta[1,2-c]furan-2,4,7(3H,8H)-trione, 9-(1,1-dimethylethyl)dihydro-8,9-bis[(trimethylsilyl)oxy]-, (3aS,5aR,8R,8aS,9R,10aS)-	$C_{17}H_{12}O_6$		6.70
12	2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-[2,3-bis[(trimethylsilyl)oxy]-2-propenyl]-1,3-dimethyl-5-(1-methylbutyl)-	$C_{20}H_{38}N_2O_5Si_2$		9.77
13	12-Methyl-E,E-2,13-octadecadien-1-ol	$C_{19}H_{36}O$		4.98
14	Glycine, N-[(3α,5β)-24-oxo-3-[(trimethylsilyl)oxy]cholan-24-yl]-, methyl ester	$C_{30}H_{53}NO_4Si$		1.84
15	Acetic acid, 17-acetoxy-4,4,10,13-tetramethyl-7-oxo-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl (ester)	$C_{25}H_{36}O_5$		2.52
16	Spirost-8-en-11-one, 3-hydroxy-, (3β,5α,14β,20β,22β,25R)-	$C_{27}H_{40}O_4$		3.45

17	Ethyl iso-allocholate	C ₂₆ H ₄₄ O ₅		5.34
18	Glycine, N-[(3 α ,5 β)-24-oxo-3-[(trimethylsilyl)oxy]cholan-24-yl]-, methyl ester	C ₃₀ H ₅₃ NO ₄ Si		4.28
19	9-Octadecenoic acid, (2-phenyl-1,3-dioxolan-4-yl)methyl ester, cis-	C ₂₈ H ₄₄ O ₄		3.20
20	[1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester	C ₂₁ H ₃₈ O ₂		3.50

3. Results

,4-Dioxaspiro[4.5]decane-7-butanoic acid, 6-methyl-, 2-(methylsulfonyloxy)ethyl ester (12.59%), 2-octadeca-9,12-dienoxyethanol (8.59%), 12-Methyl-E,E-2,13-octadecadien-1-ol (8.26%), 2,4,6(1H,3H,5H)-Pyrimidinetrione, 5-[2,3-bis[(trimethylsilyl)oxy]-2-propenyl]-1,3-dimethyl-5-(1-methylbutyl)-(9.77%), Ethyliso-allocholate (6.67%), 4H,5aH,9H-Furo[2,3-b]furo[3',2':2,3]cyclopenta[1,2-c]furan-2,4,7(3H,8H)-trione, 9-(1,1-dimethylethyl)dihydro-8,9-bis[(trimethylsilyl)oxy]-, (3aS,5aR,8R,8aS,9R,10aS) - (6.70%) with high content (more than 5%), Dipalmitin (2.87%), 1,2-Dipalmitin (4.43%), Glycine, N-[(3 α ,5 β)-24-oxo-3-[(trimethylsilyl)oxy]cholan-24-yl]-, methyl ester (1.81% - 1.84%), Acetic acid, 17-acetoxy-4,4,10,13-tetramethyl-7-oxo-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl (ester) (2.52%), Spirost-8-en-11-one, 3-hydroxy-, (3 β ,5 α ,14 β ,20 β ,22 β ,25R)- (3.45%), 9-Octadecenoic acid, (2-phenyl-1,3-dioxolan-4-yl)methyl ester, cis- (3.20%), [1,1'-Bicyclopropyl]-2-octanoic acid, 2'-hexyl-, methyl ester with medium content (2-5%) and Pregn-5-ene-3,11-dione, 17,20:20,21-bis[methylenebis(oxy)]-, cyclic 3-(1,2-ethanediyl acetal) (1.47%) with low content (less than 2%) and an unknown compound, 5.17%.

4. Conclusion

In summary, GC-MS analysis revealed a diverse chemical composition of melissa essential oil, including several key components such as 1,4-Dioxaspiro[4.5]decane-7-butanoic acid, 6-methyl-, 2-(methylsulfonyloxy)ethyl ester and 2-octadeca-9,12-dienoxyethanol, which constitute a significant portion of the oil content. These findings provide further insight into the potential therapeutic properties of melissa essential oil and its use in medicine and cosmetology.

Overall, melissa essential oil is a unique and valuable natural product due to its rich chemical composition and multiple therapeutic properties. However, in order to fully utilize it, it is necessary to continue research aimed at deepening the understanding of its properties, improving production techniques and developing new products. As a result of such efforts, melissa products will be able to take an even more significant place in medicine, cosmetology, aromatherapy and other fields.

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