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Gas chromatography for β-caryophyllene determination in St. John's wort infused oil

Vida Vičkačkaitė*,

Sandra Petrokaitė,

Vilius Poškus

Department of Analytical and Environmental Chemistry, Vilnius University, 24 Naugarduko Street, 03225 Vilnius, Lithuania

Hypericum Perforatum L., commonly known as St. John's wort, is one of the best-known medicinal herbs. St. John's wort infused oils are mostly used externally, but can be taken orally for stomach ulcers, are used as a food supplement. Therefore, it is important to develop methods that allow a rapid and reliable determination of β-caryophyllene, which is one of the main active components of St. John's wort.

In this work, two gas chromatographic techniques, static headspace gas chromatography (SHS-GC) and solid phase microextraction, combined with gas chromatography-mass spectrometry (SPME-GC-MS), were examined for the determination of β-caryophyllene in St. John's wort infused oils. A comparison of these two techniques revealed that SPME-GC-MS can be successfully applied for the analysis. The other method, SHS-GC, is simple and fast, but because of its high detection limit, it can only be applied to oil samples with β-caryophyllene concentration higher than 0.1 mg/g.

Keywords: headspace sampling, gas chromatography, *Hypericum Perforatum* L., β-caryophyllene

INTRODUCTION

Hypericum Perforatum L., commonly known as St. John's wort, is one of the best-known medicinal herbs. It is famous for its neuroprotective, antineuralgic and antiviral properties, is beneficial for premenstrual syndrome, polycystic ovary syndrome, perimenopause and menopause, eczema and psoriasis. For a long time, St. John's wort has been used in traditional medicines for healing skin wounds, burns, diseases of the alimentary tract, and psychological disorders, especially depression. St. John's wort has recently been shown to have antioxidant, anticonvulsant, analgesic, anti-inflammatory, cytotoxic and antidiabetic activities [1–4]. Due to its healing properties St. John's wort is used as a nutraceutical, phytopharmaceutic, and an ingredient in cosmetics [5]. Its leaves and flowers since the ancient times are used to make herbal tea and to prepare infused oils. It is known that St. John's wort infused oils help to overcome skin problems – relieve irritation, reduce itching, soften, disinfect, regenerate cells, act against herpes, hepatitis, flu viruses, relieve muscle, joint and bone pain. St. John's wort infused oils are mostly used externally, but can be taken orally for stomach ulcers, are used as a food supplement [6].

Since many of the active components of St. John's wort are poorly soluble in water but have a high hydrofobicity, it can be expected that the concentrations of these substances in St. John's wort infused oils will be higher, and the medical properties of infused oils will be stronger than in herbal tee. Moreover, *Hypericum* extracts show a significant antioxidant activity, inhibiting free radical generation and lipid peroxidation [7]. So St. John's wort infused oils, in addition to their therapeutic efficacy, should also be more resistant to ageing.

There have been numerous investigations of St. John's wort essential oils and they have shown

* Corresponding author. Email: vida.vickackaite@chf.vu.lt

a wide variability in composition. One of the main constituents of St. John's wort is β-caryophyllene. Its quantity depends on the region and varies in a broad range. For example, β-caryophyllene content in the essential oil of St. John's wort from northern Turkey is 4.1–5.9% [8], from southeastern France 0.2–28.4% [9], from Greece 6.6–10.3% [10], from Uzbekistan 11.7% [11] and from Lithuania 1.6–14.2% [12].

β-Caryophyllene as well as St. John's wort demonstrantes analgesic, antioxidant, anti-inflammatory, antidepressant and cancer cell growth inhibitory effects [13]. The similarity of the pharmacological properties of β-caryophyllene and of St. John's wort suggests that β-caryophyllene is one of the principle substances responsible for the unique therapeutic effect of St. John's wort.

β-Caryophyllene is usually determined by gas chromatography (GC) or gas chromatography-mass spectrometry (GC-MS) [14–16]. However, the preparation of multicomponent plant samples for gas chromatographic analysis is often complex and time-consuming. A perfect choice for the determination of volatile compounds is GC combined with headspace sampling [17, 18]. One of the most convenient mathods that combines GC and headspace sampling is static headspace gas chromatography (SHS-GC). It includes an isolation of a volatile analyte in a gas phase and subsequent automatic delivery of an aliquot of vapour to the GC system.

In the case of low concentrations of volatile analytes, before GC analysis they should be preconcentrated. An effective preconcentration technique is solid phase microextraction (SPME). With SPME, the analytes are absorbed on to an absorbent coated fused silica fibre, which is part of a syringe needle. After the partitioning of the analytes from the sample matrices to the extraction phases, the fibre is inserted directly into a GC injection port for thermal desorption [19].

The aim of this work was to prepare, compare and apply SHS-GC and SPME-GC-MS techniques for β-caryophyllene determination in St. John's wort infused oil.

EXPERIMENTAL

Reagents and samples

β-Caryophyllene (≥80%) was purchased from Sigma-Aldrich (Germany). Unrefined sunflower oil 'Senoji aliejinė' (Lithuania), refined sunflower oil (Ukraine) and coconut oil 'Naturalisimo' (the Netherlands) were purchased in a local supermarket.

β-Caryophyllene stock solution in coconut oil (10 mg/g) was prepared by weighting. Working β-caryophyllene solutions in coconut oil were prepared by dilution of the β-caryophyllene stock solution with coconut oil to a required concentration.

Three samples of aereal parts of St. John's wort plants were examined. One plant sample was purchased in a local pharmacy in 2021 (Ph2021) and two plant samples were collected in the flowering period from the field in the Varėna District (Lithuania) in 2020 (V2020) and in 2021 (V2021).

For St. John's wort infused oil preparation, 100 g of sunflower oil (carrier oil) was added to 2 g of dried aereal parts of St. John's wort.

Instrumentation and conditions

Headspace extraction and sample introduction was performed on a PerkinElmer Headspace Sampler Turbomatrix 16 (PerkinElmer, USA) equipped with a balanced pressure system. Twenty millilitre headspace vials were used in all experiments. A headspace vial was positioned in the HS autosampler and equilibrated at the selected temperature. The needle temperature and the transition line temperature was 10°C higher than the headspace vial equilibration temperature. The settings of the headspace sampler were 1 min for pressurization and 0.09 min for injection. Helium was employed as carrier gas with 16.7 psi column head pressure.

Headspace gas chromatographic analysis was performed on a PerkinElmer Clarus 580 series gas chromatograph (PerkinElmer, USA) equipped with a flame ionisation detector (temperature 250°C, hydrogen flow 40 ml/min, air flow 400 ml/min and auxiliary gas (helium) flow 30 ml/min). The GC system was equipped with the Rxi®-5Sil MS capillary column (30 m × 0.25 mm id, 0.25 μm film thickness). The injector temperature was held at 110°C. The oven temperature was programmed as follows: 40°C for 1 min, from 40 to 60°C at 2°C/min, from 60 to 200°C at 40°C/min, from 200 to 250°C at 10°C/min and held for 1 min.

Solid phase microextraction was performed with a Supelco CAR/PDMS (85 μm) fibre housed in a manual holder (Supelco Bellofonte, PA, USA).

SPME was carried out in a 20 ml vial closed with a silicone rubber septum placed in a cap. The vial was placed in a water-jacketed vessel on a magnetic stirrer and kept at 80°C temperature for 20 min. Desorption was carried out in a GC-MS injection port at 250°C for 30 s.

Gas chromatographic-mass spectrometric analysis was performed on a PerkinElmer Clarus 580 series gas chromatograph equipped with a programmable temperature vaporizer injector and coupled to a PerkinElmer Clarus 560 S mass spectrometer (PerkinElmer, Shelton, USA). The system was equipped with the Elite-5MS capillary column (30 m × 0.25 mm id, 0.25 μm film thickness). Helium was employed as carrier gas with a constant flow of 1 ml/min. Injection was performed in the split mode (10:1). The oven temperature was programmed as follows: from 45 to 100°C at 2°C/min, from 100 to 250°C at 5°C/ min and held for 5 min. The transfer line temperature was 280°C. The electron ionisation ion source conditions were as follows: electron energy 70 eV and temperature 180°C. When GC-MS in the full scan mode was used, data acquisition was performed in a scan mode in a range of m/z 45–500. The qualitative identification of different compounds was performed by comparing their mass spectra with those stored in the NIST (National Institute of Standards and Technology) library. For β-caryophyllene quantification, the selected ion monitoring (SIM) mode was used. The quantification ions (m/z values) were 93 and 133.

The samples were heated in a microwave reactor Monowave 450 (Anton Paar).

RESULTS AND DISCUSSION

Preliminary analysis of St. John's wort

According to the literature, the quantitative composition of St. John's wort depends on the region and the climatic conditions and varies in a broad range. In this work, three different samples of St. John's wort have been investigated, two of them were collected in the Varėna District in 2020 and 2021, the third was bought at a pharmacy. The preliminary analysis was carried out using SPME and GC-MS.

For analysis, 0.2 g of dried arial part of St. John's wort was placed in a 20 ml vial and subjected to SPME for 30 min at 80°C temperature. Desorption of the SPME fibre was carried out in the GC-MS injection port at 250°C for 30 s.

The results of the analysis showed (Fig. 1, Table 1) that the main volatile components of St. John's wort from pharmacy were β-caryophyllene, γ murolene, caryophyllene oxide, γ-cadenen and δ-cadenen. The main volatile components of St. John's wort collected in 2021 in the Varėna District were γ-murolene, (Z)-β-farnesene, β-caryophyllene and δ-cadenene and the amounts of almost all components (except caryophyllene oxide) were higher (for nonane, 3-methylnonane, (Z)-β-farnesene and γ-murolene even more than 10 times higher) than in St. John's wort purchased at the pharmacy. This can probably be explained by the fact that the samples were collected at different locations and dried under different conditions. In addition, St. John's wort collected in the Varėna District is dominated by flowers and leaves, while St. John's wort purchased at the pharmacy is dominated by stems.

Comparing St. John's wort collected in the Varėna District in 2020 and 2021, it turned out that there are more volatile components in St. John's wort collected in 2021 (β caryophyllene 6.8 times, α-caryophyllene 13 times and γ-murolene even 19 times more). This could be explained by different meteorological conditions. However, it is more likely that St. John's wort loses some of its volatiles during long-term storage due to their evaporation or decomposition. One of the degradation products could be 2-methyloctane. Its amount in St. John's wort collected in 2020 is 3 times higher than in 2021. In addition, twice as much caryophyllene oxide was found in St. John's wort collected in 2020. It is likely to occur by oxidising β-caryophyllene [20, 21].

Investigation of St. John's wort infused oil

Since St. John's wort has many healing properties, it is widely used to prepare tea. However, many active components of St. John's wort have low solubility in water. For example, the water solubility of β-caryophyllene is 0.05011 mg/l, of trans-β-farnesene is less than 1 mg/l [22]. On the other hand, many St. John's wort substances are highly soluble in oil (β-caryophyllene logP = 4.4; trans-β-farnesene logP = 6.2), so the concentrations of these substances in St. John's wort infused oils should be higher, thus the healing properties of

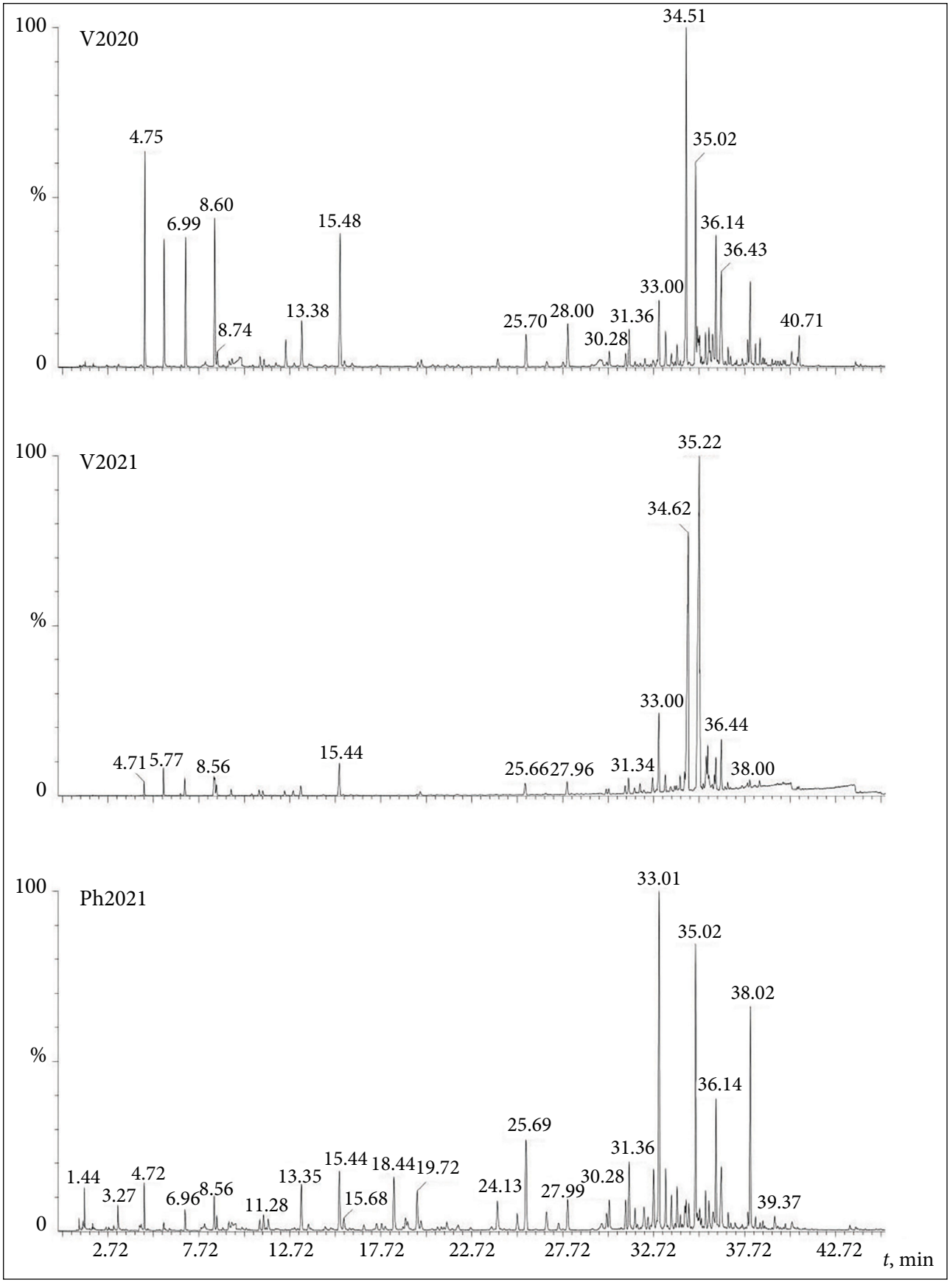

Fig. 1. SPME-GC-MS chromatograms of dry St. John's wort from local pharmacy (Ph2021) and collected in the Varėna district in 2020 (V2020) and in 2021 (V2021). For SPME-GC-MS conditions see Experimental

Table 1. **Peak areas of volatile components of St. John's wort obtained by SPME-GC-MS**

t, min	Compound	Peak area, μV × s		
		Ph2021	V2020	V2021
4.72	Octane, 2-methyl-	13793808	78196480	25722832
5.79	Nonane	2963939	52962040	61973936
6.96	1R-α-Pinene	8519788	59185956	43759196
8.56	Nonane, 3-methyl-	13677417	78984800	99312040
11.06	Benzene, 1-methyl-4-(1-methylethyl)-	5304678	6530708	16640626
13.38	Decane, 2-methyl-	24163620	31747152	35639460
15.48	Undecane	35180448	93893424	132094824
19.95	3-Cyclohexen-1-ol, 4-methyl-1-(1-methylethyl)-, (R)-	6940057	5675219	19040878
27.99	Dodecane, 2-methyl-	19314802	33462004	59760888
31.36	Copaene	32512292	22638276	55441948
33.01	β-Caryophyllene	165329984	39134476	267377440
33.38	Germacrene D	25099268	18744368	53274524
34.00	α-Himachalene	17812962	12702846	19468352
34.18	α-Caryophyllene	4605849	2739668	35446436
34.49	(Z)-β-Farnesene	9563962	178198592	1,355E+09
35.02	γ-Muurolene	116872376	106950080	2,034E+09
36.14	γ-Cadinene	48874332	62038748	85751576
36.44	δ-Cadinene	37930064	75312488	161773968
38.02	Caryophyllene oxide	85794856	46147668	23018402
38.57	Veridiflorol	2132986	13389116	22308678

the infused oils should be stronger. Additionally, β-caryophyllene is known to have antioxidant properties, so it is likely that St. John's wort-enriched oil oxidises more slowly.

St. John's wort infused sunflower oil was chosen for the study.

Determination of β-caryophyllene in infused oil by SHS-GC

SHS-GC method is cheap, fast, fully automated and thus is promissing for the determination of β-caryophyllene in complex matrices such as oils. When performing SHS-GC, it is important that the amount of analyte in the gas phase is as high as possible. This can be achieved by heating the sample. On the other hand, at high temperature, the analyte can decompose. A solution of β-caryophyllene in coconut oil was used to determine the highest temperature at which β-caryophyllene is still stable. Coconut oil was chosen because it does not oxidise or form volatile by-products when heated to 180°C.

A solution of β-caryophyllene in coconut oil (10 mg/g) was heated for 5 min in a microwave reactor at a temperature of 80–180°C. Further, 1 g of the heated solution was taken for SHS-GC analysis. The headspace vial was heated for 10 min at 80°C temperature. The obtained results showed (Fig. 2) that when the temperature exceeded 120°C β-caryophyllene started to decompose. Moreover, it is interesting to note that when β-caryophyllene was heated at 180°C, its content was significantly reduced (Fig. 3). Therefore, in order to maintain the valuable properties of β-caryophyllene, St. John's wort infused oil should not be heated above 120°C temperature.

Based on these results, a headspace vial heating temperature of 120°C was selected and the influence of the heating time on the amount of β-caryophyllene in the headspace was investigated. For that, a headspace vial was heated at 120°C temperature for 3–30 min. It was found that 10 min is enough to achieve equilibrium of the analyte between the solution and the gas phase. Previous studies have

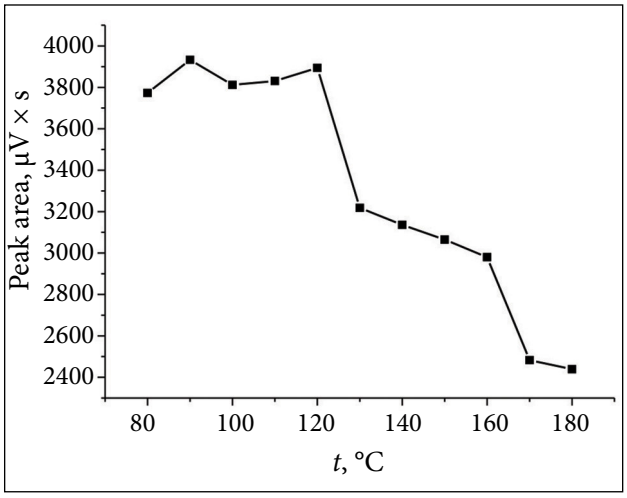

Fig. 2. Heating temperature influence on the β-caryophyllene peak area. Solution of β-caryophyllene in coconut oil (10 mg/g) heated for 5 min and analysed by SHS-GC

shown [23] that the peak area of β-caryophyllene changes little when the sample content varies from 1 up to 5 g, so 1 g of solution was taken for analysis.

Quality parameters were determined under the optimised conditions. The calibration curve was drawn with 6 calibration points with three replicate injections and was linear in the concentration range of 0.1–10 mg/g of β-caryophyllene with the correlation coefficient 0.995. The limit of detection was calculated as three times the baseline noise and was 30 μg/g. The relative standard deviation was determined by five replication analysis of the sample with the β-caryophyllene concentration 1 mg/g and was 7.4%.

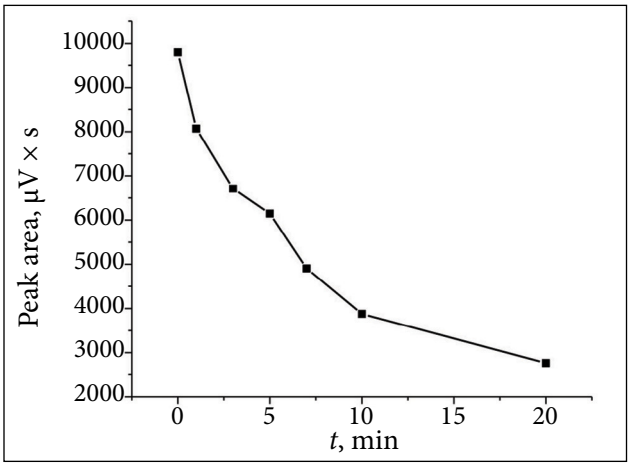

Fig. 3. Heating time influence on the β-caryophyllene peak area. Solution of β-caryophyllene in coconut oil (10 mg/g) heated at 180°C and analysed by SHS-GC

The prepared HSH-GC technique was attempted for the determination of β-caryophyllene in St. John's wort infused sunflower oil. Unfortunately, the β-caryophyllene peak was not seen in the chromatogram because of the high detection limit.

Determination of β-caryophyllene in infused oil by SPME-GC-MS

In order to reduce a detection limit of β-caryophyllene, a preconcentration by SPME was introduced. Moreover, gas chromatographic analysis was accomplished using mass spectrometric detection in the SIR mode.

For SPME of β-caryophyllene, 1 g of β-caryophyllene solution in coconut oil was placed into a 20 ml volume vial and sealed with a silicone rubber septa. The septa was pearsed with a SPME needle, the SPME fibre was exposed to the headspace of the solution and the extraction was carried out at 80°C temperature using 200 rpm stirring rate. As it was demonstrated above, β-caryophyllene starts to decompose when the temperature exceeds 120°C. However, for simplicity the heating of the vial was carried out in a water termostate that did not allow to reach 120°C heating temperature. The SPME extraction time was examined and it was found that after 20 min the peak area of β-caryophyllene became stable. Thus 20 min were stabilised as an optimum SPME time. The desorption was carried out in a GC injection port at 250°C for 30 s.

The calibration curve was drawn with 6 calibration points with three replicate injections. In order to improve sensitivity and reduce interferences, the peak areas of β-caryophyllene were recorded using the SIR mode (m/z 93 and 133). The calibration curve was linear in a concentration range of 0.017–100 mg/kg of β-caryophyllene with the correlation coefficient 0.999. The limit of detection was calculated as three times the baseline noise and was 5 μg/kg. The relative standard deviation was determined by five replication analysis of the sample with the β-caryophyllene concentration 10 mg/kg and was 6.1%.

The method was applied for the determination of β-caryophyllene in St. John's wort infused oil. It was determined that after 30 days infusion sunflower oil contained 35 μg/kg of β-caryophyllene and after 130 days infusion 109 μg/kg of β-caryophyllene.

Effect of heating on the composition of volatile components of St. John's wort infused oil

It was studied how heating affects St. John's wort infused sunflower oil and sunflower oil that does not contain St. John's wort. The oils were heated in a microwave reactor for 10 min at 180°C temperature and analysed by SPME-GC-MS in the full scan mode. Peak areas of volatile components of the oils are presented in Table 2, the chromatograms of unheated and heated St. John's wort infused sunflower oil are presented in Fig. 4.

As can be seen from the results presented in Table 2, after heating, large amounts of 2-propenal, 2-hexenal, 1-hexene, 4,5-dimethyl-, 1-octen-3-ol and

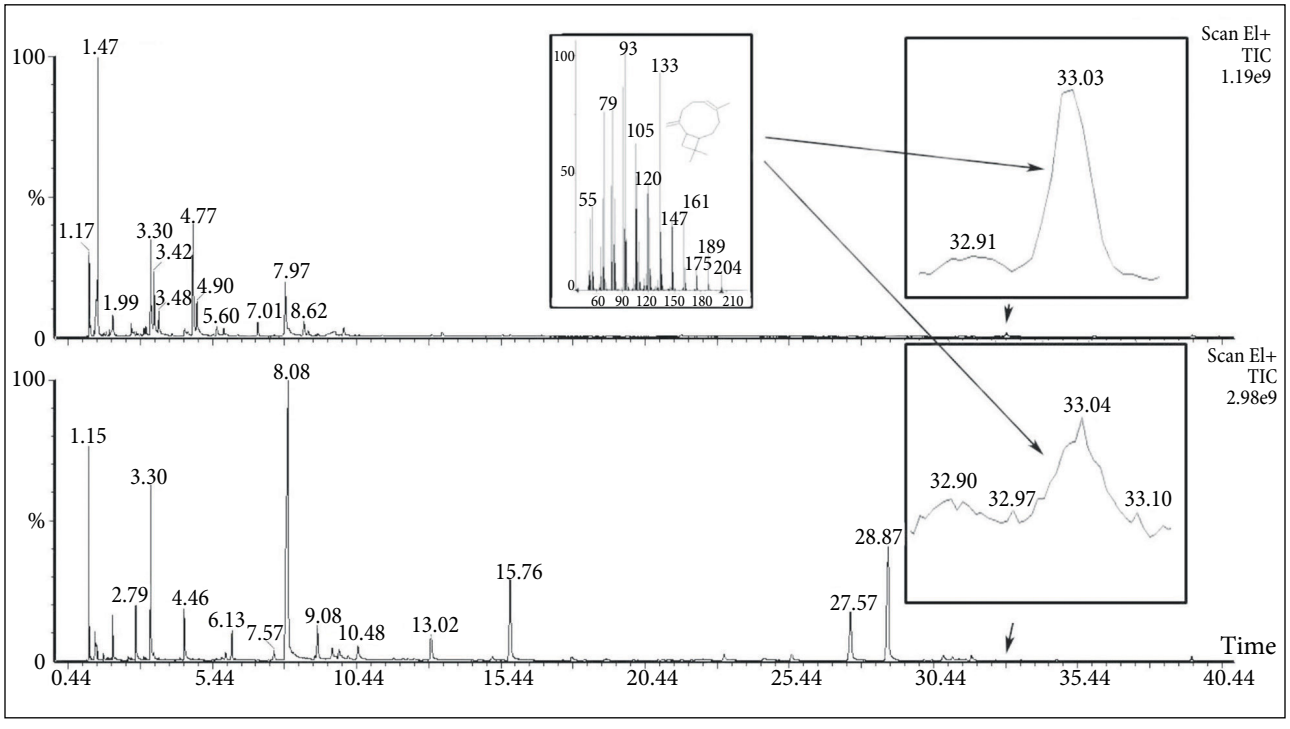

Fig. 4. SPME-GC-MS chromatograms of unheated (A) and heated (B) St. John's wort infused sunflower oil. For SPME-GC-MS conditions see Experimental

Table 2. **Peak areas of volatile components of sunflower oil and St. John's wort infused sunflower oil obtained by SPME-GC-MS**

t, min	Compound	Sunflower oil		St. John's wort infused sunflower oil	
		Unheated	Heated	Unheated	Heated
1.15	2-Propenal		32722918		33721656
1.47	3-Buten-2-ol, 2-methyl-			33185216	
1.97	Pentanal	1449532	11669884	4395838	12442286
2.77	1-Pentanol	–	19065942		19600372
3.29	Heksan	8886842	51645152	14665977	53906256
3.39	2-Octene	4379666		10786154	
4.45	2-Hexenal	–	24155194		24654786
4.77	Octane, 2-methyl			18930994	
4.86	Benzene, 1,3-dimethyl	23811238		7531230	
5.56	p-Xylene	7492343		2311124	
5.83	Nonane			1679372	
5.87	Heptanal	–	4818342	788752	3880153
6.11	1-Hexene, 4,5-dimethyl-		15858377		12694090

Table 2. **(Continued)**

t, min	Compound	Sunflower oil		St. John's wort infused sunflower oil	
		Unheated	Heated	Unheated	Heated
7.01	1R-α-Pinene			3042768	
8.05	2-Heptenal	5235565	186128112	15478443	260782960
9.06	1-Octen-3-ol		19193404		20033742
9.96	Decane	2389230		2326215	
13.00	2-Octenal	356410	14399541	475888	22503450
13.42	Decane,2-methyl-			1219417	
15.51	Undecane			506771	
15.75	Nonanal	607649	59229988	691009	72347416
21.69	Dodecane	631069		620804	
28.83	2,4-Decadienal		52287068		106233616
32.60	Tetradecane	28736194		2820554	
33.04	β-Caryophyllene			514766	
38.02	Caryophyllene oxide			46699	
39.38	Decanoic acid decyl ester		5995346		2277649

2,4-decadienal were formed. These substances were not detected in the unheated oil. Also, in the heated oil, quantities of hexanal, heptanal, 2-heptenal, 2-octenal and nonanal significantly increased. Interestingly, heating increases the amount of hexanal in pure sunflower oil by 5.8 times, and in St. John's wort-infused oil only by 3.6 times. Hexanal is a marker of lipid oxidation degree as it is the main secondary oxidation product of linoleic acid which is one of the principle fatty acids of many edible oils [24]. Therefore, it can be concluded that St. John's wort slowed down the oxidation of sunflower oil. The amount of β-caryophyllene decreased in the heated St. John's wort oil, with the peak area of β-caryophyllene before heating being 504979 and after heating being 166240. It is likely that β-caryophyllene was converted to caryophyllene oxide by temperature exposure. Before heating the caryophyllene oxide peak area was 46699, after heating it was 57412.

CONCLUSIONS

β-Caryophyllene is one of its main active components of St. John's wort, which is one of the best-known medicinal herbs with various healing properties. Many of the active components of St. John's wort are poorly soluble in water but exhibit a high hydrofobicity. Thus, the concentrations of these substances in St. John's wort infused oils should be higher, and the medical properties of infused oils should be stronger than in herbal tee.

In this work, two gas chromatographic techniques, SHS-GC and SPME-GC-MS, were proposed for the determination of β-caryophyllene in St. John's wort infused oils. A comparison of these two techniques revealed that SPME-GC-MS can be successfully applied to the analysis of edible oil. The other method, SHS-GC, is simple and fast, but because of its high detection limit, it can only be applied to oil samples with β-caryophyllene concentration higher than 0.1 mg/g.

St. John's wort has been shown to partially inhibit the oxidation of sunflower oil. In addition, heating at 180°C has been shown to reduce the amount of many active components in St. John's wort infused sunflower oil.

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DUJŲ CHROMATOGRAFIJOS METODAI β-KARIOFILENUI NUSTATYTI JONAŽOLIŲ EKSTRAKTUOSE ALIEJUJE

S a n t r a u k a

Hipericum Perforatum L., paprastai žinomas kaip jonažolė, yra plačiai naudojamas vaistinis augalas. Jonažolės ekstraktai aliejuose dažniausiai naudojami išoriškai, bet gali būti geriami sergant skrandžio opalige, vartojami kaip maisto papildas. Todėl svarbu sukurti metodus, leidžiančius greitai ir patikimai aliejuose nustatyti β-kariofileną, kuris yra vienas pagrindinių aktyvių jonažolės komponentų.

Šiame darbe, siekiant nustatyti β-kariofileną jonažolių aliejuje, ištirtos dvi dujų chromatografijos technikos – statinė viršerdvės dujų chromatografija (SHS-GC) ir kietafazė mikroekstrakcija, sujungta su dujų chromatografija-masių spektrometrija (SPME-GC-MS). Palyginus šiuos du metodus paaiškėjo, kad jonažolių ekstraktų aliejuose analizei galima sėkmingai pritaikyti SPME-GC-MS. Kitas metodas, SHS-GC, yra paprastas ir greitas, tačiau dėl aukštos aptikimo ribos jis gali būti taikomas tik aliejaus mėginiams, kuriuose β-kariofileno koncentracija yra didesnė nei 0,1 mg/g.