COMPARISON OF AERIAL PARTS ESSENTIAL OILS OF PURPLE AND WHITE FLOWERED *Vitex agnus-castus* (LAMIACEAE) POPULATIONS

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Essential oils obtained by hydrodistillation of purple and white flowered *Vitex agnus-castus* (Lamiaceae) from Hatay (Türkiye), were analyzed by GC/MS. The total ratio of 53 components in *Vitex agnus-castus* volatile components with purple flowers is 99.87%. This ratio is seen as 43 components and 98.86% in white-flowered *Vitex agnus-castus*. Eucalyptol, sabinene, α-pinene, α-terpinyl acetate and trans-caryophyllene were identified as the main components of the essential oils of *Vitex agnus-castus* with purple and white flowers. In the essential oils of purple flowering *Vitex agnus-castus*, the highest component was determined as eucalyptol with a rate of 15.41%, followed by nerolidol with 12.76%, caryophyllene oxide with 12.43% and sabinene with 9.4%. When the essential oils of white-flowered *Vitex agnus-castus* were examined, the rate of eucalyptol was determined as 21.62%. Sabinene ratio was determined as 17.6%, followed by 10.76% α-pinene and 5.69% α-terpinyl acetate, respectively.

Keywords: essential oil, GC-MS, *Vitex agnus-castus*

INTRODUCTION

Vitex agnus-castus, the fruits of which are used for gynecological disorders such as menstrual pain, irregularity and premenstrual symptoms (pms), especially proven pharmacological activity against premenstrual mastalgia (mastodynia) (Jarry *et al.*, 1991; Wuttke *et al*., 1997; Jarry *et al*., 1999) is a widely used medicinal plant. While it was in the Verbenaceae family in the past, it has been included in the Lamiaceae family as a result of molecular analyzes in recent years (Güner *et al*., 2012).

There are purple-flowered (fig. 1) or white-flowered populations of the plant. White-flowered populations have occasionally been evaluated as varieties or forms, in separate taxonomic categories, such as: *Vitex agnus-castus* var. *alba* Weston, *Vitex agnus-castus* f. *albiflora* Moldenke (IPNI, 2022; WFO, 2022). Today, these populations are considered as intraspecific variation and do not need to be evaluated in a separate taxonomic category (WFO, 2022). However, there are studies showing that populations with different flower colors have different compositions of fruit essential oils, and populations with white flowers have higher monoterpene content (Sanatore *et al.*, 2003). 1,8-cineole and sabinene are the main monoterpene compounds and beta-caryophyllene is the main sesquiterpene compound of the fruit essential oils and sabinene, 1,8-cineole, trans-beta-farnesene, α-pinene, trans-β-caryophyllene and limonene are the main compounds of the leave essential oils of *Vitex agnus-castus* (Sanatore *et al.*, 2003; Stojković *et al.*, 2011; Khalilzadeh *et al.*, 2015). Studies on the essential oils of the plant are generally about fruit essential oils, as its fruits are used more for medicinal purposes. However, aerial parts in and around Hatay are also widely used for medicinal purposes such as menstrual pains, depilatory-weakening the hair, and care is taken for flower color in these uses, and it is stated that purple-flowered plants are more effective (Guzel *et al.*, 2015). Although there is a study comparing fruit essential oils of populations with different colors, there is no study comparing aerial parts.

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Therefore, the aim of this study was to determine and compare the essential oil compositions of *Vitex agnus-castus* populations with white and purple flowers.

Figure 1. Aerial parts of the *Vitex agnus-castus*

EXPERIMENTAL

Plant Material

The plant materials were collected from their natural habitats and identified by Yelda Güzel. Purple flowering plants from Serinyol-Yıldırım Valley-Hatay-Türkiye, white-flowered plants from Harbiye-Döver Valey-Hatay-Türkiye. Vouchers from the plants numbered Y. Güzel-3137 and Y. Güzel-3138 were stored in the herbarium of the Hatay Mustafa Kemal University, Biology Department.

Essential Oil Isolation

The essential oil was obtained from dried leaves. A total of 50 g of the ground plant samples was used for hydrodistillation experiment. A sample weight was individually and carefully placed into a 2000 mL flask. Distilled water was added until it covered the sample completely. Essential oils were obtained by hydrodistillation method which was carried out in an all-glass Clevenger-type distillation. The essential oil ratio was calculated according to dry weight of plant materials and amount of essential oils obtained. The obtained essential oil samples were dried over anhydrous sodium sulfate and stored in amber vials at +4 .

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GC-MS Analysis of the Essential Oils

Analysis of the essential oil was carried out using a Thermo Scientific Focus gas chromatograph equipped with MS, auto sampler, and TR-5MS (5% phenyl polysilphenylene-siloxane, 0.25 mm i.d. x 60 m length, film thickness 0.25 µm). The carrier gas was helium (99.9%) at a flow rate of 1 mL/min; ionization energy 70 eV. Mass range m/z 50–650 amu. Data acquired at scan mode. MS transfer line temperature 250°C; MS ionization source temperature 220°C, injection port temperature 220°C. The samples were injected with a 250 split ratio. The injection volume was 1 µL. Oven temperature was programmed from 50°C to 220°C at 3°C/min. The structure of each compound was identified by comparison of their mass spectrum with the Wiley Registry, 9th edition. Data acquisition used the Xcalibur software program.

RESULTS AND DISCUSSION

When the essential oil contents obtained from the purple flowering *Vitex agnus* plant were examined, the main components were determined as eucalyptol, nerolidol, caryophyllene oxide and sabinene, respectively. The highest component was determined as eucalyptol with a rate of 15.41%, followed by nerolidol with 12.76%, caryophyllene oxide with 12.43% and sabinene with 9.4%. In the essential oil components of *Vitex agnus-castus* with white flowers, the main components were determined as eucalyptol, sabinene, α-pinene and α-terpinyl acetate. When the components were examined, the rate of eucalyptol was determined as 21.62%. Sabinene ratio was determined as 17.6%, followed by 10.76% α-pinene and 5.69% α-terpinyl acetate, respectively. In previous study, showing that populations with different flower colors have different compositions of fruit essential oils, and populations with white flowers have higher monoterpene content (Sanatore *et al*., 2003). 1,8-cineole and sabinene are the main monoterpene compounds and β-caryophyllene is the main sesquiterpene compound of the fruit essential oils and sabinene, 1,8-cineole, trans-β-farnesene, α-pinene, trans-β-caryophyllene and limonene are the main compounds of the leave essential oils of *Vitex agnus-castus* (Sanatore *et al.*, 2003; Stojković *et al.*, 2011; Khalilzadeh *et al.*, 2015).

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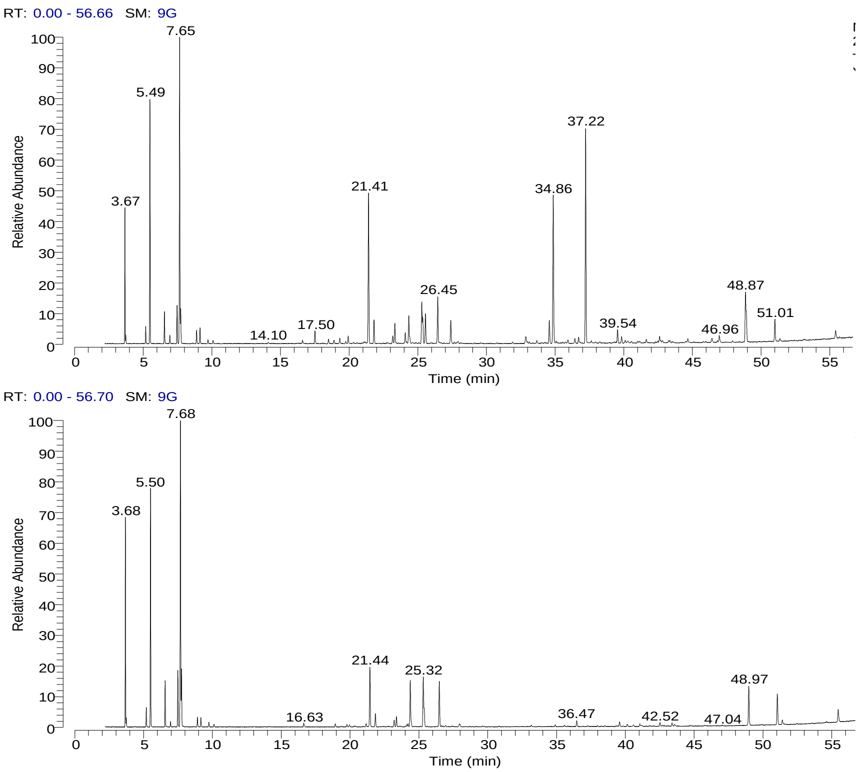

Figure 2. Essential oil chromatograms obtained from purple (above) and white (below) flowered *Vitex agnus-castus*

Table 1. Comparison of essential oil components of purple and white flowered *Vitex agnus-castus*

RT	Compound Name	Purple	White
3.67	α-pinene	4.58	10.76
5.18	β-pinene	0.71	1.19
5.49	Sabinene	9.4	17.6
6.55	Myrcene	1.37	2.95
6.94	2-carene	0.38	0.38
7.47	Limonene	1.71	3.87
7.65	Eucalyptol	15.41	21.62
8.89	γ-terpinene	0.64	0.74
9.14	trans-β-Ocimene	0.73	0.69
9.72	m-cymene	0.23	0.38
10.09	α-terpinolene	0.2	0.23
16.61	cis-sabinene hydrate	0.21	0.48
18.5	β-bourbonene	0.28	nd
18.89	α-Gurjunene	0.22	0.3

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RT	Compound Name	Purple	White
19.75	trans-sabinene hydrate	0.15	0.23
19.93	Linalool	0.45	0.22
21.16	α-bergamotene	nd	0.34
21.41	trans-caryophyllene	9.28	5.62
21.81	Terpinen-4-ol	1.43	1.22
23.17	Alloaromadendrene	0.48	0.66
23.33	Pulegone	1.26	0.94
24.08	Humulene	0.68	0.18
24.21	Citronellyl acetate		0.25
24.34	trans-β-farnesene	1.83	4.34
25.29	α-terpinyl acetate	2.39	5.69
25.35	α-terpineol	1.28	nd
25.56	Germacrene D	2.21	nd
26.45	Bicyclogermacrene	2.88	4.32
27.4	σ-Cadinene	1.54	nd
27.43	α-Copaene	nd	0.12
27.94	Citronellol	0.19	nd
27.95	β-famesene	nd	0.39
33.17	Palustrol	nd	0.18
33.66	Veridiflorol	0.21	nd
34.86	Caryophyllene oxide	12.43	0.46
35.07	exo-2-Hydroxycineole acetate;	0.13	nd
36.43	Ledol	0.35	0.81
36.71	1,2-dimethylcyclooctene	0.38	nd
37.22	Nerolidol	12.76	nd
37.64	Cubenol	0.14	nd
39.33	Tetrahydro-Ionone	nd	0.11
39.54	Spathulenol	0.87	0.6
39.84	Nerolidol-epoxyacetate	0.46	nd
40.11	Lanceol	0.19	nd
40.31	Ledene oxide	0.17	nd
41.01	α-cadinol	0.15	0.34
41.16	Alloaromadendrenoxide	0.14	nd
41.2	Ethyl linoleate	nd	0.15
41.64	Cedrenol	0.28	nd
42.61	Carvacrol	0.46	nd
42.82	Globulol	0.15	0.47
48.97	β-methylionone	4.68	3.85
51	Sclareol	1.47	3.58
55.43	Thunbergol	0.6	1.36

nd: not detected

CONCLUSIONS

In this study, it is seen that the essential oil components of purple and white flowered *Vitex agnus castus* are similar. However, although the components are similar, there are

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great differences in the ratios of the components. This study is a pioneer in terms of breeding *Vitex agnus-castus* for producers, whichever component is needed.

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