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Essential Oil Composition of Three *Centaurea* Species from Turkey: *Centaurea aggregata* Fisch. & Mey. ex. DC. subsp. *aggregata*, *C. balsamita* Lam. and *C. behen* L.

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Abstract: The essential oils of *Centaurea aggregata* subsp. a*ggregata*, *C. balsamita* and *C. behen* collected in the same habitat from Turkey, have been investigated. A total of 26, 54 and 26 components were identified in *C. aggregata* subsp. *aggregata*, *C. balsamita* and *C. behen*, respectively. The main constituents of the investigated populations of the three taxa have been revealed as follows: *Centaurea aggregata* subsp. *aggregata:* hexadecanoic acid (35.8%), phytol (7.2%), caryophyllene oxide(6.0%), spathulenol (6.0%); *C. balsamita*: hexadecanoic acid (23.0%), spathulenol (8.9%), germacrene D (2.1%); *C. behen*: hexadecanoic acid (32.7%), germacrene D (14.8%), and phytol (12.3%).

Keywords: *Centaurea aggregata* subsp. *aggregata; Centaurea balsamita*; *Centaurea behen*; Asteraceae; essential oil.

1. Plant Source

Centaurea genus is represented with 192 taxa in Turkey, 114 of which are endemic [1-3]. It is known as "peygamber çiçeği, zerdali dikeni, coban kaldiran, timur dikeni" in Turkey [3, 4]. Many species of the genus *Centaurea* have traditionally been used for their antirheumatic, diuretic, choleretic, stomachic, astringent, cytotoxic, antibacterial, antipyretic and tonic properties [4-6].

C.aggregata Fisch. & Mey. ex. DC. subsp. *aggregata* is a perennial plant, with erect, 30-75 cm tall stems and purple flowers. *C. balsamita* Lam. is an annual species, with yellow flowers and 30-120 cm tall stems. *C. behen* L. is a perennial plant with erect glabrous stem, yellow flowers [3]. The aerial

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parts of *Centaurea aggregata* subsp. *aggregata*, *C. balsamita* and *C. behen* were collected in July 2011 from Elazığ, Turkey. The plants were identified by Uğur Cakılcioglu. Voucher specimens (Numbers. 1458, 1467 and 1469 respectively) were deposited in the Herbarium of Faculty of Pharmacy, Department of Pharmacognosy, Ege University, Izmir, Turkey.

2. Previous Studies

Flavonoides, steroids, volatile constituents, sesquiterpene lactones and fatty acids have been previously isolated from this genus [7-11]. The essential oil composition of some *Centaurea* species from Turkey have been previously investigated [12-19]. In the earlier studies germacrene D, hexadecanoic acid, caryophyllene and caryophyllene oxide were reported to be the major components of the essential oils [13, 17-19].

To the best of our knowledge, the oils of *Centaurea behen* and *C. aggregata* subsp. *aggregata* have not been previously investigated.

3. Present Study

The aim of the present study was to determine the chemical composition of the essential oils of *Centaurea aggregata* subsp. *aggregata*, *C. balsamita* and *C. behen* growing wild in Elazığ, Turkey. The air-dried aerial parts of the plants were subjected to hydrodistillation for 3 h using a Clevenger-type apparatus to produce essential oils. The percentage yield (w/w) of essential oils were determined as 0.017%, 0.021% and 0.015% for *C. aggregata* subsp. *aggregata*, *C. balsamita* and *C. behen* respectively. The obtained yellow essential oils were stored at +4 ºC until the analysis.

The essential oil components were identified by comparison of Mass spectra with those in Wiley GC/MS Library, Adams Library, MassFinder Library and in Baser Library of Essential Oil Constituents which was built up by genuine compounds and components of known oils. Identification of the essential oil components were carried out by comparison of their relative retention times and their relative retention indices (RRI). Alkanes (C_9-C_{30}) were used as reference points for the calculation of relative retention indices. MS literature data was also used for the identification of compounds [22, 23].

The compositions of the essential oils of *Centaurea aggregata* subsp. *aggregata*, *C. balsamita* and *C. behen* were given in Table 1. A total of 26 compounds in *Centaurea aggregata* subsp. *aggregata*, (87.4% of oil), 54 compounds in *C. balsamita* (73.4% of oil), 26 compounds (96.3% of oil) in *C. behen* were identified and quantified. Hexadecanoic acid (35.8%), phytol (7.2%), spathulenol (6.0%), and caryophyllene oxide (6.0%) were identified as major components of the essential oil of *C. aggregata* subsp. *aggregata. C. balsamita* was characterized by its lower content of phytol (0.3%) and caryophyllene oxide (1.2%) than *C. aggregata* subsp. *aggregate*. *C. balsamita* was found to have high contents of hexadecanoic acid (23.0%) and spathulenol (8.9%). *C. behen* contained a similar content of hexadecanoic acid (32.7%) as observed in the other two *Centaurea* species. In addition, phytol (12.3%) was detected as the main component in *C. behen* essential oil. *C. behen* with producing high amount of germacrene D (14.8%) and low amount of spathulenol (0.6%) showed a little different chemical behavior from the other *Centaurea* species. The low volatile compounds were not detected. The difference in the percentages of identified components might be attributed to the distillation process which may not be suitable for volatile components sensitive to temperature. The difference of oil components among different *Centaurea* species were probably related to the different subspecies or to the geographical origin of plants. The data presented in this work differed from the G. Flamini *et al.* report about the essential oil composition of *C. balsamita* from the middle of Turkey (Konya region). Germacrene D (40.2%), bicyclogermacrene (7.1%) and spathulenol (2.2%) were reported to be the main constituents of *C. balsamita* [24]. Hexadecanoic acid (23.0%) and spathulenol (8.9%) were detected as the major components of the essential oil of *C. balsamita* whereas germacrene D (2.1%) were identidied in low percentages. These differences might be attributed to different collection times and geographic and climatic factors in Turkey.

Hexadecanoic (palmitic) acid, the most common saturated fatty acid found in animals, plants and microorganisms was known to raise plasma cholesterol concentrations and also dietary intakes of saturated fatty acids were shown to increase the risk of coronary heart disease [25]. Hexadecanoic acid was previously found as the major component of essential oils of *Centaurea aladagensis* [12], *C. luschaiana, C. tossiensis, C. wagenitzii* [14], *C. paphlagonica* [15], *C. saligna* [16], *C. iberica, C. hyalolepis* and *C. polyclada* [19] from Turkey. In the present work, hexadecanoic acid was also detected as the main component of three *Centaurea* species.

In conclusion, this is the first report on the essential oil composition of *C. aggregata* subsp. *aggregata* and *C. behen* from the southeast of Turkey (Elazığ region). The high hexadecanoic acid content might be explained about the collection time of plant materials at late flowering period. The plant materials with achenes inside the capitulum might have lead to high content of fatty acids in the essential oil [26, 27]. People should also be warned about the use of *Centaurea aggregata* subsp. *agregata*, *C. behen* and *C. balsamita* essential oils as the high content of hexadecanoic acid might cause serious cardiac problems.

Table 1. The composition of the essential oils of three *Centaurea* species.

RRI	Compound	A (%)	B (%)	C (%)	Identification
1300	Tridecane	-	-	0.8	t_R, MS
1400	Tetradecane	-	-	0.4	t_R, MS
1400	Nonanal	-	0.2	-	t_R, MS
1497	α-Copaene	-	0.2	-	MS
1500	Pentadecane	-	-	0.3	t_R, MS
1577	α-Cedrene	-	0.6	-	t_R, MS
1589	β-Ylangene	-	0.3	-	MS
1594	*trans*-β-Bergamotene	-	0.1	-	MS
1612	β-Caryophyllene	0.8	0.5	3.8	t_R, MS
1613	β-Cedrene	-	0.4	-	t_R, MS
1687	α-Humulene	-	0.3	0.8	t_R, MS
1693	β-Acoradiene	-	0.3	-	MS
1705	Zizanene	0.6	3.0	-	MS
1719	1-Heptadecene	-	0.5	-	MS
1726	Germacrene D	0.9	2.1	14.8	t_R, MS
1740	α-Muurolene	-	0.7	0.8	MS
1740	Valencene	-	0.3	-	MS
1755	Bicyclogermacrene	-	-	3.7	MS
1773	δ-Cadinene	-	-	1.2	MS
1786	*ar*-Curcumene	-	0.2	-	MS
1830	Tridecanal	-	0.6	-	t_R, MS
1838	(*E*)-β-Damascenone	-	0.2	-	MS
1849	Calamenene*	-	0.1	-	MS
1854	Germacrene-B	-	-	0.5	MS
1882	Aplotaxene	1.0	0.6	-	MS
1941	α-Calacorene	-	0.4	-	MS
1945	1,5-Epoxy-salvial(4)14-ene	1.0	1.0	0.4	MS
1958	(*E*)-β-Ionone	-	0.4	-	MS
2008	Caryophyllene oxide	6.0	1.2	3.2	t_R, MS
2037	Salvial-4(14)-en-1-one	1.8	0.7	-	MS
2041	Pentadecanal	0.9	-	0.1	t_R, MS
2050	(*E*)-Nerolidol	-	0.6	-	t_R, MS
2071	Humulene epoxide-II	1.2	0.5	-	MS
2080	Cubenol	-	0.3	-	MS
2081	1,10-*diepi*-Cubenol	-	1.0	-	MS
2104	Viridiflorol	-	0.9	-	MS
2130	Salviadienol	0.9	0.5	-	MS
2131	Hexahydrofarnesyl acetone	1.6	0.9	0.8	MS
2143	Rosifoliol	-	0.2	-	MS
2144	Spathulenol	6.0	8.9	0.6	MS
2170	β-Bisabolol	-	0.4	-	t_R, MS
2179	Nor-Copaonone	-	0.1	-	MS
2187	T-Cadinol	-	1.1	-	MS

2192	Nonanoic acid	-	0.5	-	t_R, MS
2200	3,4-dimetil-5-pentyl-5H-furan-2-one	-	0.3	-	MS
2209	T-Muurolol	-	2.2	-	MS
2219	δ-Cadinol	-	-	0.9	MS
2247	trans-α-Bergamotol	-	1.0	-	MS
2255	α-Cadinol	-	3.6	0.6	MS
2257	β-Eudesmol	4.5	-	-	t_R, MS
2267	Guaia-3,9-dien-11-ol	-	0.6	-	MS
2269	Guaia-6,10(14)-dien-4β-ol	1.3	-	-	MS
2278	Torilenol	2.2	1.3	-	MS
2300	Tricosane	1.5	1.1	0.7	t_R, MS
2324	Caryophylla-2(12),6(13)-dien-5α-ol	0.8	-	-	MS
2369	Eudesma-4(15),7-dien-4β-ol	1.9	1.8	-	MS
2392	Caryophylla-2(12),6-dien-5β-ol	1.4	-	-	MS
2500	Pentacosane	0.7	1.7	1.6	t_R, MS
2503	Dodecanoic acid	2.6	1.7	0.5	t_R, MS
2568	14-Hydroxy-α-muurolene	-	0.3	-	MS
2607	Octadecanol	-	-	2.0	t_R, MS
2622	Phytol	7.2	0.3	12.3	MS
2670	Tetradecanoic acid	1.9	1.2	2.5	t_R, MS
2700	Heptacosane	1.8	1.4	8.7	t_R, MS
2822	Pentadecanoic acid	1.1	-	-	t_R, MS
2900	Nonacosane	-	1.1	1.6	t_R, MS
2931	Hexadecanoic acid	35.8	23.0	32.7	t_R, MS
	Total	**87.4**	**73.4**	**96.3**	

A: The essential oil of *Centaurea aggregata* subsp. a*ggregata*
B: The essential oil of *C. balsamita*
C: The essential oil of *C. behen*
RRI:relative retention indices calculated against n-alkanes (C_9-C_{30}). Percentage calculated from FID data; tr:trace (<0.1%); t_R: identification based on the retention times of genuine compounds on the HP Innowax column; MS: tentatively identified on the basis of computer matching of the mass spectra with those of the Wiley and MassFinder libraries and comparison with literature data

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