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Essential Oils of Bidens tripartita L.

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Abstract

Essential oils were obtained from fresh aerial parts and air dried flower heads of *Bidens tripartita* L. (Asteraceae). Volatile constituents of the oils were analyzed by GC and GC/MS methods. The 77 components were identified representing 98.5% and 80.9% of the total components detected, respectively. The major constituents of the oil of flower heads were p-cymene (16.6%), β-caryophyllene oxide (6.0%) and humulene epoxide II (5.3%). The main constituents of the oil of fresh herb were allo-ocimene (38.3%), (Z)-β-ocimene (30.6%) and α-phellandrene (8.5%).

Key Word Index

Bidens tripartita, Asteraceae, essential oil composition, p-cymene, allo-ocimene, (Z)-β-ocimene.

Introduction

Bidens tripartita L. (Asteraceae) is a perennial, branched herb, which is widely distributed throughout most of Europe, except extreme north and extreme south of Europe. The plant is mainly found in waste, damp, wet places on lowland up to the lower mountains passage (1-3).

The herb of *B. tripartita*, commonly known as bur-marigold (4), is used in folk medicine as a diuretic, sudorific and an anti-inflammatory agent. It is also used in the treatment of skin diseases and as a stimulant of immunological system. It has been employed in treating fevers, gravel, stone and bladder and kidney troubles, and was considered also a good styptic and an excellent remedy for ruptured blood vessels and bleeding of every description. It is of benefit to consumptive patients (5,6). Previous chemical studies of bur-marigold herb proved the presence of flavones, flavanones, chalcones and aurones (7-11). *Bidens tripartita* has been reported to contain coumarins (12,13) and a volatile oil (8,11,12,14). Phytochemical investigations resulted in the identification of lower amounts of vitamin C (8), polysaccharides (9), carotenoids, γ-lactones, amines as well as mineral elements (12,15). The lipophilic fraction contains phosphatides, wax and glycerides (16). The green parts of *B. tripartita* afforded the identification of acetylenic compounds, linoleic acid and ocimene. The flower heads were reported to contain additionally thiophene and traces of cosmene and eugenol (17).

Experimental

Plant material used in this study was collected on August 2001 in Bielsk Podlaski area (Poland) and identified by J. Nazaruk. The voucher specimen was deposited in the Herbarium of Department of Pharmacognosy, Medical University of Białystok, Poland (No. BT97005).

The oil was hydrodistilled (3 h) from the freshly picked-up flowering aerial parts of the herb (500 g) using a Deryng-type apparatus, as described in the Polish Pharmacopoeia V (18). The oil has been obtained also from dried flowers heads (210 g) that were in a cool, airy place using the same distillation method. The amount of oil calculated for the fresh herb (BTH) was 0.12% (v/w) and 0.06% for the flower heads (BTF).

GC analysis of both oils was performed on a Carlo-Erba Instruments Chromatograph MEGA HRQC 5300 equipped with a flame-ionization detector FID, injector SSL using CP Sil 5-CB (Chrompack), (film thickness 0.25 μm) and Carbowax/BTR (Quadrex), (film thickness 0.5 μm) columns (30 m x 0.32 mm) and nitrogen as a carrier gas. The oven temperature was programmed from 50°-300°C (15 min isothermal), at 4°C/min. The injector and detector temperatures were 320°C and 310°C, respectively, and the flow rate of carrier gas (N_2) was 1 mL/min. GC/MS analysis was carried out using GC 8000 Fisons Instruments combined with an MD 800 mass spectrometer using CP Sil 5-CB (Chrompack). The conditions were as follows: temperature program 50°C (3 min isothermal) to 300°C (at 4°C/min). The flow-rate of the carrier gas (He) was 0.8 mL/min, the ion source temperature was 200°C and the electron impact energy was 70 eV.

The components of the oils were identified on the basis of the comparison of the retention times with reference compounds under the same conditions, retention indices of essential oils

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Table I. Chemical composition (%) of the essential oils of *Bidens tripartita*

Peak number	Compound	RI	Percentage BTH	Percentage BTF	Mode of identification
1	tricyclene	915	t	-	MS, RI
2	α-thujene	925	0.1	-	MS, RI
3	α-pinene	934	3.5	1.2	MS, RI
4	camphene	946	0.1	0.1	MS, RI
5	sabinene	964	0.2	t	MS, RI
6	β-pinene	966			
7	myrcene	985	0.5	0.5	MS, RI
8	α-phellandrene	1006	8.5	0.3	MS, RI
9	α-terpinene	1182 [1]	t	-	MS, RI
10	p-cymene	1020	5.2	16.6	MS, RI
11	limonene	1025 1208[1]	0.1[1]	1.3	MS, RI
12	β-phellandrene	1217 [1]	0.1[1]	-	MS, RI
13	(Z)-β-ocimene	1042	30.6	2.2	MS, RI
14	(E)-β-ocimene	1046	0.8	-	MS, RI
15	γ-terpinene	1053	0.2	-	MS, RI
16	*cis*-linalool oxide †	1059	-	0.5	MS, RI
17	*trans*-linalool oxide †	1076	-	0.4	MS, RI
18	terpinolene	1077	1.2	-	MS, RI
19	linalool	1090	0.4	3.1	MS, RI
20	α-campholenal	1101	-	0.2	MS, RI
21	perillene	1111	t	-	MS, RI
22	sabinol [2]	1136	-	0.3	MS, RI
23	allo-ocimene [2]	1138	38.3	-	MS
24	allo-ocimene [2]	1155	0.1	-	MS
25	terpinen-4-ol	1164	0.3	0.9	MS, RI
26	p-cymen-8-ol	1168	-	2.6	MS, RI
27	α-terpineol	1179	0.1	1.0	MS, RI
28	*trans*-p-mentha-1,8-dien-2-ol	1188	0.1	-	MS, RI
29	*cis*-p-mentha-1,8-dien-2-ol	1193	0.1	0,2	MS, RI
30	cumin aldehyde	1205	-	0.6	MS, RI
31	carvone	1217	-	0.8	MS, RI
32	piperitone	1225	-	0.2	MS, RI
33	(E)-anethole	1269	0.1	-	MS, RI
34	thymol	1293	-	1.4	MS, RI
35	β-elemene	1387	2.1	0.9	MS, RI
36	β-caryophyllene	1413	0.9	0.3	MS, RI
37	α-humulene	1447	1.0	0.5	MS, RI
38	germacrene D	1472	0.4	-	MS, RI
39	ar-curcumene	1477	-	1.1	MS, RI
40	β-selinene		0.1		
41	zingiberene	1483	0.3	-	MS, RI
42	valencene	1488	0.1	-	MS, RI
43	α-selinene	1492	0.1	0.6	MS, RI
44	β-bisabolene	1507	-	0.3	MS, RI
45	δ-cadinene	1513	t	-	MS, RI
46	(E)-nerolidol	1549	0.1	0.2	MS, RI
47	caryophyllene oxide	1568	t	6.0	MS, RI
48	clovenol [3]	1573	-	0.3	MS
49	salvial-4(14)-en-1-one (mintketone)	1578	-	0.1	MS, RI
50	humulene epoxide II	1586	0.4	5.3	MS, RI
51	dodecanoic acid	1600	-	0.3	MS
52	humulenol II	1615	-	1.5	MS, RI
53	caryophylladienol [4]	1618	-	0.4	MS
54	T-muurolol	1622	0.1	-	MS, RI
55	eugenyl butyrate	1632	0.1	2.3	MS
56	intermedeol	1639	0.1	-	MS, RI
57	sesquiterpene alcohol [3]	1692	t	1.7	MS, RI
58	sesquiterpene alcohol [3]	1695	-	1.8	MS
59	methyldibenzothiophene [2]	1716	t	-	MS
60	eugenyl valerate	1729	0.1	0.2	MS
61	eugenyl isovalerate	1745	-	0.1	MS
62	tetradecanoic acid	1758	-	1.0	MS

Table I. continued

Peak number	Compound	RI	Percentage BTH	Percentage BTF	Mode of identification
63	methyldibenzothiophene [2]	1777	1.9	1.1	MS
64	hexahydrofarnesyl acetone	1826	-	1.5	MS, RI
65	pentadecanoic acid	1853	-	0.2	MS
66	hexadecanoic acid	1978	-	9.8	MS
67	phytol [3]	2101	0.1	0.3	MS, RI
68	octadecanoic acid	2142	-	6.9	MS
69	tricosane	2296	t	0.2	MS, RI
70	tetracosane	2396	-	t	MS, RI
71	pentacosane	2494	t	0.5	MS, RI
72	hexacosane	2596	-	0.1	MS, RI
73	heptacosane	2698	t	0.7	MS, RI
74	octacosane	2797	-	t	MS, RI
75	nonacosane	2897	t	0.3	MS, RI
76	triacontaane	2996	-	t	MS, RI
77	hentriacontane	3095	-	t	MS, RI
	Total percentage			**98.5%**	**80.9%**

RI = retention indices; MS = mass spectral fragments; BTH = essential oil obtained from fresh plant material; BTF = essential oil obtained from dried flower heads; [1]results from Carbowax/BTR column; [2]correct isomer not identified; [3]tentatively identified compound; [4]tentatively identified, correct isomer of sesquiterpene alcohol not identified; [†]furanoid form; t = trace (< 0.1%); mass spectra of tentatively identified compounds: [m/z (rel.int.)]: clovenol RI = 1573, 41(100), 161(80), 44(74), 91(73), 67(49), 55(48), 77(45), 105(44), 79(43), 119(36), 220(3) [M+]; caryophylladienol RI = 1618, 41(100), 91(59), 79(56), 55(55), 136(51), 69(50), 43(43), 77(40), 56(39), 67(38), 220(1) [M+]; sesquiterpene alcohol RI = 1692, 93(100), 105(89), 91(89), 133(83), 107(68), 41(66), 131(56), 79(53), 77(50), 119(47), 220(19) [M+]; sesquiterpene alcohol RI = 1695, 41(100), 43(98), 79(87), 81(85), 67(77), 55(70), 91(70), 53(63), 93(57), 77(52), 220(13) [M+]; methyldibenzothiophene RI = 1716, 197(31), 165(30), 69(30), 152(17), 171(17), 199(16), 198(100) [M+]; methyldibenzothiophene RI = 1777, 197(35), 165(27), 171(16), 199(14), 153(10), 198(100) [M+]; phytol RI = 2101, 43(100), 71(86), 41(46), 55(46), 95(44), 68(40), 82(35), 123(28), 97(17), 111(10)

components with those from data bank and comparison of mass spectra published in computerized library spectrum NIST. The quantitative data obtained were from the electronic integration of FID area percents without the use of correction factors.

Results and Discussion

The quantitative and qualitative composition for both oils can be seen in Table I. The oil obtained from fresh plant (BTH) was limpid, pale yellow, lighter than water with an unpleasant odor. The amount of oil obtained for that sample of *B. tripartita* was 0.12% (v/w). As can be seen from Table I, 49 components were identified representing an average of 98.5% of the volatile fraction of fresh material. The major constituents of this oil were allo-ocimene (isomer I) (38.3%), (Z)-β-ocimene (30.6%), and α-phellandrene (8.5%), which constituted altogether about 77.4% of the oil.

The oil obtained from the dried flower heads (BTF) was limpid, yellow and lighter than water with a very unpleasant odor. The average yield was 0.06% (calculated per weight of dried plant material). Fifty-seven components that were identified in the oil represented 80.9% of that volatile fraction with the main compounds being p-cymene (16.6%), caryophyllene oxide (6.0%), humulene epoxide II (5.3%), which together constituted 27.9% of the oil. The content of hexadecanoic acid (9.8%) in the oil was noted.

Analysis of the oils showed that the main components might be classified in the following groups: monoterpene hydrocarbons and their oxidation products, sesquiterpene hydrocarbons, oxygenated derivatives of mono- and sesquiterpenes and their oxidation products, phenylpropane derivatives as well as derivatives of benzothiophene. A comparison between the oil from fresh plants and that from the flower heads of *B. tripartita* showed significant differences. The oil prepared from fresh plant material was characterized by a high content of monoterpene fraction (85.3%) with the monoterpene hydrocarbons such as allo-ocimene (isomer I) (38.3%), (Z)-β- ocimene (30.6%) and α-pinene (3.5%) dominating. Both allo-ocimene isomers are unstable compounds and they undergo chemical decomposition during storage of the oil. Among other compounds of the fresh herb oil, a phenylpropane derivatives (5.6% mainly p-cymene), sesquiterpene hydrocarbons (5.7% mainly, β-elemene, α-humulene, β-caryophyllene) and benzothiophene derivatives (1.9% mainly methyldibenzothiophene - unknown position of methyl group) were found. On the other hand, oxygenated derivatives of monoterpenes and sesquiterpenes appeared to be present only in small amounts.

The composition of the oil obtained from air-dried flower heads of *B. tripartita* was more complex. Phenylpropanes derivatives and sesquiterpenes with their oxydation products constituted 23.2% of the whole oil with major constituents such as p-cymene (16.6%), p-cymen-8-ol (2.6%), eugenyl butyrate (2.3%), thymol (1.4%) and from the sesquiterpene fraction caryophyllene oxide (6.0%), humulene epoxide II (5.3%) were noted. In addition, studies proved the occurrence of fatty acids such as palmitic acid (9.8%) and myristic acid (1.0%).

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