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Chemical composition of volatile oil of *Thymus vulgaris* L. from Western Ghats of India

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Abstract

The aerial parts of *Thymus vulgaris* collected from Western Ghats of India were analysed for essential oil by Gas Chromatography. Forty eight compounds were detected among which 36 compounds, which constituted 98.63% of the oil were identified, with thymol (61.6%), p-cymene (11.2%), ϒ-terpinene (7.4%), methyl thymol (3.9%), methyl carvacrol (3.3%) and β-caryophyllene (2.3%) as major chemical constituents.

Keywords: essential oil composition, *Thymus vulgaris*

Thymus vulgaris L. (Labiate) is cultivated for its essential oil. Many chemo-variants (Granger & Passet 1973; Piccaglia & Marotti 1993) and phytochemical investigations (Mohammad *et al*. 2002) have been reported on the species. Geraniol, linalool, α-terpineol, carvacrol, thymol, 1, 8-cineole and trans-thuyanol-4 along with terpenine-4-ol are the major components of each chemo-type. Schwarz *et al*. (1996) discussed the strong antioxidant activity of p-cymene-2, 3-diol (2, 3-dihydroxy-4-isopropyl-1-methyl-benzene), a phenolic compound isolated from the hexane extract of thyme, which was greater than those of α-tocopherol and butylated hydroxyanisole. Generally thymol and carvacrol along with linalool are the important chemical principles of this herb. Not much work was carried out on the chemical profile of the essential oil of the species available in India, the cultivation of which is restricted to few regions of south India. During our survey in search of potential essential oil bearing aromatic plants in Western Ghats, we have collected the plant from a wild source in Nilgiri Hills. The essential oil obtained by hydro distillation of the aerial parts of the plant and studied for detailed chemical investigation, using Gas Chromatography (GC) and Gas Chromatography/Mass Spectroscopy (GC-MS), is presented in this paper.

The aerial parts of *T. vulgaris* were collected during April 2005 from Nilgiri Hills. A voucher specimen was deposited at the herbarium at Central Institute of Medicinal and Aromatic Plants (CIMAP), Resource Centre, Bangalore. Aerial parts collected were hydro distilled using Clevenger type apparatus for 5 h to obtain the essential oil (0.3 % v/w). The oil sample after drying over anhydrous Na_2SO_4 was stored at 4°C till the sample was subjected for GC and GC-MS analysis. GC analysis of the essential oil sample was done on a Varian CP-3800 gas

Table 1. Chemical composition of *Thymus vulgaris* oil

S. No	Compound	Composition (%)	Kovat Index (obtained)	Kovat Index (lit. value)	Method of identification
1	α-Thujene	0.37	926	931	a,b
2	α-Pinene	0.26	935	942	a,b,c
3	Camphene	0.05	948	954	a,b
4	Sabinene	0.66	964	976	a,b
5	β-Pinene	0.1	974	981	a,b,c
6	Octen-3-ol	0.06	980	983	a,b
7	Myrcene	0.89	983	986	a,b
8	α-Phellandrene	0.1	997	1002	a,b
9	δ-Carene	0.05	1006	1009	a,b
10	α-Terpinene	0.83	1010	1016	a,b
11	p-Cymene	11.28	1014	1020	a,b,c
12	Limonene + 1,8-cineole	0.4	1023	1025	a,b
13	ϒ-Terpinene	7.47	1053	1056	a,b
14	E-Sabinene hydrate	0.24	1057	1060	a,b
15	Terpinolene	0.07	1081	1074	a,b
16	Linalool	0.59	1084	1092	a,b,c
17	Camphor	0.07	1127	1136	a,b,c
18	Isoborneol	0.1	1154	1157	a,b,c
19	Borneol	0.25	1163	1164	a,b,c
20	Cymen-8-ol	0.49	1166	1167	a,b,c
21	Terpinene-4-ol	0.15	1177	1175	a,b
22	α-Terpineol	0.06	1184	1185	a,b
23	Methyl thymol	3.96	1215	1221	a,b
24	Methyl carvacrol	3.35	1227	1226	a,b
25	Thymol	61.63	1272	1287	a,b,c
26	Carvacrol	0.93	1277	1297	a,b,c
27	Thymol acetate	0.08	1331	1329	a,b
28	β-Caryophyllene	2.31	1428	1427	a,b,c
29	Germacrene D	0.17	1479	1480	a,b
30	α-Humulene	0.09	1461	1465	a,b
31	α-Muurolene	0.23	1500	1496	a,b
32	ϒ-Cadinene	0.08	1521	1518	a,b
33	δ-Cadinene	0.76	1536	1524	a,b
34	Caryophyllene oxide	0.28	1577	1576	a,b
35	β-Eudesmol	0.16	1624	1635	a,b,c
36	α-Cadinol	0.06	1646	1643	a,b
	Total % of compounds identified	98.63			

a=Retention index in comparison with literature value; b=Mass spectra; c=Co-injection with authentic sample

chromatograph equipped with two Flame Ionization Detectors and split/split less capillary injectors and Star workstation software. 100% Dimethylpolysiloxane column (CP-Sil 5 CB 50 m x 0.32 mm I.D., film thickness 0.25µm of Chrom Pack and CP-Wax 52 CB column (60 m x 0.25 mm I.D., film thickness 0.25µm) were used with nitrogen as carrier gas with a pressure of 16 and 17 psi, respectively. The sample (0.2 µl) was injected in split mode (split ratio 1:100). The column was initially held at 60°C for 5 min., then heated to 220°C at 5°C per min., held for 3 min. and to 250°C at 5°C per min., held for 4 min. Injector and detector temperatures were kept at 250°C and 300°C, respectively.

The GC-MS analysis was carried out on a Perkin-Elmer Turbomass Auto XL Instrument at 70eV fitted with column (5% phenyl 95%, dimethylpolysiloxane) of 50 m x 0.32 mm with a film thickness of 0.33 µm. Oven temperature was programmed from 100–280°C at 3°C min^{-1} with initial hold of 2 min. Helium was used as the carrier gas at 10 psi. Injector and detector temperatures were kept at 220°C and 300°C, respectively.

The compounds were identified by comparison of the retention indices of the peaks on non polar and polar columns with literature values (Jennings & Shibamot 1989; Davies 1990; Adams 1995), computer matching against library spectra built up using pure substances and components of known essential oil, and finally confirmed by comparison of the mass spectra of peaks with published data. Relative amounts of individual components are based on peaks obtained without FID response factor correction. The Kovat indices were obtained from the gas chromatograms by comparing with the natural homologous series of hydrocarbons. The identity was further confirmed by matching their mass spectra with those recorded in Wiley and NIST library search.

The aerial parts of the *T. vulgaris* on hydro distillation gave an essential oil yield of 0.3% on fresh weight basis and exhibited 48 peaks on GC analysis. Thirty-six peaks accounting for 98.6% of the oil were identified and listed along with respective concentration of each component and Kovat indices are indicated in Table 1 in the order of their elution on 100% dimethylpolysiloxane column. Monoterpenes, sesquiterpenes, aromatic compounds, alcohols and ester compounds were present in the oil. Hydroxylated compounds were the dominant aroma principles in this oil. Thymol (61.63%) was the major compound, which is the potential principle of *T. vulgaris* in agreement with earlier reports. Earlier reports indicate thymol (9.6% – 78.2%), carvacrol (0.2% – 71.6%), p-cymene (2.4 – 46.4%), -terpinene (2.2% – 22.8%) as major components (Lawrence 2003, 2004). Methyl thymol and methyl carvacrol were reported in the essential oils by few authors (Pino *et al*. 1997; Asllani & Toska 2003; Mirza & Bahr 2003). Recently Bahman *et al*. (2005) reported 74.7% of thymol along with 3.6% of methyl carvacrol from *T. daenensis* subsp. *daenensis*. The oil in the present investigation showed thymol (61.63%) and its biosynthetic precursor p-cymene (11.28%), γ-terpinene (7.47%), methyl thymol (3.96%), methyl carvacrol (3.35%) and β-caryophyllene (2.31%), which constitute 89.4% of total essential oil with less carvacrol (0.93%). The total phenolic contents in the present oil account for 69% of the total oil. The composition and contents in the thyme oil available in Western Ghats is comparable with the oils available in the international trade. The higher content of thymol is a good source for flavour industry and also for further value addition. It can be concluded that the thyme can be cultivated in India and is a potential source of thymol as well as its essential oil.

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