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Comparative terpenoid composition of the leaf and root essential oil of *Tithonia diversifolia* (Hemsl.) A. Gray

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Abstract
The terpenoid composition of *Tithonia diversifolia* (Hemsl.) A. Gray leaf and root collected from Nainital, Uttarakhand (India) was determined with the help of GC and GC-MS. A total of 34 compounds were identified, accounting 93.6 % and 92.2 % of the leaf and root oil, respectively, showed the qualitative and quantitative terpenoid diversity in their volatile constituents. The leaf oil of *Tithionia diversifolia* was characterized by the presence of *α*-pinene as a major constituent followed by the presence of *β*-pinene, germacrene D, *δ*-cadinene and *β*-cubebene. On the other hand, the root oil showed the presence of thymol, *α*-bisabolol, carvacrol and *β*-eudesmol as major constituents.

Keywords: *Tithonia diversifolia*, Asteraceae, *α*-pinene and thymol

1. Introduction
Tithonia diversifolia (Hemsl.) A. Gray is a 2.5-5 m tall shrub or undershrub and belongs to the family Asteraceae with subterranean stolons, stem brown to green, round, glabrous to villous. Leaves alternate, deltoids, 3-5 lobed accuminate with attenuate base, serrate on margins, shortly hairy above. It is very common in ravine slopes and marshy wastelands [1]. It is widely used in folk medicine in the treatment of various diseases, it is commonly known as Mexican sunflower, shrub sunflower or Japanese sunflower [2].
Previously the volatile constituents obtained by hydrodistillation was found to contain *α*-pinene *β*-caryophyllene, germacrene D, *β*-pinene and 1,8-cineole in its leaf oil while germacrene D, *β*-caryophyllene and bicyclogermacrene were characterized in flower oil [3]. Another report on the leaf oil of this species revealed the presence of α-pinene, *(Z)-β*-ocimene and limonene as major constituents [4]. Ethnobotanical studies have shown that extracts from the plant exhibited antidiarrhoeic, antiinflammatory, antibacterial, antimalaria, antiproliferation properties and its effectiveness in the treatment of wounds had been shown as well [5-9]. The leaf extract is reported to contain sequiterpene lactones taginin C as an active component against *Plasmodium* [9]. Three new sesquiterpenoids along with eight known sequiterpene lactones, were isolated for their potentials as cancer chemopreventive agents [10]. Sesquiterpene lactones were also reported from the leaf extract of *T. diversifolia* which showed inhibitory effects on germination of reddish, cucumber and onion seeds [11-13]. The decoction of a leaf of *Tithonia diversifolia* in Thailand is used for stomach pain, the decoction is drunk or leaves are heated and placed on stomach [6]. In Kenya it is also used orally to treat gastrointestinal problems [14]. In Thailand the decoction of dried leaf and stem is used orally by adults to treat hepatitis and for diabetes [8, 15-17]. The hot water extract of dried aerial parts in Guatemala and that of the entire plant in Mexico is used for malaria [11]. Apart from all these uses, in Rodrigues Islands the decoction of flowers is used for skin eczemas [18]. To best of our knowledge, there is no report on the essential oil composition of the roots of *Tithonia diversifolia*, so in this present investigation first time there is a comparison of the tepenoid constituents of leaf and root essential oil of *Tithonia diversifolia*.

2. Material and Methods
2.1 Plant material
The fresh aerial part of *Tithonia diversifolia* was collected from Nainital, Uttarakhand, Plant herbaria were identified from the Botanical Survey of India, Dehradun (Acc. No. 113564) and voucher specimen were deposited in the Phytochemistry laboratory, Chemistry Department, Kumaun University, Nainital.

2.2 Extraction of the oil

The fresh plant material (2 kg) was subjected to steam distillation. The distillates were extracted with *n*-hexane and dichloromethane. The organic phase was dried over anhydrous Na_2SO_4 and the solvent was distilled off. The major compounds were isolated by fractionation of the essential oil on silica gel CC (230-400 mesh, Merck, 600 × 25 cm column) packed with hexane, using Et_2O-hexane as mobile phase with gradually increasing concentration of ether (2-10%).

2.3 GC and GC-MS analysis

The oil was analyzed by using Nucon 5765 gas chromatograph equipped with Rtx-5 non-polar fused silica capillary column (30 m × 0.32 mm, 0.25 µm film coating). The oven temperature (60-210 ºC) was programmed at 3 ºC min^{-1} using N_2 as carrier gas at 4 Kg cm^{-2}. The injector temperature was 210 ºC, detector temperature 210 ºC and the injection volume 0.5 mL, using a 10% solution of the oil in *n*-hexane. GC-MS was conducted on a ThermoQuest Trace GC 2000 interfaced with a Finnigan MAT PolarisQ ion trap mass spectrometer equipped with Rtx-5 non-polar fused silica capillary column (30 m × 0.25 mm, 0.25 µm film coating). The oven temperature (60-210 ºC) was programmed at 3 ºC min^{-1} using helium as carrier gas at 1.0 min^{-1}. The injection, ion source and MS transfer line temperatures were 210 ºC, 220 ºC and 275 ºC, respectively, the injection volume was 0.1 mL, and the split ratio was 1:40. MS were taken at 70 eV with mass range of 40-450 amu.

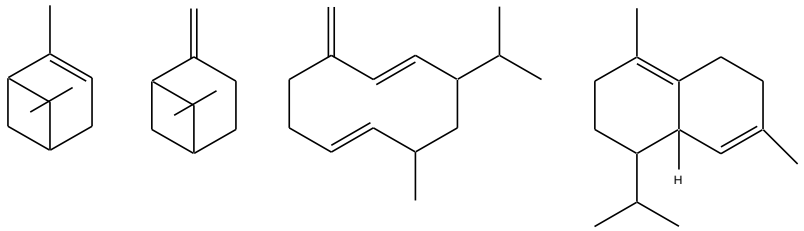
2.4 Identification of constituents

Characterization of constituents was done on the basis of Linear Retention Index (LRI, determined with reference to homologous series of *n*-alkanes C_9-C_{24}) under identical experimental condition, co-injection with available compounds, MS Library search (NIST and WILLEY) and by comparing with the MS literature data [16]. The relative contents of individual components were calculated GC response on FID without using correction factor.

Table 1: Volatile constituents of *Tithonia diversifolia* (Hemsl.) Grey

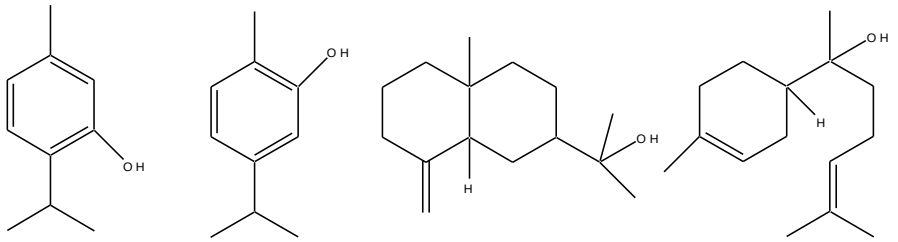
S. No.	Compounds	LRI	%FID Leaf oil	%FID Root oil	Mode of identification
1.	*α*-thujene	933	2.1	1.2	a,b
2.	*α*-pinene	941	33.6	5.1	a,b
3.	sabinene	978	0.2	0.4	a,b
4.	*β*- pinene	982	8.6	2.6	a,b
5.	*α*-phellandrene	1009	1.2	-	a,b
6.	*α*-terpinene	1019	1.9	-	a,b
7.	*p*-cymene	1029	1.3	1.2	a,b
8.	*β*- phellandrene	1032	0.9	t	a,b
9.	limonene	1033	1.9	1.5	a,b
10.	*(Z)- β*-ocimene	1042	0.2	0.5	a,b
11.	*(E)- β*-ocimene	1051	0.1	2.3	a,b
12.	borneol	1167	0.9	-	a,b
13.	terpinen- 4-ol	1180	0.2	0.4	a,b
14.	bornyl acetate	1285	1.3	0.6	a,b
15.	thymol	1288	0.3	20.6	a,b
16.	carvacrol	1296	t	10.8	a,b
17.	*δ*- elemene	1339	0.4	8.5	a,b
18.	*α*- longipinene	1350	1.3	t	a,b
19.	*α*- cubebene	1357	t	t	a,b
20.	*α*-copaene	1378	2.5	t	a,b
21.	*β*-maaliene	1384	2.6	t	a,b
22.	*β*-cubebene	1390	4.2	t	a,b
23.	*β*-cedrene	1410	t	t	a,b
24.	*β*-caryophyllene	1418	t	t	a,b
25.	*α*-humulene	1454	3.6	t	a,b
26.	*ϒ*-murrolene	1475	0.9	t	a,b
27.	germacrene D	1480	8.1	5.5	a,b,c
28.	valencene	1494	2.5	t	a,b
29.	*δ*-cadinene	1524	5.1	t	a,b,c
30.	*β*-bisabolene	1535	1.2	t	a,b
31.	caryophyllene oxide	1584	1.3	3.6	a,b
32.	cubenol	1647	2.9	5.2	a,b
33.	*β*-eudesmol	1651	2.3	10.8	a,b
34.	*α*-bisabolol	1685	t	11.4	a,b,c
Total identified			93.6 %	92.2 %	
Monoterpene hydrocarbons			52.0 %	14.8 %	
Oxygenated monoterpenes			2.7 %	32.4 %	
Sesquiterpene hydrocarbons			32.4 %	14.0 %	
Oxygenated sesquiterpene			6.5%	31.0 %	

*a= Linear Retention Index (LRI), b=MS (GC-MS), c=NMR (^1H & ^{13}C), t = trace, less than 0.1%



α-pinene *β*-pinene germacrene D *δ*-cadinene

Fig 1: Major constituents of the leaf essential oil of *Tithonia diversifolia*



thymol carvacrol *β*-eudesmol *α*-bisabolol

Fig 2: Major constituents of the root essential oil of *Tithonia diversifolia*

3. Result and discussion

Literature search revealed *α*-pinene, *β*-caryophyllene, germacrene D, *β*-pinene and 1, 8-cineole as constituents of the leaves of *Tithonia diversifolia* while germacrene D, *β*-caryophyllene and bicyclogermacrene characterized in flower oil [3]. Another reports on the leaf oil of this species revealed the presence of α-pinene, *(Z)-β*-ocimene and limonene as major constituents [4]. The fresh leaves and roots of of *Tithonia diversifolia* was collected from Nainital. Their volatile constituents were obtained by steam distillation. The identified constituents are listed in Table 1. A total of 34 compounds were identified, accounting 93.6 % and 92.2 % of the leaf and root oil respectively. The leaf oil of *Tithionia diversifolia* was characterized by the presence of *α*-pinene (33.6 %) as a major constituent followed by the presence of *β*-pinene (8.6 %), germacrene D (8.1 %), *δ*-cadinene (5.1 %) and *β*-cubebene (4.2 %). On the other hand, the root oil showed the presence of thymol (20.6 %), *α*-bisabolol (11.4 %), carvacrol (10.8 %) and *β*-eudesmol (10.8 %) as major constituents. It is interesting to note that thymol, *α*-bisabolol and carvacrol are the major constituents of the root oil while these are present in a trace amount in its leaf oil. The *β*-eudesmol also showed the major presence 10.8 % in root oil while in leaf oil it only constitutes 2.3 %. *α*-Bisabolol is a biologically active ingredient for use in high value and expensive cosmetics. The action of *α*-bisabolol in the skin is very well known. The most important effects of *α*-bisabolol are anti-inflammatory, anti-bacterial, anti-mycotic, anti-phlogistic and non-allergic [21]. Therefore, the root oil of *Tithonia diversifolia* can be used in the perfumery and pharmaceutical industry because of *α*-bisabolol content in it. The total monoterpene hydrocarbons account for leaf oil is 52.0 % while only 14.8 % in root oil. The root oil was found to be rich in oxygenated monoterpenes accounting 32.4 % as compared to 2.7 % in the leaf oil. The oxygenated sesquiterpene also showed the remarkable presence (31.0 %) in root oil as compared to 6.5 % in leaf oil. So, based on these results it was concluded that the leaf oil of *Tithonia diversifolia* is rich in monoterpene and sesquiterpene hydrocarbons while the root oil was found to rich in oxygenated monoterpenes and sesquiterpene compounds and has commercial potential because of the presence of *α*-bisabolol. This is the first report on the essential oil composition of the roots of *Tithonia diversifolia*.

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