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The essential oil of *Tagetes erecta* L. occurring in Iran

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ABSTRACT: Hydro-distilled volatile oils from the leaves and stems and the flowers of *Tagetes erecta* L. were analyzed by a combination of GC and GC/MS. Thirty-three components in leaf and stem oil and 34 components in flower oil were identified. The main characterized constituents were β-caryophyllene (8.5 and 35.2%), terpinolene (18.4 and 6.3%), (E)-ocimenone (12.6 and 9.8%), (Z)-β-ocimene (10.4 and 13.7%), piperitenone (10.4 and 2.6%), (Z)-ocimenone (5.5 and 7.7%) and limonene (6.2 and 2.5%) in leaf and stem and flower oils respectively.

KEY WORDS: *Tagetes erecta* L.; Compositae; essential oil composition; β-caryophyllene; terpinolene; (E)-ocimenone; (Z)-β-ocimene; piperitenone; (Z)-ocimenone; limonene

Introduction

The genus *Tagetes*, with the common name of marigold, presents 30–40 species that are endemic from Arizona to Argentina.[1,2] Some of the *Tagetes* species are cultivated in Iran as ornamental. *T. erecta*, with beautiful yellow flowers, is one of these cultivated ornamental species.

The oils of *T. erecta* and *T. patula* were found to contain limonene, α-terpinolene, piperitone and caryophyllene components.[3] Analysis of composition of volatile flower oil of yellow *T. erecta* in Yanbian region by GC/MS showed *trans*-caryophyllene (33.18%), β-cubebene, limonene (4.81%), and α-terpinolene (4.44%) to the main components.[4]

The larvicidal effects of essential oil from the leaves of *T. erecta* and some other plants had been evaluated against *Anopheles stephensi*, *Culex quinquefasciatus* and *Ades aegypti*. *T. erecta* oil was found to be the most effective at lower concentration.[5]

In this research chemical composition of the flower oil and also stem and leaf oil of *T. erecta*, cultivated in Iran, were investigated.

Experimental

Plant material

The aerial parts of *Tagetes erecta*, cultivated in National Botanical Garden of Iran (Tehran), were collected, at full flowering stage, in July–August 2001. The voucher specimen has been deposited in the Herbarium of the Research Institute of Forests and Rangelands (TARI).

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Isolation procedure

Dried plant materials (80–100 g flower, 90–100 g leaves and stems, three times) were subjected individually to hydro-distillation for 4 h using a Clevenger-type apparatus to produce oils at 0.37% (w/w for leaves and stems) and 0.35% (w/w for flowers) yield.

The oils were dried over anhydrous sodium sulfate and stored in sealed vials at low temperature before analysis.

Gas chromatography

GC analyses were performed using a Shimadzu GC-9A gas chromatograph equipped with a DB-1 fused silica column (60 m × 0.25 mm i.d., film thickness 0.25 μm).

Oven temperature was held at 40 °C for 5 min and then programmed to 280 °C at a rate of 4 °C/min; injector and detector (FID) temperature was 290 °C; carrier gas, helium with a linear velocity of 32 cm/s.

Percentages of components were calculated by electronic integration of FID peak areas without the use of response factor correction.

Gas chromatography–mass spectrometry (GC-MS)

GC-MS analyses were carried out on a Varian 3400 GC-MS system equipped with a DB-1 fused silica column (60 m × 0.25 mm i.d.). Oven temperature was 40–250 °C at a rate of 4 °C; transfer line temperature was 260 °C; carrier gas was helium with a linear velocity of 31.5 cm/s; split ratio was 1/60; ionization energy was 70 eV; scan time was 1 s ; mass range was 40–300 amu.

Identification of components

The components of the oils were identified by comparison of their mass spectra with those of a computer library or with authentic compounds and confirmed by comparison of their retention indices either with those of authentic compounds or with data published in the literature.[6,7]

Results and Discussion

The oils isolated by hydro-distillation from the flowers and leaves and stems of *T. erecta* were found to be yellow liquids and obtained in yields of 0.35 and 0.37% (w/w) based on dry weight, respectively. The constituents were identified by matching their mass spectra and retention indices with those recorded in the SATURN Data system and literature.

Thirty-three components in leaf and stem oil and 34 components in flower oil were identified. The main characterized constituents were β-caryophyllene (8.5 and 35.2%), terpinolene (18.4 and 6.3%), (E)-ocimenone (12.6 and 9.8%), (Z)-β-ocimene (10.4 and 13.7%), piperitenone (10.4 and 2.6%), (Z)-ocimenone (5.5 and 7.7%) and limonene (6.2 and 2.5%) in leaf and stem and flower oils respectively.

The chemical composition of the oils of *T. erecta* can be seen in Table 1. The components are listed in order of their elution on the DB-1 column. Comparing the composition of *T. erecta* leaf and stem oil with flower oil showed some similarities and differences. While the main component of the flower oil was β-caryophyllene, the major compound of stem and leaf oil was terpinolene. The percentages of other major components in both oils were also different. In addition, some components like *p*-cymene-8-ol, terpinen-4-ol, α-terpineole and verbenone were found only in stem and leaf oil and some components

Table 1. Percentage composition of the essential oil of *Tagetes erecta*

Compound	Retention index	Leaves and stems (%)	Flowers (%)	Method of identification
α-Thujene	937	—	t	MS, RI
α-Pinene	942	0.3	t	MS, RI, CoI
Camphene	953	t	t	MS, RI
Sabinene	972	0.5	0.3	MS, RI, CoI
β-Pinene	976	t	t	MS, RI
Myrcene	987	0.1	0.2	MS, RI, CoI
α-Phellandrene	999	0.3	t	MS, RI, CoI
α-Terpinene	1011	t	t	MS, RI
p-Cymene	1014	t	t	MS, RI
Limonene	1022	6.2	2.5	MS, RI, CoI
(Z)-β-Ocimene	1028	10.4	13.7	MS, RI, CoI
(E)-β-Ocimene	1038	0.9	1.7	MS, RI, CoI
γ-Terpinene	1049	t	t	MS, RI
Terpinolene	1078	18.4	6.3	MS, RI, CoI
Linalool	1081	0.3	1.2	MS, RI, CoI
Fenchol	1109	2.6	1.9	MS, RI, CoI
t-Menth-2-en-1-ol	1114	0.4	0.4	MS, RI
Terpinen-1-ol	1119	1.7	2.4	MS, RI
(E)-Tagetone	1122	2.2	1.3	MS, RI
(Z)-Tagetone	1127	3.7	1.5	MS, RI
p-Cymene-8-ol	1153	0.6	—	MS, RI
Terpinen-4-ol	1157	0.2	—	MS, RI
α-Terpineole	1166	0.3	—	MS, RI
Verbenone	1183	0.2	—	MS, RI
(Z)-Ocimenone	1203	5.5	7.7	MS, RI
(E)-Ocimenone	1211	12.6	9.8	MS, RI, CoI
Piperitone	1222	4.2	0.6	MS, RI, CoI
Lavandulyl acetate	1272	0.2	—	MS, RI
Piperitenone	1305	10.4	2.6	MS, RI, CoI
β-Bourbonene	1381	—	0.2	MS, RI, CoI
β-Caryophyllene	1419	8.5	35.2	MS, RI, CoI
(Z)-β-farnesene	1441	1.2	0.4	MS, RI, CoI
α-Humulene	1448	—	0.7	MS, RI, CoI
Germacrene D	1473	3.0	4.1	MS, RI
Bicyclogermacrene	1488	1.6	2.1	MS, RI
δ-Cadinene	1511	—	0.2	MS, RI
Spathulenol	1561	—	0.3	MS, RI
Caryophyllene oxide	1567	0.2	1.2	MS, RI
T-Muurolol	1633	—	0.3	MS, RI

RI, retention indices in elution order from DB-1 column; MS = mass spectroscopy; CoI = co-injection; t = less than 0.05%.

like β-bourbonene, α-humulene, δ-cadinene, spathulenol and T-muurolol were found only in flower oil.

Comparing these results with those obtained from results in other countries,[3,4] some compounds like piperitenone and ocimenone were found in the Iranian sample at relatively high percentages.

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