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# Identification of Non-Polar Chemical Compounds *Acroptilon repens* Growing in Iran by GC-MS

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**Abstract:** The aerial part of the plant *Acroptilonrepens* belongs to the family Asteraceae were collected on June 2012 from Pnu university of Bojnourd (North Khorasan Province of Iran) the essential oils of the plant were isolated by solvent extraction (solvent : n-hexane). Accounting for 94% of the total oil. The oil of *Acroptilonrepens* was characterized by Tetradecane(18.2%), Bis (2-ethylhexyl) phthalate (14.6%), Hexadecane (13.5%), 2,4-Bis (1,1-dimethylethyl) phenol (6.9%).

**Key words:** *Acropetilonrepens* · Medicinal Plant · Chemical Composition · Asteraceae · N-Hexane Extraction

## INTRODUCTION

Plants have always an important role to play in medicinal and public health. The knowledge on the use of medicinal plants was acquired by trial and error and handing on from generation to generation [1]. *Acroptilonrepens* (L.)DC. (Russian knapweed) belongs to the family Astraceae. This plants is herbaceous. The stem is numerous branched from the base, densely leafy. The leaf is numerous branched from the base, densely leafy. The leaf is rigid, heraseous membranose sessile with variable form, the flower is purple-pink capitalum. Fruit is achene the flowering period June-July [2]. Although some sources include this species in the genus *Centaurea,* molecular phylogeny results, the structure of the flower and the chromosome number support recognizing it as a separate genus. Only one species of this plant is known in Iran. This species has allelopathic effects. *A. repens* has been shown to produce phytotoxic compounds which may contribute to its competitive behavior. Studies of the extracts from root and callus tissue of *A. repens* have suggested the presence of plant growth inhibitors [3]. The genus *A. repens* have been the subject of several investigations, from which several sesquiterpene lactones and flavones with substantial toxicity have been isolated [4, 5]. The phytotoxin in the root exudates of *A. repens* was identified as 7,8-benzoflavone [6]. *A. repens* of is a medicinal plant with antipyretic properties. owing this character and the important of the allelopathic effects of this species and belief of its being toxic and causing chewing disease in horses Essential oils found in its aerial tissues have antimicrobial activity against gram-positive bacteria [7,8].Aerial tissues of *A. repens* possess aromatic amines and sterols [9]. Therefore we aimed to study its essential oil components.

**Plant Material:** The plant *Acroptilonrepens* were collected during flowering stage from the Bojnourd, Iran, in June. 2012, and identified at the Pnu university of Bojnourd, Iran. A voucher specimen has been deposited in the Environmenta Department of Bojnourd Herbarium (EDBH:00115)

**Isolation of Chemical Compounds:** *Acroptilonrepens* were air-dried for 4 days before isolation of essential oil. The plant material (100g) was cut into small pieces. The plant powdered was macerated in 95% pure n-hexane as a solvent for 48 hours, filtered through a Whatman

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Table 1: The percentage composition of the various oil components are listed in

| No. | Compound | Retention Index (RI[a]) | Percentage | Method of Identification |
|---|---|---|---|---|
| 1 | Hexanoicacid,ethyl ester | 953 | 0.4 | MS-GC |
| 2 | 2-ethyl hexanol | 1016 | 0.3 | MS-GC |
| 3 | 2-methyl decane | 1069 | 0.6 | MS-GC |
| 4 | 1,1,3-triethoxy-propane | 1194 | 0.9 | MS-GC |
| 5 | Octanoicacid,ethyl ester | 1173 | 3.5 | MS-GC |
| 6 | Dodecane | 1199 | 3.6 | MS-GC |
| 7 | 2-methyl naphthalene | 1289 | 0.3 | MS-GC |
| 8 | Tridecane | 1299 | 0.4 | MS-GC |
| 9 | Germacrene-D | 1325 | 0.6 | MS-GC |
| 10 | Tridecane,5-methyl | 1395 | 0.5 | MS-GC |
| 11 | 1-tetradecene | 1389 | 0.7 | MS-GC |
| 12 | Decanoicacid,ethyl ester | 1397 | 5.7 | MS-GC |
| 13 | Tetradecane | 1399 | 18.2 | MS-GC |
| 14 | Tridecane,3-methyl | 1410 | 0.9 | MS-GC |
| 15 | Pentadecane | 1500 | 1.3 | MS-GC |
| 16 | 2,4-Bis(1,1-dimethylethyl) phenol | 1520 | 6.9 | MS-GC |
| 17 | 5-methyl pentadecane | 1551 | 0.6 | MS-GC |
| 18 | 3-methyl pentadecane | 1570 | 0.9 | MS-GC |
| 19 | Caryophyllene oxide | 1583 | 0.6 | MS-GC |
| 20 | 1-hexadecene | 1593 | 0.6 | MS-GC |
| 21 | Hexadecane | 1600 | 13.5 | MS-GC |
| 22 | Heptadecane | 1700 | 0.3 | MS-GC |
| 23 | 3-methyl-heptadecane | 1770 | 0.5 | MS-GC |
| 24 | Octadecane | 1800 | 4.4 | MS-GC |
| 25 | 7,9-Di-tert-butyl-1-oxaspiro[4.5]deca-6,9-diene-2,8-dione | 1919 | 0.7 | MS-GC |
| 26 | Palmitic acid | 1956 | 1.6 | MS-GC |
| 27 | Dibutyl phthalate | 1961 | 0.5 | MS-GC |
| 28 | Hexadecanoicacid,ethyl ester | 1989 | 1.2 | MS-GC |
| 29 | Eicosane | 1995 | 1.2 | MS-GC |
| 30 | Phytol | 2110 | 0.9 | MS-GC |
| 31 | Linoleic acid | 2129 | 0.3 | MS-GC |
| 32 | Ethyl linoleolate | 2135 | 1.8 | MS-GC |
| 33 | Octadecanoicacid,ethyl ester | 2189 | 0.5 | MS-GC |
| 34 | Bis(2-ethylhexyl) phthalate | 2290 | 14.6 | MS-GC |
| 35 | *Gamma-sitosterol* | 2448 | 0.7 | MS-GC |
| 36 | Pentacosane | 2500 | 0.4 | MS-GC |
| 37 | Heptacosane | 2700 | 0.4 | MS-GC |
| 38 | Cyclotetracosane | 2892 | 1.2 | MS-GC |
| 39 | Alpha-tocopherol | 3111 | 1.8 | MS-GC |
| Total | 94 | | | |

a: Retention Indices on RTX-5MS

paper then evaporated off the solvent in vacuum by rotary evaporator (IKA, RV10) to yield light yellow oil and dried over by adding anhydrous $Na_2SO_4$. In absolute oil recovery, concentrated oil was dissolved in minimum volume of absolute alcohol to remove the natural fats and waxes present in the essential oil. It was kept in -14°C for 48 hours and then it was filtered through a filter paper. Alcohol was removed by distillation and traces of alcohol were removed by passing nitrogen gas through it [7].

**Gas Chromatography and Mass Spectrometry:** GC analysis of the oil from the aerial parts of the plant was performed using an Hewlett-Packard (HP) 6890A gas chromatograph equipped with flame ionization (FID) and a RTX-5MS (95% Diphenyl / 5% Dimethyl Polysiloxan) (15m×250µm.i.d., film thickness 0.25µm). The oven temperature was programmed 50-290°C at a rate of 5°C/mm; the carrier gas was helium with a flow rate of 1ml/min the sample was injected using the split sampling technique 1:10. The percentage composition of the oil was calculated automatically from peak areas without any correction. Retention indices (RI) compounds were determined by comparing to the retention times of a series of n-alkanes with linear interpolation. Identification of each component was confirmed by comparison of its retention index either with those of authentic compounds or with data in the literature [10, 11].

## RESULTS AND DISCUSSION

The average yield of chemical composition of the plant *Acroptilonrepens* was about 9.28%. Table 1 report the chemical composition of the phytochemical components under study. Fifty component were

identified, accounting for %94 of the total oil. The various compounds were identified by comparison of their Kovats retention indexes, determined utilizing a non-logarithmic scale on non-polar (Rtx-5MS) columns and by comparison of the mass spectra of each GC component with those of standards and with reported data (4). High resolution gas Chromatography-mass spectrometric (HP GC-MS) analysis and Kovats Index values showed that its principal components are the Tetradecane (18.2%), Bis (2-ethylhexyl) Phthalate (14.6%), Hexadecane (13.5%), 2,4-Bis(1,1-dimethylethyl) phenol (6.9%).

In previous works, ethanol extract of *A. repens* was isolated and purified by means of chromatography. These compounds were identified by their spectral data and 11 compounds were isolated and identified [12]. Volatile oil from the aerial parts of A.repens with steam distillation was investigated by GC and GC–MS. Twenty-two components, representing 99.7% of the oil, were identified [13]. A new sesquiterpene lactone-acroptilin-isolated from *A. repens* has been assigned to the sesquiterpene lactones of the guaiane or germacrane type [14]. Phytotoxic polyacetylenes from roots of Russian knapweed (*Acroptilon repens* (L.) DC.) were isolated [15].

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