Volatile compounds of essential oil *Centaurea behen* L. grown in Iran

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**ABSTRACT**

The essential oils from Compositae specie of Iran: *Centaurea behen* L. obtained by hydrodistillation was analyzed by GC and GC/MS. β-Caryooyllane (24.5%), β-selinene (13.9%) and valencene (11.7%) were the main components among the sixteen constituents characterized in the oil of *Centaurea behen* representing 93.7% of the total components detected.

**Keywords:** *Centaurea behen*; compositae; essential oil; composition; β-caryooyllane.

**INTRODUCTION**

Seventy-four species of the genus *Centaurea* are found in Iran, among which thirty-eight are endemic [1,2]. Previous chemical investigation on *Centaurea* species have shown the presence of flavonoids [3] sesquiterpene lactones specially guaianolides [4-6] and germacranolide types sesquiterpene lactones [3]. Sesquiterpene lactones have been reported to have multiple biological effects including cytotoxic antibacterial, anti-inflammatory, hypotensive and many others. Volatile constituents studies are available in the literature on *Centaurea* species: *C. thessala* subsp. drakiensis, *C. zuzcariniana*, *C. spruneri*, *C. raphanina* subsp. mixta, and *C. petia* [10, 11], *C. calcitrapa* and *C. solstitialis* [12-14], *C. calcitrapa*, *C. gloriosa*, and *C. moschata* [15-17], *C. pseudoscabiosa* subsp. pseudoscabiosa, and *C. hadimensis* [18], and *C. kotschyi* var. kotschyi and *C. kotschyi* var. decumbens [19]. Our study deals with the analysis of the volatile oil isolated from *Centaurea behen* L. growing wild in Iran.

**MATERIALS AND METHODS**

**Plant materials:** The aerial parts of *Centaurea behen* L., were collected in June 2009 from Givi, Khalkhal road (Ardabil province) in the northwest of Iran at an altitude of 1400 m. A voucher specimen (No: 1563) has been deposited at the Herbarium of the Agriculture Research Centre (A.R.C.) Ardabil, Iran.

**Extraction of the oils:** The air-dried aerial parts of *Centaurea behen* was separately subjected to hydrodistillation using a Clevenger-type apparatus for 4 h. After decanting and drying of the oils over anhydrous sodium sulfate, the corresponding oils were isolated in yield of 0.16% (w/w).

**Analysis:** GC analysis was performed on a Shimadzu 15A gas chromatography equipped with a split/ splitless injector (250°C) and a flame ionization detector (250°C). N2 was used as carrier gas (1 mL/min) and the capillary column used was DB-5 (50 m × 0.2 mm, film thickness 0.32 µm).

The column temperature was kept at 60°C for 3 min and then heated to 220°C with a 5°C/min rate and kept constant at 220°C for 5 min.

GC/MS analysis was performed using a Hewlett-Packard 5973 with a HP-5MS column (30 m × 0.25 mm, film thickness 0.25 µm). The column temperature was kept at 60°C for 3 min and programmed to 220°C at a rate of 5°C/min, and kept constant at 220°C for 3 min. The flow rate of Helium as carrier gas was (1 mL/min). MS were taken at 70 eV. Identification of the constituents of each oil was made by comparision of their mass spectra and retention indices (RI) with those given in the literature and those authentic samples [7]. Relative percentage amounts were calculated from peak area using a Shimadzu C-R4A chromatopac.
RESULTS

The essential oil, with yellow color, was obtained by hydrodistillation in a Clevenger-type apparatus from whole plant of *C. behen* with the yields of 0.16% (w/w) on dry weight. The essential oil of *C. behen* was analyzed by GC–MS with HP-5 column. The composition of the essential oils of *C. behen* was listed in Table I, in which the percentage and retention indices of components are given. As it is shown, about 93.7% (16 compounds) was identified. The oil of *Centaurea behen* consisted of five monoterpenes (7.8%), eleven sesquiterpene hydrocarbons (85.9%). Caryooyllane (24.5%), β-selinene (13.9%) and valencene (11.7%) were the major components in this oil, followed by δ-cadinene (8.7%), Epi-α-muurolene (7.6%), α-humulene (6.5%) and α-copane (4.0%).

Table 1. Chemical composition (%) of the essential oils of aerial part of *Centaurea behen* L.

<table>
<thead>
<tr>
<th>Compound</th>
<th>RI^6</th>
<th>%</th>
</tr>
</thead>
<tbody>
<tr>
<td>α-pinene</td>
<td>939</td>
<td>3.0</td>
</tr>
<tr>
<td>myrcene</td>
<td>928</td>
<td>2.8</td>
</tr>
<tr>
<td>trans-cymene</td>
<td>1026</td>
<td>1.0</td>
</tr>
<tr>
<td>α-terpinene</td>
<td>1063</td>
<td>0.7</td>
</tr>
<tr>
<td>(E)-β-ocimene</td>
<td>1067</td>
<td>0.3</td>
</tr>
<tr>
<td>α-copane</td>
<td>1376</td>
<td>6.2</td>
</tr>
<tr>
<td>β-bourbonene</td>
<td>1384</td>
<td>0.2</td>
</tr>
<tr>
<td>aromadendrene</td>
<td>1397</td>
<td>0.5</td>
</tr>
<tr>
<td>β-caryooyllane</td>
<td>1418</td>
<td>24.5</td>
</tr>
<tr>
<td>α-humulene</td>
<td>1452</td>
<td>6.5</td>
</tr>
<tr>
<td>Epi-α-muurolene</td>
<td>1641</td>
<td>7.6</td>
</tr>
<tr>
<td>β-selinene</td>
<td>1660</td>
<td>13.9</td>
</tr>
<tr>
<td>δ-cadinene</td>
<td>1664</td>
<td>8.7</td>
</tr>
<tr>
<td>Valencene</td>
<td>1670</td>
<td>12.5</td>
</tr>
<tr>
<td>selina,3,7(11)-diene</td>
<td>1680</td>
<td>5.0</td>
</tr>
<tr>
<td>β-selinene</td>
<td>1705</td>
<td>0.3</td>
</tr>
</tbody>
</table>

DISCUSSION

Piperitone (35.2%) and elemol (14.1%) were the main components among the twenty-six constituents characterized in the oil of *Centaurea behen* representing 90.5% of the total components detected [8]. The oil of *Centaurea depressa* consisted of four oxygenated monoterpenes (36.5%), six sesquiterpene hydrocarbons (5.9%), ten oxygenated sesquiterpenes (39.7%), five aliphatic hydrocarbons (4.4%) and one aliphatic acid (4.0%). Eighteen components were identified in the oil of *Centaurea solstitialis* representing 86.6% of the total oil with hexadecanoic acid (30.8%) and caryophyllene oxide (25.2%) as major constituents [9]. The oil of *C. solstitialis* consisted of eight monoterpenes (16.5%), nine sesquiterpenes (39.3%) and one aliphatic acid (30.8%). Hexadecanoic acid (plamitic acid) (30.8%) and caryophyllene oxide (25.2%) were the major compounds in this oil, followed by 1,8-cineole (9.6%) and β-caryophyllene (6.2%). Our results, comparing these results with our previous investigation on oils of the *Centaurea* genus, showed also dominated by sesquiterpenes. Piperitone (35.2%) and elemol (14.1%) were the main components among the twenty-six constituents characterized in the oil of *Centaurea depressa* representing 90.5% of the total components detected [8]. Mirza et al., (2003) reported that Iran collected in the Tehran province ((Bomehen) forms of *C. behen* contained twenty-one compounds and in this plant in other local in Iran were identified that constitute 91% of the oil. The main constituents of the essential oil were β-caryophyllene (40.3%), β-sesquiphellandrene (18.4%), and caryophene oxide (9.9%) (21). So, in research shown The structure of a guaianolide and lactones previously reported from this plant by Rustaiyan (4). Comparing samples of GC-MS spectra showed previous study reported only two major compound (β-caryophyllene and β-sesquiphellandrene), and in this study have less compounds with three major compounds (β-Caryooyllane, β-selinene and valencene). In this different results can be return to collected locals. So percentage monoterpenoids were more in previous study. That can be concluded that *C. behen* collected from Givi, Khalkhal road (Ardabil province) were mostly flowers in the Tehran province (Bomehen). The oil of *Centaurea depressa* consisted of four oxygenated monoterpenes (36.5%), six sesquiterpene hydrocarbons (5.9%), ten oxygenated sesquiterpenes (39.7%), five aliphatic hydrocarbons (4.4%) and one aliphatic acid (4.0%). Eighteen components were identified in the oil of *Centaurea solstitialis* representing
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REFERENCES