

## Chemical Composition of the Essential Oil of *Heracleum persicum* Seeds of Iran

AVAT (ARMAN) TAHERPOUR\*, MOSTAFA YOUSEFIRAD  
and RAMIN KARIMZADEH

Department of Chemistry, Graduate School, Islamic Azad University  
P.O. Box 38135-567, Arak Branch, Arak, Iran

E-mail: avatarman.taherpour@gmail.com; avat\_1@yahoo.co.uk

Volatile chemical constituents of the essential oil of *Heracleum persicum* seeds, which is growing wild in Ardebile, Iran were investigated by GC and GC/MS technique. 29 Compounds, representing 75 % of the total oil were identified and 12 unknown compounds detected. The main components are hexylbutyrate (37.7 %), hexylbutanoate (36.7 %), octylacetate (16.3 %), hexyl-2-methylbutanoate (5.7 %), hexylisobutyrate (4.7 %), hexylhexanoate (4.3 %), heptyl-2-methylbutyrate (2.3 %), *n*-butylbutanoate (2.25 %), hexylvalerate (1.9 %), octylbutanoate (1.7 %) and linalole (1.5 %).

**Key Words:** *Heracleum persicum*, Octylacetate, Essential oil compounds, Hexyl-2-methylbutanoate.

### INTRODUCTION

*Heracleum* genus has 10 species in Iran. *H. persicum* Desf. Ex Fischer (syn. *H. pubescens* Rech., *H. glabrescens* Boiss. & Hohen.) (Apiaceae) is an annual herb, indigenous to the Alborz region, the northern part of Iran, where it grows at an altitude ranging from 2000 to 3000 m<sup>1,2</sup>. The genus *Heracleum* are noted for their rich furanocoumarin content. Furanocoumarins are effective dermal photosensitizing agents and are widely used in the treatment of leucoderma and in various suntan lotions. *Heracleum persicum* Desf (umbellifereae) is an annual plant which grows in the northern parts of Iran. The seeds of this plant is used as spices and the young stems are used for making pickles<sup>3</sup>. The *Heracleum persicum* materials of this study were collected from Ardebil-Iran in Aug. of this year. A voucher specimen has been deposited in herbarium of Research Institute of Forest and Rangelands, Ardebil, Iran. Its fruits are used commonly in Iran as spices, while the fruits and the young shoots are used in the preparation of pickles. From the aerial parts of this herb, especially the fruits were administered because of their carminative activity in local medicine by folks<sup>1</sup>.

## EXPERIMENTAL

Dried aerial parts of *Heracleum persicum* were subjected to hydro-distillation for 5 h using Clevenger-type apparatus to produce a yellow oil in 0.28 % (w/w) yield. The oil of the aerial parts of *Heracleum persicum* was examined by GC/MS (GC:HP 6890, MS:HP 5973), column (HP5-MS, 30 m × 0.25 mm fused silica capillary column, film thickness 0.32 μm) by temperature program 60 °C (3 min) -210 °C (2 min) at the rate of 6 °C/min (injection temperature 250 °C, carrier gas: helium (with purity 99.99 %), detector temperature 150 °C, ionization energy in mass was 70 eV, mass range 10-300 amu and scan time was 1 s.

The list of identified components is presented in Table-1. The constituents were identified by comparing their MS spectra with those in computer library or with authentic compounds. The identifications were confirmed by comparison of their retention indices either with those of authentic compounds or with data in the literature<sup>4-6</sup>.

In the aerial parts of *H. persicum* the major identified components and the relative amounts based on peak area are: hexylbutyrate (37.7 %), hexylbutanoate (36.7 %), octylacetate (16.3 %), hexyl-2-methylbutanoate (5.7 %), hexylisobutyrate (4.7 %), hexylhexanoate (4.3 %), heptyl-2-methylbutyrate (2.3 %), *n*-butylbutanoate (2.25 %), hexylvalerate (1.9), octylbutanoate (1.7 %) and linalole (1.5 %).

## RESULTS AND DISCUSSION

Plants from genus *Heracleum* have been previously studied and reported in the literature. There are some nice studies of the chemical composition of essential oil of *Heracleum* species<sup>7-11</sup>. A report in literature shows that roots of *Heracleum persicum* have been investigated because of their furanocoumarins; five of which compounds were isolated and identified<sup>7</sup>. The literature survey of such compounds in leaves and seeds of this species<sup>8</sup>. From the diethyl ether extracts of the fruits of *Heracleum persicum*, an aglycone was identified which was demonstrated to be quercetin<sup>9</sup>. In this investigation, the volatile constituents of the essential oil of *H. persicum* growing wild in Ardebile-Iran were investigated by GC and GC/MS technique. As could see in Table-1, two component *i.e.* hexylbutyrate (37.7 %) and hexylbutanoate (36.7 %) have the highest percentage and more than 35 % among the known compounds in the essential oil of this herb. Some other components like octylacetate (16.3%) and hexyl-2-methylbutanoate (5.7 %), are located in the second level of the concentration in the essential oil. According to the data in Table-1, some components *i.e.*: hexylisobutyrate (4.7 %), hexylhexanoate (4.3 %), heptyl-2-methylbutyrate (2.3 %), *n*-butylbutanoate (2.25 %), hexylvalerate (1.9 %), octylbutanoate (1.7 %)

TABLE-1  
 ESSENTIAL OIL CONSTITUENTS OF *Heracleum persicum*

No.	Name of compounds	Scan	Kovats index	Retention time	%
1	Unknown	15	846.478	4.131	0.938
2	Unknown	62	846.788	4.260	2.368
3	Butyl-2-methylpropanoate	496	940.258	5.444	2.368
4	Isobutylbutanoate	515	942.500	5.496	0.308
5	Unknown	592	951.551	5.706	0.505
6	<i>n</i> -Butylbutanoate	846	981.422	6.399	2.250
7	<i>n</i> -Octanal	909	988.836	6.571	1.017
8	Isobutyl-3-methylbutanoate	932	991.551	6.634	0.490
9	Hexylethanoate	994	998.836	6.803	1.501
10	<i>para</i> -Cymene	1102	1010.120	7.098	1.057
11	<i>cis</i> - $\beta$ -Ocimene	1208	1020.783	7.387	0.320
12	<i>n</i> -Butyl-2-methylbutanoate	1238	1023.843	7.469	0.402
13	Butylpentanoate	1278	1029.910	7.578	1.057
14	$\gamma$ -Terpinene	1398	1040.111	0.905	0.784
15	1-Octanol	1504	1050.932	8.195	0.929
16	Linalol	1759	1076.865	8.890	1.529
17	Hexylpropinoate	1796	1080.634	8.991	0.714
18	Unknown	1945	1095.820	9.398	0.343
19	Hexylisobutyrate	2180	1119.029	10.039	4.703
20	Hexylbutanoate	2628	1162.050	11.235	32.710
21	Hexylbutyrate	2628	1163.021	11.262	37.760
22	Unknown	2659	1166.043	11.346	5.454
23	Unknown	2670	1167.122	11.376	0.393
24	Decanal	2695	1169.604	11.445	0.200
25	Octylacetate	2772	1177.517	11.655	16.297
26	Hexyl-2-methylbutanoate	2958	1195.396	12.162	5.745
27	Hexylvalerate	2987	1198.237	12.241	1.902
28	Unknown	3731	1273.137	14.272	0.188
29	Octylisobutyrate	3823	1282.399	14.523	1.383
30	Unknown	4078	1308.423	15.219	0.447
31	Hexylhexanoate	4162	1317.231	15.448	4.307
32	Octylbutanoate	4182	1319.308	15.502	1.676
33	Unknown	4237	1325.077	15.652	0.247
34	Unknown	4436	1345.962	16.195	0.121
35	Heptyl-2-methylbutyrate	4524	1355.231	16.436	2.286
36	Octylvalerate	4554	1358.346	16.517	0.714
37	Unknown	5618	1475.875	19.421	0.220
38	Heptyloctanoate	6940	1627.387	23.028	0.200
39	Unknown	2840	1183.813	11.840	0.178
40	<i>n</i> -Octylpropinoate	3486	1248.450	13.603	0.141
41	Undeca-6-ol	3636	1263.542	14.012	0.093

and linalole (1.5 %) have the medium up to low relative percentages, could see some important compounds with effects like mold and mildew preventive, microscopy, preservative and antioxidant with percentages under 1.5 %. Biological and aroma effects of the main and minor compounds of the essential oil of *Heracleum persicum* are discussable in terms of their possible use in medicine, cosmetics and foods. Perhaps, the high densities of the main compounds give some biological activities to the essential oil or to this herb. Although no records of toxicity have been found for this plant, it belongs to a family that includes many poisonous plants so some caution is advised<sup>5,6</sup>.

### Conclusion

*Heracleum persicum* is one of the *Heracleum* genus of that was collected from west area in Iran. It is utilized as the medicinal herb for the various purposes in local and traditional medicine by folks in Iran. 29 Compounds, representing 75 % of the total oil were identified and 12 unknown compounds detected. These components were identified by GC and GC/MS technique. In this herb, hexylbutyrate (37.7 %) and hexylbutanoate (36.7 %) have the most percentages among compounds of the essential oil. Some other components like octylacetate (16.3 %) and hexyl-2-methylbutanoate (5.7 %) are located in the second level of the concentration in the essential oil. The folks in common medicinal have been used from the aerial parts of this herb because of their carminative activity.

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